With Metal or Not? A Computationally Predicted Rule for Dirhodium Catalyst in [3+3] Cycloadditions of Triazole with Thiirane

Shi-Jun Li,[a] Xue Li,[a] Ling-Bo Qu,[a] Donghui Wei,*[a] Yu Lan*[ab]

[a]College of Chemistry, and Institute of Green Catalysis, Zhengzhou University, 100 Science Avenue, Zhengzhou, Henan, 450001, P. R. China

[b]School of Chemistry and Chemical Engineering, and Chongqing Key Laboratory of Theoretical and Computational Chemistry, Chongqing University, Chongqing 400030, P. R. China

S1. Computational Details

All theoretical calculations in this study were performed in the Gaussian16 program package.[1] All structures were optimized using B3LYP,[2] in conjunction with the DZVP basis set.[3] The self-consistent reaction field (SCRF) polarizable continuum model (PCM)[4] with IDSRCF radii[5] was applied to simulate the solvent effect and toluene was employed as solvent, which is methodologically abbreviated as the B3LYP-IDSCRF/DZVP. All the optimized stationary points had been identified as minima (zero imaginary frequencies) and transition states (one imaginary frequency), *via* the vibrational analysis. The solution-translational entropy correction has been calculated with THERMO program.[6] The entropy model has been successfully applied to typical cyclization reactions to predict activated entropy in solution. Furthermore, the single point energy at B2PLYP[7]/def2-TZVP[8]+CPCM[9] level has been also computed by using ORCA 4.1.0 program to confirm the results.

Based on the atoms-in-molecules (AIM) theory, the topological properties of the electron density distribution have been analyzed with the wave functions, and the 2-dimensional Laplacian graphs have been plotted with the AIM98PC program package.[11]

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi ,R.; Normand, J.; Raghavachari, K.; Rendell, A. P.;Burant, J. C.;Iyengar, S. S.;Tomasi,J.; Cossi, M.; Millam, J. M.; Klene,M.;Adamo,C.;Cammi,R.;Ochterski, J. W.; Martin, R. L.;Morokuma,K.;Farkas,O.;Foresman, J. B.; Fox, D. J. *Gaussian16*, Gaussian, Inc., Wallingford, CT, **2016**.

2. (a) Lee, C.; Yang, W.; Parr, R.G.; Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density, Phys. Rev. B: Condens. Matter Mater. Phys. 1988, 37, 785-789; (b) Becke, A.D. Density-Functional Thermochemistry. III. The role of Exact Exchange, J. Chem. Phys. 1993, 98, 5648-5652.
3. (a) Godbout, N.; Salahub, D. R.; Andzelm, J.; Wimmer, E. Optimization of Gaussian-Type Basis-Sets for Local Spin-Density Functional Calculations .1. Boron Through Neon, Optimization Technique and Validation, Can. J. Chem. 1992, 70, 560−571. (b) Sosa, C.; Andzelm, J.; Elkin, B. C.; Wimmer, E.; Dobbs, K. D.; Dixon, D. A. A Local Density Functional Study of the Structure and Vibrational Frequencies of Molecular Transition-Metal Compounds, J. Phys. Chem. 1992, 96, 6630−6636.
4. Scalmani, G.; Frisch, M. J. Continuous Surface Charge Polarizable Continuum Models of Solvation. I. General formalism, *J. Chem. Phys.* **2010**, *132*, 114110-24.
5. Tao, J.-Y.; Mu, W.-H.; Chass, G. A.; Tang, T.-H.; Fang, D.-C. Balancing the Atomic Waistline: Isodensity-based SCRF Radii for Main-group Elements and Transition Metals, *Int. J. Quantum Chem.* **2013**, *113*, 975−984.
6. Fang, D.-C. THERMO; Beijing Normal University, Beijing, People's Republic of China, 2013.
7. Grimme, S. "Semiempirical hybrid density functional with perturbative second-order correlation," J. Chem. Phys., **2006**, 124, 034108.
8. Weigend F.; Ahlrichs, R. "Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy," Phys. Chem. Chem. Phys., **2005**, 7, 3297-305.
9. Barone, V. Cossi, M. "Quantum calculation of molecular energies and energy gradients in solution by a conductor solvent model," J. Phys. Chem. A, **1998**,102, 1995-2001.
10. (a) Neese, F. Wennmohs, F. ORCA(4.1.0)-An ab initio, DFT and semiempirical SCF-MO package, Max-Planck-Institute for Chemical Energy Conversion, Stiftstr. 34-36, 45470 Mulheim a. d. Ruhr, Germany; (b) Neese, F. Wiley Interdiscip. Rev.: Comput. Mol. Sci., **2012**, 2, 73–78
11. (a)Bader, R. F. W.; Atoms in Molecules: A Quantum Theory, Oxford University, Oxford, 1990.(b) D.-C. Fang, T.-H. Tang, AIM98PC, Beijing Normal University, Beijing,China, 1998.

S2. The energies, entropies and Gibbs free energies in both gas-phase and solution-phase.

Species	E	S	S^{sol}	G^{sol}	G	G^1
R1	-1292.29853	165.7	130.9	-1292.09190	-1292.10560	-1291.55889
CAT	-11221.13495	281.7	242.0	-11220.54141	-11220.56564	-2065.039989
COM1	-12513.42602	343.0	403.2	-12512.60516	-12512.64190	-3356.584495
TS1	-12513.39425	344.1	404.9	-12512.57689	-12512.61405	-3356.562657
M1	-12513.41227	408.9	347.8	-12512.59536	-12512.63267	-3356.58272
TS2	-12513.39710	407.3	347.3	-12512.58246	-12512.61911	-3356.570842
M2	-12403.88712	335.9	393.0	-12403.07561	-12403.11051	-3247.099653
N_2	-109.53766	47.5	32.0	-109.54743	-109.55694	-109.5129854
R2	-707.84337	97.2	70.2	-707.73667	-707.75313	-707.4463722
TS3	-13111.73047	447.3	380.1	-13110.79514	-13110.83621	-3954.533079
M3	-13111.74955	449.9	382.0	-13110.81362	-13110.85508	-3954.558487
TS4	-13111.73799	448.0	380.1	-13110.80238	-13110.84381	-3954.544152
P	-1890.66566	206.6	164.4	-1890.33860	-1890.36436	-1889.567814
TS1'	-1292.26627	167.9	130.2	-1292.06193	-1292.08492	-1291.530507
M1'	-1292.28203	172.3	134.3	-1292.07840	-1292.10161	-1291.548276
TS2'	-1292.23670	176.8	137.3	-1292.03838	-1292.06246	-1291.5092
M2'	-1182.70833	161.8	125.1	-1182.51320	-1182.53562	-1182.019517

S^{sol} and G^{sol} are calculated using the Fang's method while the S and G are computed based the output file from Gaussian calculation. G^1= G^{sol}-E+E(B2PLYP/def2-TZVP+CPCM)

The computed results at B2PLYP/def2-TZVP+CPCM level shows the free energy barrier of three pathways are 22.7, 31.2 and 17.6 kcal/mol, respectively, which would show the similar tendency with the results at B3LYP/DZVP+PCM level. However, the barriers for the reaction would be underestimated which would be not suitable in the system.

S3 . The estimation of rate determined free energy barrier

Reaction condition: 1a (0.5 mmol, 1.0 equiv.), phenylthiirane 2a (1.0 mmol, 2 equiv.), Cat. (0.01 mmol, 0.02 equiv.), solvent (2 mL), 110 °C.
Yield: 69%

For the pseudo-first-order reaction, the rate constant can be calculated using eq. 1.

$$k = \frac{ln[1/(1-x]}{t * [Cat.]} \quad (1)$$

x should be the yield. t should be the reaction time. And [Cat] would be the concentration of *Cat.*

For this system, the yield is 69% when the reaction time is 4h. So, the concentration of *Cat.* would be 0.005 mol/L, the rate constant would be $1.63*10^{-2}$ L/mol/s., hence the corresponding free energy barrier be **25.8** kcal/mol.

S4 . The energies, entropies and Gibbs free energies for the different catalysts at 383.15 K.

Species $Rh(XCOO)_4$		E	G^{sol}
X=Me	Cat	-10289.43826	-10289.43826
	TS2	-11581.86464	-11581.49077
$X=CF_3$	Cat	-11480.72250	-11480.67494
	TS2	-12773.00466	-12772.73816
X=H	Cat	-10132.27404	-10132.21483
	TS2	-11424.54781	-11424.27200
$X= CHF_2$	Cat	-11083.64550	-11083.55878
	TS2	-12375.92743	-12375.62110
$X=CH_2F$	Cat	-10686.59248	-10686.46682
	TS2	-11978.87068	-11978.52808
X=Ph	Cat	-11056.61578	-11056.26781
	TS2	-12348.88675	-12348.31710
X=p-OMePh	Cat	-11514.33774	-11514.33774
	TS2	-12807.07041	-12806.38623
$X=p-NMe_2Ph$	Cat	-11592.56765	-11591.95516
	TS2	-12884.83574	-12884.00142
$X=2,4,6-Cl_3Ph$	Cat	-16571.30531	-16571.10023
	TS2	-17863.58153	-17863.15552
$X=C_6F_5$	Cat	-13041.65555	-13041.49983
	TS2	-14333.93182	-14333.55707
X=*t*-Bu	Cat	-10761.40566	-10760.93565
	TS2	-12053.67546	-12052.98198
$X=p-NO_2Ph$	Cat	-11874.77914	-11874.43931
	TS2	-13167.05551	-13166.49318

S5. The transformation of α ,β-unsaturated Rh-carbene **M2**

When α,β-unsaturated Rh-carbene complex **M2** is formed through a mixed processes in Pathway 3, the electronic character of this complex is interesting because it may enable further transformation by stepwise [3+3] cycloaddition. The electrostatic potential map of **M2** shown in **Figure S1** clearly reveals that the carbene moiety exhibits positive character. Therefore, this moiety can be nucleophilically attacked by an extra nucleophile. In these reaction conditions, the lone-pair electrons on the sulfur atom in thiirane act as nucleophiles, reacting with M2 through an intermolecular nucleophilic addition via transition state **TS3**. As shown in **Figure S1**, the calculated activation free energy for this step is only 8.4 kcal/mol. Then the zwitterionic thiiranium intermediate **M3** is formed, a process that is 3.4 kcal/mol exergonic. The C-S bond in **M3** is 0.13 Å longer than that in **R2**, which indicates that this bond is weakened by the formation of cationic sulfur. Subsequently, an intramolecular nucleophilic substitution by the imine group takes place via transition state TS4, leading to the ring opening of thiiranium. The calculated free energy barrier for this step is only 7.1 kcal/mol. In the computed geometry of **TS4**, the bond angle of N-C-S is 116°, the bond lengths of the forming C9-N1 and breaking C9-S7 are 2.61 and 2.91 Å, respectively, which indicates a suprafacial concerted substitution. The irreversible release of thiazine product **P** regenerates active catalyst **Cat** to accomplish the catalytic cycle.

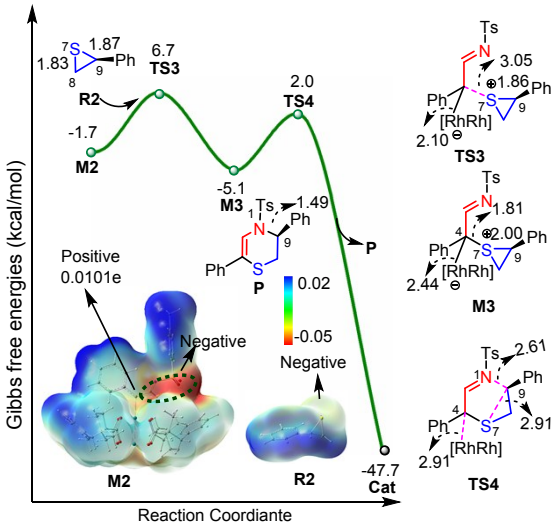

Figure S1. Free energy profiles for the [3+3] cycloaddition process of unsaturated Rh-carbene and thiirane. The electrostatic potential map of total density for **M2** and **R2** are also given.

S6. The coordinates of stationary points

R1			
N	-1.47930	-0.07343	-1.55128
N	-0.28127	0.43213	-1.53836
C	-2.10247	0.15087	-0.34005
C	-1.21490	0.83794	0.46852
N	-0.10650	0.99694	-0.31379
H	-1.26440	1.22812	1.47488
C	-4.19874	-0.99044	-1.06206
C	-5.50356	-1.42387	-0.81514
C	-3.47626	-0.30278	-0.07008
H	-6.04991	-1.95385	-1.59245
C	-6.10883	-1.17877	0.42328
C	-4.09150	-0.06010	1.17173
H	-7.12529	-1.51619	0.61347
H	-3.55474	0.47186	1.95445
C	-5.39626	-0.49452	1.41574
H	-5.85753	-0.29757	2.38107
H	-3.73079	-1.18013	-2.02383
S	1.42788	1.77081	0.11571
O	1.17885	2.25091	1.47242
O	1.74589	2.66467	-0.98735
C	2.56669	0.40396	0.13935
C	2.77694	-0.28468	1.33823
C	3.23696	0.05636	-1.03912
C	3.67912	-1.34966	1.34668
C	4.13222	-1.01171	-1.00446
C	4.36489	-1.73185	0.18117
H	2.26059	0.01430	2.24627
H	3.06490	0.61173	-1.95660
H	3.85545	-1.88528	2.27705
H	4.66108	-1.28711	-1.91467
C	5.31703	-2.90469	0.19105
H	5.66986	-3.12853	1.20157
H	4.82048	-3.80399	-0.19381
H	6.18790	-2.71674	-0.44443

R2			
C	-0.21324	0.30227	0.09059
C	-0.62677	-1.04116	0.13134
C	-1.18809	1.30313	-0.05154
C	-1.98086	-1.36972	0.04558
C	-2.54614	0.97467	-0.13844
C	-2.94769	-0.36339	-0.08789
H	0.11441	-1.83403	0.20524
H	-0.88417	2.34799	-0.09141
H	-2.28488	-2.41397	0.07666
H	-3.28659	1.76429	-0.24739
H	-4.00182	-0.62292	-0.15754
C	1.21865	0.70937	0.22019
C	2.18157	-0.01381	1.09393
S	2.55308	-0.23159	-0.68883
H	1.37524	1.78392	0.15180
H	1.82796	-0.90403	1.60960
H	2.90600	0.57601	1.65184

Cat.			
C	-1.89208	-1.82783	0.15218
O	-1.48986	-1.43020	-0.98997
O	-1.43039	-1.41295	1.27068
Rh	0.09051	0.01311	1.29295
Rh	-0.01049	0.03267	-1.09859
C	1.87560	-1.91637	0.00074
O	1.43006	-1.46382	-1.10437
O	1.50315	-1.51436	1.15574
C	-1.84064	1.91678	0.19377
O	-1.46020	1.52512	-0.95927
O	-1.34175	1.51989	1.30039
C	1.95135	1.88809	0.03202
O	1.47184	1.48897	-1.07911
O	1.58387	1.46154	1.18009
C	-3.01621	-2.87950	0.20927
C	-2.97609	2.95468	0.24351
C	3.04233	2.97408	0.00415
C	2.92770	-3.03970	-0.04538
C	2.49432	4.20941	0.75733
H	2.22698	3.96077	1.78797
H	3.25493	4.99801	0.77605
H	1.60617	4.61326	0.25836
C	3.38719	3.36255	-1.44350
H	4.15752	4.14244	-1.43799
H	3.76193	2.51100	-2.01584
H	2.50942	3.75460	-1.96502

C	0.39281	-2.23513	1.82307
O	0.62925	-1.05226	1.41367
O	-0.58872	-2.95695	1.43071
Rh	-1.90130	-2.21332	0.00569
Rh	-0.59451	-0.20383	-0.04399
C	-2.77407	-0.17193	1.90805
O	-1.83042	0.54810	1.44659
O	-3.03553	-1.36429	1.52753
C	0.29917	-2.28186	-1.91568
O	0.56051	-1.08795	-1.54774
O	-0.68978	-2.97226	-1.49658
C	-2.87616	-0.20181	-1.88144
O	-1.89806	0.51925	-1.49820
O	-3.13234	-1.37636	-1.44746
C	1.33424	-2.86072	2.86899
C	1.24128	-2.93065	-2.94706
C	-3.82020	0.35727	-2.96177
C	-3.66308	0.41431	3.02026
C	-3.68801	-0.55137	-4.20755
H	-3.94580	-1.58795	-3.97324
H	-4.35945	-0.19629	-4.99760
H	-2.66629	-0.53147	-4.60356
C	-3.43686	1.79948	-3.32984
H	-4.11987	2.17327	-4.10194
H	-3.48720	2.46748	-2.46774
H	-2.41837	1.84454	-3.72659
C	1.04585	-2.15041	-4.27199

C	-2.36388	4.29128	-0.25037
H	-3.13017	5.07433	-0.24491
H	-1.97217	4.19760	-1.26744
C	-3.50862	3.14209	1.67597
H	-2.71354	3.45937	2.35581
H	-4.28562	3.91502	1.67224
H	-3.94766	2.22563	2.07745
C	-2.51145	-4.06455	1.06599
H	-2.26869	-3.74700	2.08342
H	-3.28475	-4.83903	1.11741
H	-1.61497	-4.51601	0.62617
C	-3.37597	-3.37329	-1.20160
H	-4.17480	-4.12097	-1.13428
H	-3.72077	-2.55959	-1.84307
H	-2.51327	-3.84050	-1.68599
C	2.33692	-4.26837	0.68569
H	1.43426	-4.63044	0.18083
H	3.06895	-5.08372	0.68813
H	2.07932	-4.02983	1.72109
C	3.26086	-3.41442	-1.49942
H	3.66157	-2.56561	-2.05790
H	4.00674	-4.21771	-1.50725
H	2.37147	-3.77083	-2.02699
C	4.21134	-2.58178	0.72666
H	4.92879	-3.40813	0.65924
H	3.94718	-2.47163	1.78298
C	4.30961	2.45755	0.76610
H	5.05795	3.25673	0.70821
H	4.04386	2.34233	1.82142
C	-4.26710	-2.26005	0.92350
H	-4.98816	-3.07497	1.05510
H	-3.95840	-1.94279	1.92539
C	4.85126	-1.29840	0.23366
C	5.87622	-1.29683	-0.72568
C	4.40260	-0.06499	0.72762
C	6.41437	-0.08908	-1.18326
H	6.26115	-2.23951	-1.11044
C	4.89865	1.15791	0.25271
H	3.63620	-0.05611	1.49744
C	5.92319	1.13140	-0.70672
H	7.21870	-0.09891	-1.91596
H	6.34455	2.06435	-1.07679
C	-4.93638	-1.10725	0.19839
C	-4.32242	0.15553	0.17611
C	-6.14807	-1.27244	-0.48463
C	-4.84374	1.23263	-0.54993
H	-3.41238	0.27566	0.75090
C	-6.71645	-0.19559	-1.17711
H	-6.64968	-2.23850	-0.47712
C	-6.06641	1.04003	-1.21807
H	-7.66401	-0.32479	-1.69607
H	-6.50743	1.86131	-1.78138
H	-1.54871	4.61467	0.40624
C	-4.11343	2.55789	-0.73659
H	-4.84945	3.37106	-0.71569
H	-3.69513	2.55625	-1.75008

H	1.68725	-2.57643	-5.05147
H	1.30283	-1.09403	-4.15262
C	0.88816	-4.41169	-3.17205
H	-0.14066	-4.52695	-3.52420
H	1.55980	-4.83051	-3.93035
H	0.99785	-5.00297	-2.25987
C	0.47576	-3.20085	4.11124
H	-0.31583	-3.91501	3.86830
H	1.11136	-3.63642	4.89029
H	0.00986	-2.29977	4.52586
C	2.45209	-1.88131	3.26036
H	3.10405	-2.35544	4.00385
H	3.06259	-1.58696	2.40504
H	2.03909	-0.96956	3.70201
C	-3.47066	-0.46367	4.28005
H	-2.43085	-0.43524	4.62473
H	-4.10243	-0.08715	5.09257
H	-3.74013	-1.50537	4.08491
C	-3.25966	1.86427	3.33399
H	-3.36117	2.51368	2.46184
H	-3.89817	2.25482	4.13539
H	-2.22008	1.91745	3.66938
C	-5.16580	0.32697	2.58871
H	-5.75394	0.74039	3.41680
H	-5.42987	-0.73185	2.50509
C	-5.29894	0.27950	-2.45319
H	-5.92935	0.67781	-3.25721
H	-5.55774	-0.77730	-2.33572
C	1.92621	-4.19840	2.30674
H	2.45520	-4.68051	3.13697
H	1.08778	-4.85225	2.04219
C	-5.52353	1.03808	1.29734
C	-6.02007	2.35086	1.28381
C	-5.34630	0.38331	0.06996
C	-6.30855	2.98540	0.07080
H	-6.18970	2.87638	2.22229
C	-5.58802	1.01513	-1.15849
H	-5.00256	-0.64655	0.07065
C	-6.08351	2.32817	-1.14373
H	-6.70707	3.99819	0.07184
H	-6.30340	2.83596	-2.08156
C	2.87019	-4.06414	1.12496
C	2.37866	-3.64374	-0.12032
C	4.24082	-4.32762	1.24421
C	3.21017	-3.41608	-1.22254
H	1.31093	-3.49852	-0.21067
C	5.08575	-4.16533	0.13912
H	4.65064	-4.65878	2.19717
C	4.57858	-3.70412	-1.07828
H	6.14767	-4.38466	0.23315
H	5.25343	-3.55159	-1.91964
H	0.00831	-2.21804	-4.61846
C	2.72443	-2.76415	-2.51065
H	3.34015	-3.13048	-3.34161
H	2.93360	-1.69153	-2.42619
N	1.46970	2.88642	1.62034
N	2.54556	2.16023	1.59068
C	0.86951	2.89629	0.37427
C	1.63327	2.09868	-0.46431
N	2.65711	1.66011	0.33245
H	1.56429	1.82423	-1.50744
C	-1.01734	4.32517	1.15042
C	-2.10221	5.16437	0.89034
C	-0.30754	3.73174	0.09181
H	-2.64398	5.61578	1.71874
C	-2.49424	5.42460	-0.42803
C	-0.70944	3.99400	-1.22943

H	-3.33904	6.07972	-0.62935
H	-0.17065	3.54965	-2.06323
C	-1.79356	4.83479	-1.48654
H	-2.08983	5.03289	-2.51424
H	-0.71088	4.12500	2.17276
S	4.16320	0.86786	-0.16851
O	3.88421	0.46563	-1.54355
O	4.49064	-0.07380	0.88780
C	5.32929	2.21623	-0.15559
C	5.55405	2.93342	-1.33369
C	6.00439	2.52067	1.03293
C	6.47642	3.98255	-1.31279
C	6.91862	3.57199	1.02832
C	7.16800	4.31921	-0.13816
H	5.03290	2.66953	-2.24977
H	5.81876	1.94522	1.93530
H	6.66146	4.54157	-2.22748
H	7.44902	3.81522	1.94701
C	8.16026	5.45837	-0.11466
H	9.14305	5.11558	0.22754
H	8.28281	5.90737	-1.10381
H	7.83361	6.24462	0.57557

TS1

C	0.46350	-2.18987	1.71883
O	0.66349	-0.97993	1.36839
O	-0.52346	-2.90420	1.33342
Rh	-1.92088	-2.11588	0.01590
Rh	-0.63326	-0.07696	-0.00167
C	-2.72016	-0.18023	2.06393
O	-1.81513	0.58169	1.58856
O	-2.98278	-1.35458	1.64073
C	0.18675	-2.06326	-2.01163
O	0.46549	-0.88890	-1.59319
O	-0.78129	-2.77678	-1.58711
C	-3.02149	-0.04601	-1.72116
O	-2.03103	0.67078	-1.36526
O	-3.24380	-1.23981	-1.32419
C	1.45795	-2.86406	2.68409
C	1.08178	-2.65541	-3.11772
C	-4.03270	0.54486	-2.72210
C	-3.55659	0.33398	3.25205
C	-3.96336	-0.31153	-4.00945
H	-4.19195	-1.36088	-3.80324
H	-4.68517	0.06403	-4.74379
H	-2.96727	-0.25888	-4.46348
C	-3.68791	2.00480	-3.05326
H	-4.41388	2.39748	-3.77546
H	-3.70251	2.64028	-2.16587
H	-2.69069	2.08247	-3.49448
C	0.84001	-1.79897	-4.38639
H	1.44381	-2.18460	-5.21544
H	1.11273	-0.75321	-4.21800
C	0.70495	-4.11846	-3.41227
H	-0.33857	-4.20509	-3.72748
H	1.34096	-4.49808	-4.22043
H	0.84631	-4.76149	-2.54034
C	0.66392	-3.23889	3.95953
H	-0.15224	-3.93102	3.73463
H	1.33389	-3.71374	4.68496
H	0.23721	-2.34763	4.43382
C	2.61328	-1.91931	3.04932
H	3.29413	-2.43170	3.73979
H	3.18455	-1.60516	2.17369
H	2.24058	-1.01843	3.54609
C	-3.28813	-0.60688	4.45076
H	-2.23238	-0.58045	4.74368
H	-3.88285	-0.28669	5.31376

M1

C	-0.29928	-2.33875	-1.64602
O	-0.54217	-1.11038	-1.39584
O	0.68911	-2.99494	-1.17352
Rh	2.01643	-2.08000	0.14550
Rh	0.66474	-0.08933	-0.03544
C	2.84445	-0.25590	-2.00058
O	1.89406	0.50703	-1.61566
O	3.12848	-1.38297	-1.48057
C	-0.18027	-1.96250	2.06930
O	-0.48198	-0.83388	1.55114
O	0.82896	-2.66893	1.73847
C	2.95976	0.13624	1.79209
O	1.96605	0.79347	1.34048
O	3.24714	-1.06833	1.47941
C	-1.24545	-3.10062	-2.59423
C	-1.10002	-2.50305	3.18086
C	3.89201	0.82802	2.80539
C	3.71165	0.20607	-3.18719
C	3.82776	0.02303	4.12528
H	4.12624	-1.01789	3.97325
H	4.49821	0.47292	4.86639
H	2.81445	0.03301	4.54261
C	3.44685	2.27612	3.06333
H	4.11107	2.73580	3.80496
H	3.47272	2.87914	2.15406
H	2.42518	2.31077	3.45162
C	-0.94284	-1.54288	4.38723
H	-1.56764	-1.88732	5.21878
H	-1.24578	-0.52490	4.12638
C	-0.68405	-3.92368	3.60182
H	0.34679	-3.94604	3.96636
H	-1.34163	-4.26641	4.40915
H	-0.76283	-4.63441	2.77582
C	-0.40711	-3.51147	-3.82960
H	0.42439	-4.16420	-3.54945
H	-1.04241	-4.04417	-4.54600
H	0.00283	-2.63129	-4.33829
C	-2.42370	-2.21677	-3.03511
H	-3.07449	-2.79050	-3.70566
H	-3.02245	-1.87170	-2.18927
H	-2.07077	-1.33480	-3.57824
C	3.57027	-0.84858	-4.31034
H	2.53562	-0.90936	-4.66618
H	4.20099	-0.56938	-5.16191

H	-3.55162	-1.64059	4.21120	H	3.87253	-1.84030	-3.96394
C	-3.15871	1.77090	3.62768	C	3.25158	1.57643	-3.71095
H	-3.34089	2.46974	2.80789	H	3.34369	2.35649	-2.95130
H	-3.74584	2.09884	4.49353	H	3.86682	1.86497	-4.57115
H	-2.09947	1.82948	3.89395	H	2.20793	1.54427	-4.03682
C	-5.07830	0.24864	2.89256	C	5.21263	0.25058	-2.74134
H	-5.62960	0.61432	3.76723	H	5.78909	0.59020	-3.61016
H	-5.33419	-0.80833	2.77053	H	5.52883	-0.77492	-2.52699
C	-5.47811	0.42639	-2.13250	C	5.36368	0.77769	2.27164
H	-6.15898	0.85153	-2.87955	H	5.98578	1.29175	3.01407
H	-5.71974	-0.63734	-2.04561	H	5.68010	-0.26971	2.25726
C	1.99477	-4.18767	2.04014	C	-1.75229	-4.40750	-1.89532
H	2.55956	-4.71043	2.82094	H	-2.26839	-4.99506	-2.66360
H	1.13158	-4.81713	1.79766	H	-0.87417	-4.98644	-1.58904
C	-5.50540	1.01570	1.65535	C	5.51518	1.12965	-1.54279
C	-6.00231	2.32678	1.72738	C	5.90312	2.47191	-1.68157
C	-5.39215	0.41682	0.39219	C	5.39333	0.60469	-0.24789
C	-6.35227	3.01479	0.56027	C	6.14053	3.25957	-0.54948
H	-6.12577	2.80782	2.69649	H	6.03299	2.90032	-2.67419
C	-5.69777	1.10231	-0.79252	C	5.58712	1.38668	0.90033
H	-5.04652	-0.61054	0.32951	H	5.13094	-0.44258	-0.12892
C	-6.19082	2.41278	-0.69249	C	5.97370	2.72592	0.73325
H	-6.75235	4.02485	0.62722	H	6.45990	4.29344	-0.66774
H	-6.45916	2.96166	-1.59376	H	6.15668	3.35081	1.60593
C	2.87685	-4.02319	0.81471	C	-2.68376	-4.21082	-0.71192
C	2.33578	-3.52157	-0.37884	C	-2.21047	-3.60455	0.46132
C	4.24084	-4.34000	0.84399	C	-4.02876	-4.59875	-0.76294
C	3.11537	-3.26575	-1.51214	C	-3.04097	-3.31172	1.54874
H	1.27186	-3.33246	-0.40314	H	-1.15897	-3.35999	0.50650
C	5.03124	-4.14737	-0.29573	C	-4.86680	-4.37127	0.33566
H	4.68876	-4.73410	1.75508	H	-4.42489	-5.07466	-1.65883
C	4.47772	-3.60617	-1.45827	C	-4.38213	-3.72424	1.47479
H	6.08863	-4.40406	-0.27035	H	-5.90917	-4.68155	0.29413
H	5.11278	-3.42911	-2.32525	H	-5.05632	-3.51911	2.30516
H	-0.21181	-1.83724	-4.69199	H	0.09556	-1.51709	4.73671
C	2.58444	-2.53108	-2.73652	C	-2.58926	-2.46612	2.73270
H	3.15809	-2.85552	-3.61363	H	-3.18664	-2.74663	3.60903
H	2.81719	-1.46807	-2.60260	H	-2.85431	-1.42558	2.51106
N	0.96402	2.24043	1.49222	N	-0.71235	2.01139	-1.72895
N	1.89798	1.83682	2.06330	N	-0.65125	1.91476	-2.84995
C	0.71018	2.25811	0.12691	C	-0.72953	2.04877	-0.36877
C	1.89481	1.74014	-0.48705	C	-1.99827	1.58238	0.19015
N	2.85670	1.36398	0.30783	N	-3.00687	1.30380	-0.56266
H	1.96956	1.65880	-1.56967	H	-2.02517	1.48719	1.28019
C	-1.31173	3.70805	0.36800	C	1.30667	3.53712	-0.26437
C	-2.18887	4.67295	-0.12838	C	1.98789	4.63595	0.26014
C	-0.26315	3.21904	-0.43035	C	0.03925	3.18618	0.23094
H	-2.99510	5.03838	0.50371	H	2.96786	4.89375	-0.13473
C	-2.04421	5.16031	-1.43252	C	1.42961	5.38492	1.30279
C	-0.12611	3.70715	-1.74183	C	-0.52284	3.94547	1.27144
H	-2.72916	5.91215	-1.81787	H	1.96696	6.23553	1.71603
H	0.67779	3.35353	-2.38293	H	-1.51127	3.71142	1.65802
C	-1.01225	4.66636	-2.23727	C	0.17710	5.02845	1.81189
H	-0.88772	5.03434	-3.25339	H	-0.26946	5.60350	2.62002
H	-1.44349	3.32197	1.37459	H	1.76996	2.93663	-1.04191
S	4.34856	0.77225	-0.29903	S	-4.41249	0.73639	0.24260
O	4.22835	0.60795	-1.75589	O	-4.20473	0.69693	1.70299
O	4.72743	-0.34561	0.55933	O	-4.83647	-0.46851	-0.47430
C	5.44180	2.15281	0.03563	C	-5.55752	2.06640	-0.13074
C	5.70930	3.07919	-0.97488	C	-5.84976	3.01956	0.84700
C	6.01854	2.27273	1.30467	C	-6.14937	2.12202	-1.39761
C	6.56574	4.14872	-0.70063	C	-6.74535	4.04900	0.54313
C	6.86880	3.34910	1.55837	C	-7.03828	3.15874	-1.68246
C	7.15638	4.30161	0.56425	C	-7.35080	4.13632	-0.72065
H	5.26743	2.95872	-1.96022	H	-5.39454	2.94942	1.83115
H	5.81079	1.53374	2.07375	H	-5.92284	1.36337	-2.14194
H	6.77978	4.87063	-1.48619	H	-6.97812	4.79104	1.30444

H	7.31907	3.44729	2.54446	H	-7.49914	3.20648	-2.66747
C	8.10394	5.44465	0.84805	C	-8.33959	5.23570	-1.03608
H	7.93372	5.86539	1.84424	H	-8.20231	5.61605	-2.05341
H	9.14510	5.10097	0.81364	H	-9.36881	4.86288	-0.96433
H	7.99629	6.24814	0.11402	H	-8.24276	6.07475	-0.34126
TS2				M2			
C	0.22068	-2.31515	1.69503	C	0.03500	2.36663	-1.72105
O	0.50684	-1.10330	1.40416	O	0.45558	1.20918	-1.37487
O	-0.78366	-2.95632	1.24510	O	-1.03367	2.91484	-1.29943
Rh	-2.08750	-2.05747	-0.12052	Rh	-2.25782	1.92763	0.07475
Rh	-0.66381	-0.07328	0.01314	Rh	-0.61904	0.08716	0.02506
C	-2.87248	-0.13520	1.96479	C	-2.77419	-0.11986	-1.97551
O	-1.88811	0.58548	1.57644	O	-1.73354	-0.72707	-1.54138
O	-3.18880	-1.26332	1.47567	O	-3.22496	0.97698	-1.52399
C	0.12737	-2.05254	-2.03600	C	-0.08243	2.21371	2.01775
O	0.45035	-0.90794	-1.56346	O	0.36503	1.09048	1.59024
O	-0.89187	-2.72665	-1.68348	O	-1.16175	2.76303	1.64009
C	-2.95442	0.14869	-1.83937	C	-2.92637	-0.31839	1.83787
O	-1.95263	0.80125	-1.39220	O	-1.84802	-0.87125	1.42832
O	-3.27113	-1.03860	-1.50527	O	-3.35858	0.81717	1.46860
C	1.14604	-3.06783	2.67335	C	0.87844	3.16937	-2.73295
C	1.04563	-2.64703	-3.12307	C	0.76448	2.92922	3.08946
C	-3.85907	0.84084	-2.87950	C	-3.77230	-1.08770	2.87340
C	-3.74031	0.39452	3.12407	C	-3.53828	-0.76557	-3.14870
C	-3.79191	0.00905	-4.18232	C	-3.85467	-0.21641	4.14882
H	-4.11329	-1.02220	-4.01259	H	-4.28429	0.76503	3.93163
H	-4.44235	0.45634	-4.94274	H	-4.48055	-0.71365	4.89870
H	-2.77253	-0.01020	-4.58426	H	-2.86151	-0.06759	4.58774
C	-3.38484	2.27545	-3.16137	C	-3.13514	-2.44382	3.21902
H	-4.02990	2.73177	-3.92175	H	-3.74622	-2.95384	3.97317
H	-3.41445	2.89866	-2.26526	H	-3.05462	-3.09442	2.34522
H	-2.35724	2.28353	-3.53555	H	-2.12925	-2.31237	3.62789
C	0.90196	-1.73593	-4.36837	C	0.63273	2.08912	4.38561
H	1.52292	-2.12175	-5.18463	H	1.21237	2.55457	5.19065
H	1.21755	-0.71168	-4.14972	H	1.00258	1.06980	4.23919
C	0.61415	-4.07868	-3.48723	C	0.23705	4.35113	3.35384
H	-0.41690	-4.10330	-3.85081	H	-0.80439	4.33201	3.68591
H	1.26807	-4.46152	-4.27949	H	0.84119	4.81919	4.13967
H	0.68410	-4.75656	-2.63331	H	0.29275	4.98212	2.46384
C	0.28849	-3.44365	3.90613	C	-0.03927	3.50993	-3.93103
H	-0.54765	-4.09127	3.62837	H	-0.90014	4.10677	-3.61846
H	0.90816	-3.96925	4.64137	H	0.52661	4.07596	-4.67954
H	-0.11752	-2.54861	4.39171	H	-0.41118	2.59868	-4.41333
C	2.33135	-2.19209	3.11131	C	2.08972	2.35935	-3.22184
H	2.96737	-2.76170	3.79945	H	2.66246	2.95955	-3.93895
H	2.94411	-1.86962	2.26671	H	2.75830	2.07267	-2.40826
H	1.98445	-1.29642	3.63604	H	1.77122	1.44212	-3.72639
C	-3.62465	-0.61594	4.29001	C	-3.52349	0.23964	-4.32437
H	-2.59306	-0.68124	4.65393	H	-2.49988	0.42756	-4.66768
H	-4.25456	-0.29189	5.12630	H	-4.08996	-0.16881	-5.16909
H	-3.94304	-1.61507	3.98129	H	-3.96933	1.19509	-4.03576
C	-3.26442	1.77819	3.59595	C	-2.87619	-2.08140	-3.59024
H	-3.32052	2.52484	2.80008	H	-2.86514	-2.82370	-2.78860
H	-3.89382	2.11748	4.42702	H	-3.42868	-2.50246	-4.43850
H	-2.23015	1.74111	3.94935	H	-1.84202	-1.91620	-3.90505
C	-5.23646	0.44390	2.66423	C	-5.02665	-0.99937	-2.72170
H	-5.81627	0.81774	3.51670	H	-5.53083	-1.46574	-3.57659
H	-5.56367	-0.58373	2.47902	H	-5.48941	-0.01934	-2.57080
C	-5.33834	0.82849	-2.36570	C	-5.22239	-1.27391	2.31261
H	-5.94273	1.33338	-3.12887	H	-5.78566	-1.83048	3.07122
H	-5.67142	-0.21317	-2.32884	H	-5.68053	-0.28319	2.23476
C	1.64630	-4.39417	2.00745	C	1.33249	4.51547	-2.07069
H	2.14652	-4.97211	2.79348	H	1.79971	5.11271	-2.86255
H	0.76496	-4.96869	1.70204	H	0.43266	5.05344	-1.75304
C	-5.52001	1.28938	1.43677	C	-5.22925	-1.84492	-1.47878
C	-5.90684	2.63575	1.53367	C	-5.43173	-3.23269	-1.54790
C	-5.38602	0.72747	0.15850	C	-5.20761	-1.23982	-0.21329

C	-6.13426	3.39086	0.37753
H	-6.04436	3.09218	2.51266
C	-5.57017	1.47627	-1.01354
H	-5.12328	-0.32273	0.07269
C	-5.95753	2.82002	-0.88803
H	-6.45403	4.42785	0.46314
H	-6.13424	3.41931	-1.77990
C	2.59260	-4.23262	0.83062
C	2.13270	-3.66109	-0.36520
C	3.93586	-4.62218	0.90721
C	2.97346	-3.41051	-1.45531
H	1.08197	-3.41568	-0.42747
C	4.78502	-4.43361	-0.19036
H	4.32174	-5.07043	1.82167
C	4.31228	-3.82593	-1.35590
H	5.82592	-4.74554	-0.12869
H	4.99389	-3.65308	-2.18759
H	-0.13580	-1.71102	-4.71981
C	2.53431	-2.60935	-2.67421
H	3.13027	-2.93318	-3.53660
H	2.81321	-1.56443	-2.49436
N	0.85012	1.83085	1.89128
N	0.57134	1.78716	2.96523
C	0.62968	1.73395	0.13338
C	1.97028	1.35083	-0.29267
N	2.98333	1.25932	0.49715
H	2.02392	1.08897	-1.35765
C	-1.22037	3.42213	0.01959
C	-1.69754	4.68434	-0.32926
C	0.11831	3.06878	-0.24943
H	-2.72902	4.94908	-0.10925
C	-0.85950	5.60185	-0.97626
C	0.95988	4.01017	-0.88220
H	-1.23963	6.58167	-1.25789
H	2.00075	3.76628	-1.07922
C	0.46867	5.26001	-1.25972
H	1.12212	5.97127	-1.75947
H	-1.87350	2.70448	0.50321
S	4.42598	0.62855	-0.20886
O	4.26290	0.44966	-1.66418
O	4.83052	-0.49954	0.63441
C	5.55057	1.99765	0.07172
C	5.85437	2.86604	-0.97883
C	6.11748	2.16624	1.33976
C	6.73578	3.92614	-0.74738
C	6.99240	3.23195	1.55154
C	7.31607	4.12649	0.51538
H	5.41939	2.70630	-1.96170
H	5.88368	1.47057	2.14117
H	6.97815	4.60212	-1.56509
H	7.43411	3.36752	2.53715
C	8.29127	5.25681	0.75397
H	8.13615	5.71756	1.73482
H	9.32411	4.88815	0.72750
H	8.19902	6.03551	-0.00850

C	-5.58987	-3.98409	-0.37782
H	-5.48134	-3.72599	-2.51734
C	-5.32519	-1.97894	0.97346
H	-5.08928	-0.16191	-0.14972
C	-5.52694	-3.36506	0.87578
H	-5.76867	-5.05584	-0.44363
H	-5.64953	-3.96039	1.77919
C	2.29614	4.38354	-0.90611
C	1.83753	3.89677	0.32862
C	3.65359	4.70249	-1.03497
C	2.69653	3.65897	1.40727
H	0.77641	3.70299	0.42384
C	4.52275	4.52471	0.04849
H	4.03563	5.08355	-1.98072
C	4.05191	3.99803	1.25248
H	5.57593	4.77861	-0.05477
H	4.74687	3.82803	2.07370
H	-0.41155	2.03425	4.71285
C	2.26411	2.95135	2.68585
H	2.81212	3.38746	3.53060
H	2.60997	1.91337	2.61091
C	0.73894	-1.45797	0.13360
C	2.10177	-0.96417	0.24285
N	3.00544	-1.33909	-0.60354
H	2.29132	-0.20218	1.01056
C	-0.85445	-3.34292	-0.04431
C	-1.13292	-4.70154	0.03480
C	0.45424	-2.85266	0.23896
H	-2.13207	-5.06359	-0.19424
C	-0.12858	-5.60285	0.41646
C	1.45926	-3.79351	0.62359
H	-0.35351	-6.66551	0.48472
H	2.46248	-3.44743	0.84789
C	1.16635	-5.14665	0.71436
H	1.93686	-5.85319	1.01302
H	-1.62340	-2.64240	-0.34043
S	4.53608	-0.54931	-0.42975
O	4.59489	0.21627	0.82866
O	4.81672	0.10806	-1.71038
C	5.59072	-1.99200	-0.26935
C	6.04675	-2.37510	0.99400
C	5.94752	-2.70807	-1.41748
C	6.87029	-3.49938	1.10418
C	6.76799	-3.82850	-1.28641
C	7.24232	-4.24183	-0.02822
H	5.77321	-1.79623	1.87205
H	5.59411	-2.38880	-2.39424
H	7.23197	-3.79713	2.08652
H	7.04685	-4.38842	-2.17726
C	8.15736	-5.43931	0.09206
H	8.17303	-5.83294	1.11241
H	7.85092	-6.24575	-0.58189
H	9.18639	-5.16729	-0.17346

TS3			
C	-0.91948	-1.82271	2.41462
O	-0.21241	-1.08575	1.64656
O	-2.13925	-2.13165	2.22039
Rh	-3.14178	-1.43696	0.52436
Rh	-1.03440	-0.32697	-0.12240
C	-2.84040	1.31238	1.53712
O	-1.70608	1.34010	0.94545
O	-3.63450	0.32221	1.55423
C	-1.35302	-3.12031	-1.07155
O	-0.56179	-2.11451	-1.12837
O	-2.49740	-3.12042	-0.52339

M3			
C	-0.99979	-2.34958	2.07242
O	-0.29611	-1.36534	1.66399
O	-2.10861	-2.72118	1.56766
Rh	-2.92868	-1.70469	-0.05149
Rh	-0.95888	-0.25403	-0.02086
C	-3.23235	0.64548	1.66696
O	-2.04882	0.96691	1.31228
O	-3.85622	-0.39414	1.28225
C	-0.69007	-2.70953	-1.64221
O	-0.04707	-1.66044	-1.29714
O	-1.90342	-2.95633	-1.34275

C	-3.28369	0.01730	-2.01806
O	-2.05843	0.32935	-1.83238
O	-3.99218	-0.69167	-1.23626
C	-0.25461	-2.38615	3.68835
C	-0.86838	-4.42026	-1.74515
C	-3.96653	0.52910	-3.30384
C	-3.27705	2.57641	2.30690
C	-4.38798	-0.70920	-4.12984
H	-5.05610	-1.35879	-3.55803
H	-4.90674	-0.38965	-5.04097
H	-3.51309	-1.29619	-4.43195
C	-3.01197	1.40049	-4.13613
H	-3.51981	1.72885	-5.05093
H	-2.68339	2.28628	-3.58820
H	-2.11836	0.83996	-4.42499
C	-0.89639	-4.15900	-3.27296
H	-0.55819	-5.05267	-3.80958
H	-0.24252	-3.32549	-3.54621
C	-1.80708	-5.59679	-1.41995
H	-2.83082	-5.38832	-1.74199
H	-1.45603	-6.49311	-1.94438
H	-1.83340	-5.82007	-0.35082
C	-1.12169	-1.95869	4.89551
H	-2.14044	-2.34577	4.81101
H	-0.67857	-2.33830	5.82333
H	-1.17745	-0.86676	4.97379
C	1.17317	-1.84302	3.85705
H	1.61546	-2.25383	4.77259
H	1.81637	-2.11047	3.01626
H	1.16627	-0.75219	3.94162
C	-3.40656	2.18747	3.79874
H	-2.44002	1.87275	4.20817
H	-3.75051	3.05129	4.37922
H	-4.11976	1.37005	3.93497
C	-2.24516	3.70647	2.15965
H	-2.13103	4.02263	1.11984
H	-2.56850	4.57521	2.74550
H	-1.26170	3.39580	2.52195
C	-4.68482	3.03095	1.79508
H	-4.95931	3.92120	2.37378
H	-5.40404	2.24684	2.05066
C	-5.25982	1.32354	-2.91867
H	-5.71086	1.66758	-3.85722
H	-5.96234	0.61894	-2.46316
C	-0.25635	-3.95196	3.61795
H	0.09175	-4.31218	4.59332
H	-1.29557	-4.27985	3.50738
C	-4.77701	3.33278	0.31127
C	-4.60541	4.63110	-0.19536
C	-5.02786	2.29376	-0.59720
C	-4.66705	4.86698	-1.57344
H	-4.43537	5.46165	0.48793
C	-5.05548	2.50110	-1.98444
H	-5.19651	1.29181	-0.21393
C	-4.87974	3.80878	-2.46434
H	-4.55231	5.88029	-1.95423
H	-4.92098	4.00317	-3.53495
C	0.60072	-4.55515	2.52158
C	0.16241	-4.50885	1.18787
C	1.85194	-5.12097	2.79477
C	0.95779	-4.94471	0.12244
H	-0.82808	-4.11106	1.00272
C	2.64562	-5.60811	1.74873
H	2.21315	-5.17421	3.82071
C	2.20839	-5.51057	0.42702
H	3.61815	-6.04601	1.96505
H	2.85346	-5.85394	-0.38023

C	-2.92430	0.35112	-2.13065
O	-1.79176	0.71090	-1.66958
O	-3.62924	-0.61266	-1.68541
C	-0.50904	-3.18291	3.27826
C	0.04981	-3.75363	-2.50253
C	-3.49125	1.13272	-3.33257
C	-3.97796	1.57040	2.65248
C	-3.58944	0.14796	-4.52173
H	-4.22779	-0.70644	-4.27994
H	-4.00954	0.66073	-5.39476
H	-2.59974	-0.23072	-4.80105
C	-2.57413	2.30713	-3.71045
H	-2.99922	2.84050	-4.56930
H	-2.45273	3.01406	-2.88720
H	-1.57781	1.95267	-3.98870
C	0.28492	-3.09611	-3.88717
H	0.78535	-3.80852	-4.55300
H	0.91253	-2.20485	-3.80450
C	-0.80264	-5.02356	-2.68523
H	-1.76274	-4.79480	-3.15570
H	-0.26269	-5.72709	-3.32970
H	-1.00805	-5.52473	-1.73611
C	-1.61041	-3.12446	4.36306
H	-2.55343	-3.53507	3.99345
H	-1.29794	-3.70093	5.24136
H	-1.79215	-2.09318	4.68761
C	0.80356	-2.63119	3.85170
H	1.12626	-3.25061	4.69675
H	1.60282	-2.62963	3.10743
H	0.66498	-1.60901	4.21885
C	-4.27023	0.74848	3.93031
H	-3.34020	0.43321	4.41730
H	-4.83191	1.35978	4.64600
H	-4.85606	-0.14558	3.70118
C	-3.13390	2.80126	3.01958
H	-2.93056	3.43129	2.15066
H	-3.67182	3.40750	3.75801
H	-2.17434	2.50769	3.45487
C	-5.34652	1.99912	2.02303
H	-5.83832	2.65473	2.75193
H	-5.96597	1.10200	1.92795
C	-4.93586	1.63178	-2.99263
H	-5.29930	2.17052	-3.87612
H	-5.57385	0.75135	-2.86823
C	-0.33922	-4.67714	2.83808
H	-0.12799	-5.25334	3.74680
H	-1.30570	-5.02257	2.45670
C	-5.26396	2.69495	0.67718
C	-5.23353	4.09409	0.56303
C	-5.20603	1.93176	-0.49836
C	-5.12767	4.69849	-0.69479
H	-5.30545	4.71344	1.45591
C	-5.06106	2.51561	-1.76566
H	-5.26815	0.85037	-0.42463
C	-5.03073	3.91643	-1.85102
H	-5.12213	5.78412	-0.77439
H	-4.94034	4.39831	-2.82316
C	0.74762	-4.93576	1.81209
C	0.54827	-4.55719	0.47414
C	1.97359	-5.51059	2.16957
C	1.55077	-4.67042	-0.49547
H	-0.42438	-4.16391	0.20635
C	2.97443	-5.68364	1.20422
H	2.14946	-5.82384	3.19777
C	2.77042	-5.25599	-0.10899
H	3.92280	-6.13974	1.48264
H	3.57041	-5.35989	-0.84031

H	-1.91226	-3.92790	-3.61260
C	0.59708	-4.73986	-1.34381
H	0.88973	-5.63637	-1.90550
H	1.24014	-3.93410	-1.71570
C	0.73503	0.57616	-0.81592
C	1.82462	-0.38813	-0.91653
N	2.99342	-0.22003	-0.39110
H	1.55873	-1.31364	-1.44727
C	-0.25644	2.74307	-1.51953
C	-0.20301	3.91761	-2.26102
C	0.79294	1.78744	-1.59842
H	-1.00879	4.64334	-2.18145
C	0.88079	4.16349	-3.11625
C	1.88655	2.06239	-2.46804
H	0.91329	5.08013	-3.70189
H	2.70427	1.35313	-2.54902
C	1.92304	3.23064	-3.22188
H	2.75989	3.42134	-3.88980
H	-1.09147	2.55094	-0.85829
S	4.07724	-1.55257	-0.55423
O	3.51673	-2.60738	-1.41748
O	4.52524	-1.86878	0.80850
C	5.42616	-0.75844	-1.43444
C	5.53290	-0.91686	-2.81861
C	6.35684	0.00279	-0.71945
C	6.58514	-0.29160	-3.49314
C	7.39949	0.62136	-1.41111
C	7.53109	0.48566	-2.80453
H	4.81303	-1.52886	-3.35551
H	6.27398	0.09711	0.35991
H	6.67286	-0.41716	-4.57068
H	8.12543	1.21358	-0.85690
C	8.68518	1.13293	-3.53587
H	8.45455	1.28811	-4.59386
H	8.94535	2.10064	-3.09581
H	9.57947	0.49971	-3.48298
C	3.62945	3.82913	2.07710
C	3.25819	4.28971	3.35318
C	4.39311	4.67328	1.25380
C	3.64905	5.55571	3.79324
C	4.78607	5.94217	1.69386
C	4.41636	6.38777	2.96661
H	2.64590	3.66607	4.00074
H	4.68282	4.33390	0.26069
H	3.35284	5.89741	4.78280
H	5.37863	6.58082	1.04214
H	4.71845	7.37406	3.31210
C	3.25993	2.47586	1.56841
C	3.02852	1.30352	2.44859
S	1.48112	1.90274	1.67073
H	3.67561	2.22941	0.59411
H	3.08056	1.44482	3.52598
H	3.35758	0.33253	2.08820

H	-0.66745	-2.81638	-4.35234
C	1.43905	-4.09673	-1.90164
H	1.92035	-4.79239	-2.60103
H	2.05661	-3.19459	-1.91974
C	0.89970	1.33574	-0.15916
C	1.77742	0.61345	-1.04920
N	2.92589	0.09127	-0.72374
H	1.40659	0.54702	-2.07786
C	-0.65260	3.35723	-0.13544
C	-1.02211	4.62148	-0.59868
C	0.44636	2.67587	-0.69133
H	-1.88340	5.11943	-0.15916
C	-0.31430	5.23238	-1.63979
C	1.16265	3.31182	-1.72660
H	-0.61062	6.21297	-2.00644
H	2.03815	2.83494	-2.16021
C	0.77792	4.56740	-2.20601
H	1.34271	5.03040	-3.01272
H	-1.23417	2.88028	0.64440
S	3.78770	-0.67631	-1.97037
O	3.09492	-0.56711	-3.26912
O	4.18341	-2.00051	-1.46978
C	5.26093	0.35373	-2.03325
C	5.37405	1.34238	-3.01394
C	6.28239	0.14300	-1.10154
C	6.52475	2.13473	-3.05032
C	7.42346	0.94642	-1.15128
C	7.56403	1.95251	-2.12296
H	4.58186	1.47745	-3.74556
H	6.19107	-0.64637	-0.36009
H	6.61610	2.90138	-3.81762
H	8.21959	0.78195	-0.42730
C	8.82076	2.79077	-2.19176
H	8.62206	3.77833	-2.61881
H	9.26550	2.92875	-1.20146
H	9.57470	2.30560	-2.82414
C	3.78243	2.30599	3.10762
C	3.37292	2.18856	4.45085
C	4.72115	3.30225	2.76989
C	3.89113	3.04336	5.42559
C	5.23903	4.15347	3.74619
C	4.82451	4.02771	5.07821
H	2.65248	1.43003	4.74676
H	5.04439	3.40417	1.73565
H	3.56863	2.93992	6.45907
H	5.96492	4.91480	3.47008
H	5.22680	4.69093	5.84059
C	3.28691	1.42241	2.03980
C	2.41484	0.24332	2.23139
S	1.34859	1.58264	1.58188
H	3.83434	1.42479	1.10213
H	2.11129	-0.04403	3.23272
H	2.54062	-0.58172	1.53908

TS4			
C	0.12943	2.52267	1.62902
O	-0.23873	1.34894	1.29433
O	1.25654	3.04864	1.34535
Rh	2.56251	2.02266	0.10244
Rh	0.98044	0.20499	0.04189
C	2.96394	0.01784	2.20198
O	1.96755	-0.59743	1.70056
O	3.43064	1.12743	1.77649
C	0.61777	2.21990	-2.06875
O	0.11861	1.13241	-1.61987
O	1.62702	2.81791	-1.56842
C	3.41308	-0.21737	-1.56158
O	2.31586	-0.77659	-1.24035

P			
C	-2.77507	0.39050	-0.06153
C	-1.64029	-0.30109	0.17515
N	-0.33421	0.20799	0.39175
H	-1.68919	-1.38253	0.22508
C	-5.27255	0.27141	0.16708
C	-6.49406	-0.37892	-0.02555
C	-4.06893	-0.29285	-0.29990
H	-7.40826	0.07394	0.35250
C	-6.54412	-1.60771	-0.69387
C	-4.13635	-1.52121	-0.98735
H	-7.49559	-2.11254	-0.84577
H	-3.23080	-1.95819	-1.40118
C	-5.35792	-2.17390	-1.17455

O	3.79352	0.93619	-1.16390
C	-0.84396	3.37927	2.46104
C	-0.05978	2.85070	-3.30080
C	4.37117	-0.95454	-2.51718
C	3.66112	-0.60231	3.42884
C	4.49373	-0.09973	-3.80089
H	4.85989	0.90594	-3.57727
H	5.19080	-0.57755	-4.49892
H	3.52540	-0.00891	-4.30616
C	3.83185	-2.34676	-2.87396
H	4.51817	-2.83584	-3.57609
H	3.72708	-2.98135	-1.99278
H	2.84835	-2.28007	-3.34647
C	-0.25878	1.74763	-4.36447
H	-0.73135	2.17532	-5.25580
H	-0.89398	0.94213	-3.98857
C	0.81208	3.97845	-3.87902
H	1.78896	3.59899	-4.19573
H	0.31488	4.41115	-4.75534
H	0.98318	4.77563	-3.15284
C	-0.29357	3.37947	3.91059
H	0.72325	3.78144	3.95021
H	-0.93403	3.99590	4.55175
H	-0.28084	2.36471	4.32368
C	-2.26232	2.78096	2.46484
H	-2.91227	3.39880	3.09577
H	-2.69891	2.73918	1.46479
H	-2.25164	1.76505	2.86962
C	3.48351	0.38252	4.60881
H	2.42362	0.51827	4.85192
H	3.98444	-0.01101	5.50075
H	3.90954	1.36203	4.37507
C	3.03540	-1.95901	3.79101
H	3.15130	-2.68696	2.98452
H	3.52353	-2.36049	4.68713
H	1.96647	-1.85899	3.99828
C	5.19290	-0.75036	3.14075
H	5.64293	-1.18311	4.04239
H	5.61053	0.25447	3.02425
C	5.78883	-1.05284	-1.85907
H	6.42972	-1.58555	-2.57199
H	6.18768	-0.03797	-1.76569
C	-0.84444	4.84453	1.95025
H	-1.51865	5.41048	2.60639
H	0.15699	5.25624	2.12163
C	5.55630	-1.58927	1.93009
C	5.85505	-2.95713	2.03442
C	5.58630	-0.99948	0.65820
C	6.15433	-3.70466	0.88985
H	5.86487	-3.43801	3.01146
C	5.84370	-1.73763	-0.50633
H	5.39403	0.06539	0.57026
C	6.13836	-3.10379	-0.37386
H	6.40248	-4.76041	0.98355
H	6.36608	-3.69801	-1.25745
C	-1.20811	5.14204	0.49935
C	-1.29669	4.16669	-0.49933
C	-1.38599	6.48569	0.12252
C	-1.48500	4.49203	-1.85283
H	-1.22475	3.11473	-0.24964
C	-1.61585	6.82970	-1.21111
H	-1.33422	7.26819	0.87912
C	-1.65059	5.83849	-2.20052
H	-1.75657	7.87411	-1.48372
H	-1.80900	6.11533	-3.24171
H	0.70118	1.31487	-4.66944
C	-1.47555	3.38954	-2.89320
H	-5.38390	-3.11970	-1.71196
H	-5.25544	1.21765	0.70390
S	0.59319	-0.67318	1.56946
O	-0.21829	-1.83753	1.93993
O	1.04948	0.28114	2.58595
C	2.03255	-1.28258	0.68811
C	1.87627	-2.32342	-0.23512
C	3.29144	-0.76368	0.98707
C	3.00408	-2.83192	-0.87602
C	4.41192	-1.29264	0.33866
C	4.28913	-2.32710	-0.59958
H	0.89346	-2.73903	-0.44127
H	3.39348	0.03849	1.71131
H	2.88646	-3.64162	-1.59415
H	5.39491	-0.88771	0.57005
C	5.50240	-2.90732	-1.29026
H	5.67707	-3.94115	-0.96929
H	5.36922	-2.92501	-2.37757
H	6.40507	-2.33159	-1.06816
C	1.37301	1.95450	-0.19159
C	1.83078	1.42339	-1.40793
C	2.19976	2.83390	0.51983
C	3.09077	1.76792	-1.90278
C	3.46217	3.18215	0.02564
C	3.91033	2.65104	-1.18836
H	1.20642	0.72624	-1.96306
H	1.86074	3.23986	1.47101
H	3.43600	1.34499	-2.84379
H	4.09476	3.86326	0.59097
H	4.89170	2.91935	-1.57390
C	-0.03666	1.66999	0.31420
C	-1.03667	2.35908	-0.62856
S	-2.77620	2.17912	-0.11483
H	-0.15001	2.10685	1.30999
H	-0.93211	1.98171	-1.64935
H	-0.81773	3.42973	-0.63535

H	-1.94455	3.75289	-3.81567
H	-2.07204	2.54522	-2.53673
C	-0.74527	-2.16087	0.14234
C	-1.74965	-1.47037	-0.58056
N	-2.84507	-1.03151	0.03221
H	-1.63462	-1.38100	-1.66367
C	1.26041	-3.67805	0.16742
C	2.04254	-4.68482	-0.39754
C	0.14273	-3.15079	-0.51469
H	2.89957	-5.06783	0.15219
C	1.74480	-5.18494	-1.67108
C	-0.13363	-3.65481	-1.80621
H	2.35474	-5.97085	-2.11144
H	-0.99641	-3.29797	-2.36216
C	0.65939	-4.65258	-2.37635
H	0.41480	-5.02873	-3.36779
H	1.51730	-3.28047	1.14360
S	-3.93517	-0.22702	-0.98306
O	-4.31638	-1.05093	-2.14869
O	-3.43213	1.13473	-1.23913
C	-5.36472	-0.09932	0.09787
C	-6.62433	-0.37978	-0.43229
C	-5.22398	0.36929	1.40958
C	-7.75803	-0.19985	0.36875
C	-6.36380	0.53193	2.19690
C	-7.64808	0.25541	1.69074
H	-6.71381	-0.74049	-1.45336
H	-4.23895	0.59199	1.80827
H	-8.74004	-0.41827	-0.04659
H	-6.25501	0.88694	3.22045
C	-8.87292	0.46648	2.55210
H	-9.04708	1.53523	2.72512
H	-9.77090	0.05506	2.08266
H	-8.75581	-0.00493	3.53399
C	-4.21834	-3.89452	0.26499
C	-3.43350	-4.81336	-0.48069
C	-5.59518	-3.76670	-0.05674
C	-4.00546	-5.56152	-1.50317
C	-6.16545	-4.53727	-1.06354
C	-5.37235	-5.43287	-1.79486
H	-2.37386	-4.92532	-0.27189
H	-6.21035	-3.07238	0.50913
H	-3.39062	-6.25152	-2.07613
H	-7.22460	-4.43883	-1.28906
H	-5.81599	-6.02773	-2.59017
C	-3.68466	-3.12608	1.35234
C	-2.46954	-3.45935	2.06744
S	-0.97402	-2.20502	1.87432
H	-4.33854	-2.38675	1.80502
H	-2.06515	-4.44216	1.83206
H	-2.61264	-3.34870	3.14542

TS1'			
N	-1.70623	-0.24269	1.80368
N	-0.68010	-0.02728	2.32235
C	-2.15715	0.04000	0.54743
C	-1.09573	0.69728	-0.12493
N	0.01442	0.88686	0.54842
H	-1.20674	1.03286	-1.15500
C	-4.37389	-1.03182	0.94175
C	-5.65753	-1.37758	0.51649
C	-3.50310	-0.31914	0.09434
H	-6.31346	-1.92748	1.18783
C	-6.10041	-1.02207	-0.76317
C	-3.95679	0.03653	-1.19041
H	-7.10042	-1.29208	-1.09414
H	-3.31475	0.59195	-1.87002
C	-5.24171	-0.31366	-1.61142

M1'			
N	2.00508	-0.92103	1.79969
N	1.85740	-1.36817	2.83415
C	2.15465	-0.41396	0.57861
C	1.02238	-0.56406	-0.29439
N	-0.09990	-1.08367	0.10249
H	1.17036	-0.22624	-1.32549
C	4.63105	-0.12859	0.91105
C	5.84354	0.48028	0.58052
C	3.44633	0.22379	0.23737
H	6.74820	0.19387	1.11212
C	5.89961	1.44088	-0.43584
C	3.50746	1.19976	-0.77551
H	6.84548	1.90992	-0.69617
H	2.60558	1.51391	-1.29505
C	4.72659	1.79342	-1.11225

H	-5.57268	-0.02801	-2.60748	H	4.75452	2.54385	-1.89907
H	-4.04289	-1.31689	1.93822	H	4.61494	-0.89067	1.68782
S	1.33363	1.70488	-0.15889	S	-1.29833	-1.24664	-1.10001
O	1.73704	2.73554	0.80003	O	-1.70993	-2.65601	-1.08011
O	0.98855	2.07347	-1.54218	O	-0.86118	-0.63422	-2.37045
C	2.58534	0.42434	-0.19454	C	-2.62026	-0.24898	-0.41304
C	3.32885	0.16404	0.96230	C	-3.45069	-0.79767	0.56959
C	2.80854	-0.28578	-1.37627	C	-2.80614	1.05826	-0.87003
C	4.30125	-0.83500	0.92690	C	-4.47513	-0.01424	1.10332
C	3.78993	-1.28119	-1.39090	C	-3.83817	1.82587	-0.32452
C	4.54541	-1.57473	-0.24466	C	-4.68608	1.30546	0.66724
H	3.15663	0.74038	1.86728	H	-3.30178	-1.82087	0.90370
H	2.23895	-0.05389	-2.27204	H	-2.16262	1.46239	-1.64670
H	4.88487	-1.03794	1.82302	H	-5.12188	-0.43819	1.86928
H	3.97254	-1.83025	-2.31243	H	-3.98670	2.84365	-0.68047
C	5.58996	-2.66734	-0.25721	C	-5.82050	2.13192	1.22920
H	6.51111	-2.34242	0.23761	H	-6.01964	1.88001	2.27533
H	5.22968	-3.55438	0.27800	H	-5.60476	3.20282	1.16970
H	5.83996	-2.97343	-1.27682	H	-6.74538	1.95092	0.66739
TS2'				M2'			
N	2.12309	-1.38028	1.80366	C	-2.62165	-1.24108	-0.10287
N	2.38066	-1.94822	2.72348	C	-1.29401	-1.41567	0.22389
C	2.37020	-0.86207	-0.06362	N	-0.24552	-1.29979	-0.56945
C	1.06707	-0.94517	-0.52438	H	-1.18627	-1.82516	1.24905
N	-0.02707	-1.24253	0.14216	C	-4.84892	-0.30222	-0.41644
H	1.05396	-0.84796	-1.62427	C	-5.72684	0.77427	-0.40292
C	4.71854	-0.11599	0.01301	C	-3.48002	-0.12860	-0.05259
C	5.68349	0.88584	-0.05785	H	-6.76897	0.64092	-0.68169
C	3.34258	0.20010	-0.09830	C	-5.25722	2.04263	-0.02527
H	6.73822	0.63643	0.02854	C	-3.03031	1.17580	0.32526
C	5.29067	2.21763	-0.25651	H	-5.94550	2.88564	-0.01341
C	2.96442	1.55435	-0.28259	H	-1.98676	1.31475	0.59682
H	6.04523	2.99888	-0.32085	C	-3.91356	2.24601	0.33751
H	1.90912	1.80647	-0.35575	H	-3.57455	3.23854	0.62390
C	3.93354	2.55118	-0.37453	H	-5.18012	-1.29651	-0.70470
H	3.63920	3.58664	-0.52859	S	1.19116	-1.88265	0.08992
H	5.00798	-1.15556	0.14689	O	1.74258	-2.88124	-0.83984
S	-1.37561	-1.59640	-0.80322	O	1.02363	-2.25290	1.51528
O	-1.90065	-2.89280	-0.34624	C	2.24044	-0.42332	0.01798
O	-1.09845	-1.40230	-2.24439	C	2.80891	-0.04754	-1.20414
C	-2.53245	-0.31926	-0.28826	C	2.48578	0.30994	1.18008
C	-3.20755	-0.45553	0.92968	C	3.62173	1.08524	-1.25460
C	-2.74900	0.78829	-1.10990	C	3.30675	1.44066	1.11135
C	-4.10025	0.54090	1.32583	C	3.88483	1.84638	-0.10134
C	-3.64987	1.77602	-0.69798	H	2.62315	-0.63771	-2.09750
C	-4.33668	1.67021	0.52127	H	2.05272	-0.00736	2.12481
H	-3.04168	-1.33147	1.55107	H	4.06353	1.37921	-2.20527
H	-2.23094	0.86889	-2.06165	H	3.50347	2.00888	2.01869
H	-4.62620	0.43656	2.27335	C	4.79361	3.05348	-0.16886
H	-3.82298	2.63722	-1.34069	H	4.57295	3.67023	-1.04647
C	-5.33066	2.72566	0.95196	H	4.69577	3.68066	0.72192
H	-5.22011	2.96788	2.01416	H	5.84388	2.74608	-0.24439
H	-5.21090	3.64889	0.37769				
H	-6.35942	2.37457	0.80458				
$Rh_2(CH_3COO)_4$				$Rh_2(CF_3COO)_4$			
C	-1.92550	1.83801	0.00046	C	-1.88471	1.82687	0.01224
O	-1.50709	1.42863	-1.13425	O	-1.50267	1.43694	-1.12782
O	-1.50591	1.42954	1.13505	O	-1.48218	1.44988	1.14822
Rh	0.00014	-0.00027	1.19791	Rh	0.01215	0.00744	1.20772
Rh	0.00004	-0.00003	-1.19763	Rh	-0.01207	-0.00773	-1.20775
C	-1.83807	-1.92573	0.00002	C	-1.82538	-1.88611	0.03566
O	-1.42863	-1.50716	-1.13460	O	-1.45317	-1.50083	-1.10927
O	-1.42966	-1.50631	1.13470	O	-1.43238	-1.48537	1.16679
C	1.83825	1.92543	0.00028	C	1.82551	1.88577	-0.03568
O	1.42871	1.50709	-1.13440	O	1.43254	1.48501	-1.16681
O	1.42994	1.50578	1.13491	O	1.45321	1.50056	1.10924
C	1.92567	-1.83831	-0.00014	C	1.88481	-1.82715	-0.01226

O	1.50716	-1.42870	-1.13473
O	1.50619	-1.43007	1.13458
C	-2.98602	2.91467	0.00035
H	-3.59711	2.84748	0.90229
H	-2.49057	3.89187	-0.00781
H	-3.60615	2.83787	-0.89469
C	-2.91477	-2.98622	-0.00011
H	-2.84388	-3.60089	0.89913
H	-3.89197	-2.49073	-0.00191
H	-2.84168	-3.60279	-0.89789
C	2.91497	2.98589	0.00018
H	2.84572	3.59896	0.90064
H	3.89215	2.49038	-0.00441
H	2.84027	3.60406	-0.89638
C	2.98617	-2.91499	-0.00038
H	3.60071	-2.84431	0.89898
H	2.49069	-3.89220	-0.00250
H	3.60288	-2.84167	-0.89805

O	1.48221	-1.45024	-1.14824
O	1.50281	-1.43718	1.12780
C	-2.92142	-2.98960	0.02677
F	-4.05090	-2.49555	-0.51706
F	-2.51519	-4.03597	-0.71444
F	-3.19635	-3.42124	1.26281
C	-2.98325	2.92768	-0.00967
F	-2.47348	4.05718	-0.53973
F	-4.01944	2.53170	-0.76968
F	-3.43325	3.19919	1.22064
C	2.92170	2.98911	-0.02680
F	2.51586	4.03534	0.71482
F	4.05126	2.49472	0.51656
F	3.19633	3.42105	-1.26280
C	2.98343	-2.92788	0.00964
F	4.01966	-2.53174	0.76953
F	2.47382	-4.05737	0.53984
F	3.43334	-3.19944	-1.22069

TS2($Rh_2(CH_3COO)_4$)			
C	-1.27569	-2.54173	1.33138
O	-0.56936	-1.48879	1.15182
O	-2.47111	-2.71033	0.93403
Rh	-3.42338	-1.18955	-0.13716
Rh	-1.35068	0.09944	0.06176
C	-3.27774	0.52828	2.23996
O	-2.12280	0.90776	1.83045
O	-4.03857	-0.29972	1.65293
C	-1.51942	-1.64201	-2.30874
O	-0.74921	-0.80153	-1.72534
O	-2.67002	-1.99910	-1.90484
C	-3.50428	1.42603	-1.44506
O	-2.29928	1.59901	-1.05328
O	-4.23014	0.40878	-1.20894
N	0.89699	0.99185	1.96248
N	0.66640	0.95106	3.04804
C	0.56950	1.20827	0.22288
C	1.57882	0.34001	-0.36547
N	2.44679	-0.33415	0.30752
H	1.47375	0.24516	-1.45447
C	-0.42201	3.49484	0.43787
C	-0.36474	4.87217	0.23307
C	0.63579	2.66687	0.00639
H	-1.17990	5.50446	0.57735
C	0.73147	5.44140	-0.42897
C	1.74606	3.25492	-0.63844
H	0.76664	6.51549	-0.59853
H	2.57982	2.63601	-0.96092
C	1.78373	4.62987	-0.87096
H	2.63628	5.07038	-1.38246
H	-1.27795	3.04751	0.93204
S	3.37416	-1.46406	-0.60600
O	3.14555	-1.29550	-2.05304
O	3.15257	-2.77213	0.02206
C	5.03531	-0.90841	-0.22373
C	5.75620	-0.18893	-1.17875
C	5.59063	-1.21834	1.02302
C	7.05383	0.23217	-0.87191
C	6.88506	-0.78659	1.31109
C	7.63674	-0.05696	0.37179
H	5.31488	0.02606	-2.14812
H	5.02261	-1.79368	1.74915
H	7.61985	0.78882	-1.61625
H	7.32024	-1.02479	2.28003
C	9.04910	0.37727	0.69172
H	9.40369	1.14012	-0.00709
H	9.12077	0.78293	1.70622
H	9.73871	-0.47365	0.63291

TS2($Rh_2(CF_3COO)_4$)			
C	0.58553	-2.57647	-1.17550
O	-0.05651	-1.49057	-1.06458
O	1.73977	-2.86237	-0.76558
Rh	2.83429	-1.38854	0.24081
Rh	0.86136	0.09158	-0.06443
C	2.83102	0.17963	-2.21051
O	1.71567	0.68775	-1.87875
O	3.53333	-0.66113	-1.59986
C	0.88441	-1.47775	2.38894
O	0.17582	-0.62671	1.77541
O	1.98193	-1.99011	2.04953
C	3.11948	1.27629	1.35035
O	1.94891	1.55941	0.95851
O	3.76802	0.20702	1.22264
N	-1.31207	1.02665	-1.99962
N	-1.18870	0.88514	-3.09287
C	-0.91704	1.38127	-0.31472
C	-2.02796	0.72161	0.37824
N	-2.96592	0.08563	-0.22353
H	-1.94722	0.76977	1.47272
C	0.32755	3.51092	-0.77673
C	0.43177	4.89776	-0.70047
C	-0.80309	2.85158	-0.24843
H	1.30392	5.39677	-1.11557
C	-0.57563	5.64636	-0.07756
C	-1.82430	3.61990	0.35492
H	-0.48429	6.72805	-0.00795
H	-2.71257	3.13578	0.75278
C	-1.70104	5.00500	0.45439
H	-2.48463	5.58481	0.93591
H	1.11442	2.93534	-1.25182
S	-4.06542	-0.76974	0.81793
O	-3.87556	-0.34892	2.21585
O	-3.93911	-2.18084	0.44351
C	-5.62750	-0.13079	0.22592
C	-6.30493	0.83138	0.97832
C	-6.15346	-0.62032	-0.97540
C	-7.52946	1.31532	0.50907
C	-7.37472	-0.12160	-1.42703
C	-8.08145	0.85057	-0.69531
H	-5.88946	1.18346	1.91857
H	-5.62160	-1.38230	-1.53892
H	-8.06341	2.06101	1.09464
H	-7.78819	-0.49835	-2.36072
C	-9.41865	1.35615	-1.18607
H	-9.70708	2.28410	-0.68451
H	-9.40324	1.53999	-2.26519
H	-10.20512	0.61616	-0.99381

C	-3.75093	1.10856	3.55565
H	-3.28832	0.54582	4.37398
H	-3.43943	2.15150	3.64806
H	-4.83521	1.02246	3.64210
C	-0.60997	-3.66597	2.09353
H	0.36511	-3.88131	1.64811
H	-0.43792	-3.34751	3.12690
H	-1.23766	-4.55802	2.08762
C	-1.00333	-2.23704	-3.60026
H	-1.02739	-1.46851	-4.38024
H	0.03626	-2.55045	-3.47576
H	-1.62348	-3.08007	-3.90786
C	-4.10831	2.52730	-2.29107
H	-3.65450	3.49056	-2.05069
H	-3.90715	2.30724	-3.34545
H	-5.19050	2.56300	-2.15101

$Rh_2(HCOO)_4$

C	-1.86813	-1.82160	0.15594
O	-1.51188	-1.42042	-0.99560
O	-1.41960	-1.44088	1.28185
Rh	0.07542	0.00465	1.29832
Rh	-0.02395	0.02815	-1.10694
C	1.86142	-1.87834	0.00137
O	1.42506	-1.46362	-1.11732
O	1.51720	-1.48759	1.16010
C	-1.80968	1.91138	0.19000
O	-1.46755	1.51861	-0.96868
O	-1.37159	1.49832	1.30861
C	1.91965	1.85437	0.03543
O	1.46926	1.47559	-1.09042
O	1.56525	1.45125	1.18684
H	2.70858	2.62040	0.01036
H	-2.57410	2.70128	0.22922
H	-2.65691	-2.58778	0.18097
H	2.62628	-2.66783	-0.03790

C	3.84012	2.44741	2.07754
F	3.08892	2.89742	3.10098
F	5.03369	2.07841	2.55790
F	4.02850	3.47005	1.21392
C	3.37306	0.69488	-3.57403
F	3.49994	2.03894	-3.54015
F	4.56418	0.16536	-3.87125
F	2.50727	0.38230	-4.56045
C	-0.15958	-3.73140	-1.90480
F	-1.22680	-3.28610	-2.58290
F	0.66560	-4.34676	-2.77264
F	-0.57515	-4.64013	-1.00053
C	0.34232	-1.95226	3.76794
F	-0.85962	-1.43122	4.04109
F	0.24466	-3.29387	3.79179
F	1.20006	-1.57426	4.74047

TS2($Rh_2(HCOO)_4$)

C	-1.69627	-2.46752	1.45924
O	-0.90284	-1.49599	1.23649
O	-2.89241	-2.60121	1.07062
Rh	-3.73715	-1.08736	-0.10178
Rh	-1.57472	0.08795	0.06207
C	-3.49436	0.72961	2.17193
O	-2.31149	1.01769	1.78824
O	-4.31480	-0.06491	1.63429
C	-1.83770	-1.74764	-2.20242
O	-1.01350	-0.93239	-1.67427
O	-3.00876	-2.02958	-1.81742
C	-3.62599	1.45093	-1.51953
O	-2.42095	1.58804	-1.13282
O	-4.42600	0.50266	-1.27092
N	0.72930	0.89478	1.92113
N	0.53260	0.88895	3.01362
C	0.39459	1.10082	0.18749
C	1.37212	0.19016	-0.40034
N	2.22169	-0.49954	0.27645
H	1.26491	0.09390	-1.48908
C	-0.48862	3.43899	0.36490
C	-0.36526	4.80778	0.13445
C	0.52736	2.55275	-0.05127
H	-1.14976	5.48413	0.46567
C	0.75759	5.31137	-0.53567
C	1.66560	3.07521	-0.70451
H	0.84432	6.37918	-0.72496
H	2.46889	2.41224	-1.01619
C	1.77015	4.44226	-0.96043
H	2.64352	4.83162	-1.47813
H	-1.36477	3.04630	0.86950
S	3.13657	-1.64812	-0.63657
O	2.91702	-1.46570	-2.08251
O	2.88305	-2.95105	-0.01245
C	4.80246	-1.12066	-0.23952
C	5.54026	-0.40482	-1.18457
C	5.34409	-1.44820	1.00882
C	6.84143	-0.00489	-0.86532
C	6.64247	-1.03730	1.30904
C	7.41105	-0.31148	0.38051
H	5.10931	-0.17669	-2.15562
H	4.76275	-2.02074	1.72660
H	7.42086	0.54881	-1.60146
H	7.06730	-1.28903	2.27911
C	8.82703	0.10015	0.71352
H	9.19474	0.86847	0.02765
H	8.89878	0.48976	1.73424
H	9.50589	-0.75866	0.64535
H	-3.83201	1.24268	3.08593
H	-1.47727	-2.26403	-3.10518

				H	-1.28053	-3.28550	2.06725
				H	-4.01589	2.26612	-2.14930
$Rh_2(CHF_2COO)_4$				$Rh_2(CH_2FCOO)_4$			
C	0.57818	-2.61515	-1.11291	C	0.59371	-2.60928	-1.18814
O	-0.06427	-1.53355	-0.93739	O	-0.04205	-1.51338	-1.04301
O	1.76571	-2.87578	-0.76741	O	1.76885	-2.86675	-0.79276
Rh	2.85104	-1.38769	0.19341	Rh	2.82492	-1.37719	0.20186
Rh	0.92549	0.04806	-0.02234	Rh	0.90598	0.05026	-0.05193
C	2.78012	0.16845	-2.24646	C	2.82854	0.20585	-2.23020
O	1.66742	0.64979	-1.86744	O	1.71460	0.70058	-1.85477
O	3.50308	-0.67725	-1.64689	O	3.52399	-0.65729	-1.61813
C	1.00244	-1.51329	2.41795	C	0.91625	-1.52417	2.39069
O	0.29290	-0.63549	1.83540	O	0.20538	-0.67573	1.76171
O	2.09102	-2.01818	2.02098	O	2.02340	-2.01726	2.00607
C	3.20480	1.27064	1.28485	C	3.14361	1.26733	1.35013
O	2.02459	1.54752	0.90546	O	1.95966	1.53053	0.95557
O	3.82901	0.18094	1.14194	O	3.77709	0.18291	1.18647
C	3.91866	2.41733	2.02950	C	3.82338	2.40671	2.09805
F	3.51584	2.37581	3.34103	F	5.12337	2.08905	2.45227
F	5.26541	2.25536	1.99291	C	3.33549	0.74319	-3.56245
C	3.28871	0.72787	-3.59091	F	4.53763	0.16361	-3.93018
F	3.90166	1.92940	-3.33639	C	-0.18497	-3.69209	-1.92426
F	4.20217	-0.10572	-4.14930	F	0.53537	-4.87020	-2.02353
C	-0.20964	-3.70753	-1.86470	C	0.40033	-1.97682	3.75610
F	-0.10836	-3.44380	-3.20790	F	0.98717	-1.16197	4.73137
F	0.31943	-4.93504	-1.63117	H	-0.42250	-3.33319	-2.93092
C	0.41938	-2.01891	3.75345	H	3.47249	1.82596	-3.47703
F	-0.51200	-2.98411	3.46175	H	3.24884	2.62249	3.00473
F	1.38583	-2.57946	4.52346	H	-0.68304	-1.85244	3.81258
H	-1.26672	-3.70430	-1.58525	H	3.83381	3.29490	1.45862
H	2.46700	0.89501	-4.29263	H	0.69751	-3.00991	3.94955
H	3.65477	3.39279	1.61203	H	2.58802	0.53601	-4.33483
H	-0.07106	-1.21425	4.30797	H	-1.11676	-3.88743	-1.38419
TS2($Rh_2(CHF_2COO)_4$)				TS2($Rh_2(CH_2FCOO)_4$)			
C	0.28439	-2.51405	-1.11895	C	0.80351	-2.46368	-1.24870
O	-0.19045	-1.34126	-0.98451	O	0.17336	-1.35904	-1.11445
O	1.43056	-2.93052	-0.80576	O	1.97972	-2.72326	-0.87605
Rh	2.77453	-1.57712	0.06627	Rh	3.06866	-1.24434	0.12734
Rh	0.96391	0.10572	-0.04714	Rh	1.08067	0.19580	-0.07465
C	2.73562	0.04625	-2.35790	C	2.99772	0.41610	-2.27596
O	1.73444	0.67928	-1.89926	O	1.88322	0.90351	-1.87390
O	3.36692	-0.91024	-1.82936	O	3.70679	-0.45024	-1.70159
C	1.02887	-1.51825	2.38650	C	1.17991	-1.49870	2.32209
O	0.35004	-0.60013	1.82387	O	0.45022	-0.62153	1.74434
O	2.04882	-2.11265	1.95179	O	2.29201	-1.94564	1.93245
C	3.45509	1.02258	1.17385	C	3.35217	1.38163	1.35143
O	2.27442	1.42206	0.92303	O	2.15590	1.64705	0.98982
O	3.96877	-0.10490	0.94766	O	4.00606	0.32421	1.14039
N	-1.14922	1.38625	-1.87318	N	-1.12178	1.19797	-1.96871
N	-1.02097	1.35995	-2.97487	N	-0.92299	1.14676	-3.05973
C	-0.73236	1.53608	-0.14944	C	-0.76932	1.42227	-0.23749
C	-1.83560	0.80808	0.46771	C	-1.81056	0.60381	0.36968
N	-2.76800	0.21859	-0.19465	N	-2.68819	-0.06618	-0.29237
H	-1.73119	0.71350	1.55679	H	-1.71314	0.53197	1.46105
C	0.61335	3.63106	-0.38344	C	0.34453	3.64928	-0.47406
C	0.78779	4.99479	-0.15878	C	0.35912	5.02963	-0.28433
C	-0.54963	2.97799	0.07849	C	-0.75717	2.88270	-0.03812
H	1.68309	5.49154	-0.52437	H	1.20698	5.61526	-0.63191
C	-0.17995	5.72055	0.54881	C	-0.70948	5.66218	0.36552
C	-1.53044	3.72546	0.76842	C	-1.83903	3.53489	0.59389
H	-0.03442	6.78276	0.73304	H	-0.68925	6.73842	0.52285
H	-2.44170	3.24300	1.11391	H	-2.70544	2.96376	0.91873
C	-1.33622	5.08340	1.01730	C	-1.80549	4.91225	0.81033
H	-2.08841	5.64762	1.56325	H	-2.63622	5.40301	1.31166
H	1.37012	3.06775	-0.91952	H	1.17787	3.15358	-0.96081
S	-3.74883	-0.86771	0.72194	S	-3.61422	-1.18620	0.64116
O	-3.52406	-0.68725	2.16764	O	-3.40060	-0.97143	2.08412

O	-3.53548	-2.18754	0.11181	O	-3.34861	-2.50410	0.05089
C	-5.38730	-0.28363	0.30811	C	-5.27906	-0.67766	0.22310
C	-6.10239	0.47185	1.23993	C	-6.01660	0.07691	1.13806
C	-5.93074	-0.60503	-0.94128	C	-5.81989	-1.05599	-1.01104
C	-7.38421	0.91808	0.90532	C	-7.31683	0.46454	0.80160
C	-7.20952	-0.14718	-1.25595	C	-7.11786	-0.65671	-1.32852
C	-7.95591	0.61878	-0.34150	C	-7.88609	0.10738	-0.43109
H	-5.67017	0.69544	2.21140	H	-5.58659	0.34405	2.09949
H	-5.36737	-1.20767	-1.64857	H	-5.23911	-1.65865	-1.70409
H	-7.94683	1.50303	1.63009	H	-7.89623	1.04853	1.51392
H	-7.63647	-0.39339	-2.22640	H	-7.54254	-0.94817	-2.28739
C	-9.35200	1.08083	-0.69066	C	-9.30205	0.50507	-0.78008
H	-10.06347	0.24925	-0.61796	H	-9.65944	1.32012	-0.14455
H	-9.69512	1.87077	-0.01685	H	-9.38034	0.82487	-1.82416
H	-9.40057	1.46019	-1.71651	H	-9.98512	-0.34291	-0.64786
C	4.33756	2.10002	1.83996	C	4.01609	2.51292	2.13032
F	5.51300	1.57557	2.27305	F	5.32502	2.21263	2.47191
F	4.62164	3.06300	0.90061	C	3.46534	0.98607	-3.61120
C	3.25635	0.50808	-3.73310	F	4.68941	0.46615	-3.99703
F	2.24015	0.46979	-4.64608	C	-0.01961	-3.54797	-1.93374
F	3.68461	1.80522	-3.63583	F	0.70887	-4.71389	-2.11421
C	-0.72158	-3.50110	-1.74753	C	0.58129	-2.02786	3.62027
F	-0.81503	-3.21693	-3.09009	F	1.41950	-2.94027	4.24139
F	-0.29061	-4.78409	-1.61965	H	-0.35010	-3.18240	-2.91100
C	0.49474	-1.90487	3.78194	H	3.55443	2.07371	-3.52433
F	1.07543	-3.04805	4.22881	H	3.44418	2.69481	3.04595
F	0.81902	-0.89282	4.65473	H	0.40509	-1.18852	4.30027
H	-1.71173	-3.39554	-1.29572	H	4.00964	3.42023	1.51820
H	4.08107	-0.11648	-4.08446	H	-0.37349	-2.51439	3.39675
H	3.82307	2.57717	2.67897	H	2.72162	0.74753	-4.37855
H	-0.59237	-2.02484	3.77756	H	-0.89764	-3.76348	-1.31644
$Rh_2(PhCOO)_4$				$Rh_2(2,4,6\text{-}Cl3PhCOO)_4$			
C	1.92334	1.84420	0.00000	C	-0.18026	2.81360	0.44800
O	1.49635	1.43455	1.13456	O	0.22815	1.79168	-0.18624
O	1.49566	1.43523	-1.13452	O	-1.18484	2.86991	1.22551
Rh	0.00004	-0.00002	-1.19545	Rh	-2.36319	1.17726	1.40850
Rh	0.00005	0.00001	1.19541	Rh	-0.85573	0.00703	-0.04765
C	1.84423	-1.92331	-0.00002	C	-2.98991	1.41875	-1.43249
O	1.43461	-1.49628	1.13454	O	-2.02486	0.61678	-1.64776
O	1.43525	-1.49568	-1.13455	O	-3.39152	1.80700	-0.28951
C	-1.84415	1.92329	0.00001	C	-0.22909	-0.23460	2.79334
O	-1.43448	1.49631	1.13457	O	0.17272	-0.62257	1.65033
O	-1.43520	1.49562	-1.13451	O	-1.19431	0.56715	3.00866
C	-1.92331	-1.84415	-0.00002	C	-3.03877	-1.62923	0.91274
O	-1.49633	-1.43448	1.13453	O	-2.03405	-1.68559	0.13540
O	-1.49556	-1.43529	-1.13456	O	-3.44715	-0.60730	1.54700
C	-3.00132	-2.87646	-0.00000	C	-3.80505	-2.91459	1.10629
C	-3.51035	-3.36300	1.21540	C	-3.23887	-4.00117	1.79466
C	-3.50964	-3.36378	-1.21540	C	-5.10561	-3.07819	0.60255
C	-4.51925	-4.32865	1.21330	C	-3.93598	-5.19349	1.99529
C	-4.51853	-4.32943	-1.21329	C	-5.82545	-4.26075	0.77779
C	-5.02465	-4.81307	0.00001	C	-5.22755	-5.30594	1.48126
H	-3.11119	-2.98034	2.14997	H	-3.47803	-6.01284	2.53975
H	-3.10993	-2.98170	-2.14998	H	-6.82625	-4.36088	0.37047
H	-4.91184	-4.70384	2.15575	C	-3.70283	1.96343	-2.64326
H	-4.91056	-4.70522	-2.15573	C	-5.10998	2.08225	-2.69481
H	-5.81070	-5.56538	0.00002	C	-2.99001	2.39339	-3.78714
C	2.87656	-3.00130	0.00001	C	-5.77488	2.58078	-3.81620
C	3.36367	-3.50983	-1.21539	C	-3.63508	2.90970	-4.91256
C	3.36334	-3.51009	1.21542	C	-5.02531	2.99237	-4.91555
C	4.32934	-4.51869	-1.21327	H	-6.85793	2.64387	-3.82514
C	4.32902	-4.51896	1.21333	H	-3.05610	3.24234	-5.76765
C	4.81323	-5.02457	0.00004	C	0.58590	4.09902	0.25421
H	2.98141	-3.11030	-2.14997	C	0.01976	5.18531	-0.43463
H	2.98084	-3.11078	2.14998	C	1.88633	4.26291	0.75815
H	4.70497	-4.91089	-2.15571	C	0.71682	6.37760	-0.63558
H	4.70440	-4.91135	2.15577	C	2.60614	5.44543	0.58259

H	5.56557	-5.81060	0.00005
C	3.00129	2.87656	-0.00000
C	3.50945	3.36402	-1.21541
C	3.51042	3.36303	1.21539
C	4.51827	4.32974	-1.21332
C	4.51925	4.32875	1.21328
C	5.02449	4.81331	-0.00002
H	3.10967	2.98200	-2.14998
H	3.11141	2.98024	2.14997
H	4.91017	4.70565	-2.15576
H	4.91192	4.70387	2.15571
H	5.81049	5.56567	-0.00003
C	-2.87655	3.00121	0.00003
C	-3.36339	3.50996	1.21543
C	-3.36369	3.50971	-1.21537
C	-4.32914	4.51876	1.21334
C	-4.32943	4.51850	-1.21326
C	-4.81338	5.02434	0.00005
H	-2.98089	3.11066	2.15001
H	-2.98139	3.11021	-2.14994
H	-4.70456	4.91112	2.15579
H	-4.70508	4.91067	-2.15570
H	-5.56577	5.81031	0.00006

C	2.00831	6.49031	-0.12139
H	0.25890	7.19673	-1.18037
H	3.60686	5.54578	0.99006
C	0.48396	-0.77919	4.00407
C	1.89114	-0.89757	4.05566
C	-0.22875	-1.20953	5.14787
C	2.55618	-1.39599	5.17702
C	0.41645	-1.72569	6.27328
C	1.80671	-1.80790	6.27632
H	3.63925	-1.45874	5.18599
H	-0.16245	-2.05859	7.12833
Cl	2.91947	-0.38932	2.73293
Cl	-1.97764	-1.18555	5.22952
Cl	2.62668	-2.44328	7.68521
Cl	-1.61973	-3.89234	2.45206
Cl	-5.85934	-1.79161	-0.31176
Cl	-6.11624	-6.79584	1.71979
Cl	-1.24114	2.36877	-3.86889
Cl	-6.13841	1.57436	-1.37204
Cl	-5.84512	3.62797	-6.32443
Cl	2.63994	2.97669	1.67307
Cl	-1.59934	5.07613	-1.09207
Cl	2.89694	7.98018	-0.36036

TS2(Rh_2(PhCOO)$_4$)			
C	-0.22648	2.85000	0.55116
O	0.26208	1.84012	-0.07164
O	-1.34196	2.86878	1.16549
Rh	-2.49320	1.13449	1.28768
Rh	-0.76140	0.03265	-0.03992
C	-2.92389	1.28150	-1.60909
O	-1.83419	0.61459	-1.74122
O	-3.43984	1.63438	-0.50224
C	-0.34922	-0.07781	2.87190
O	0.17898	-0.44741	1.76248
O	-1.44181	0.56629	2.98854
C	-3.01852	-1.69123	0.76067
O	-1.91199	-1.70982	0.11601
O	-3.52491	-0.67296	1.33476
N	1.07395	0.25877	-2.49904
N	0.79698	1.02899	-3.24948
C	0.81179	-0.97985	-1.24531
C	2.04982	-0.88105	-0.48812
N	3.03189	-0.10358	-0.79168
H	2.03885	-1.49156	0.42430
C	-0.74366	-2.40411	-2.59767
C	-1.02115	-3.57434	-3.30228
C	0.51892	-2.21840	-1.99571
H	-1.99516	-3.70542	-3.76789
C	-0.05647	-4.58650	-3.39643
C	1.49061	-3.23621	-2.11708
H	-0.28112	-5.50341	-3.93731
H	2.47654	-3.10423	-1.67819
C	1.19804	-4.41862	-2.79700
H	1.94898	-5.20164	-2.87114
H	-1.49571	-1.62802	-2.50633
S	4.29672	-0.01473	0.37427
O	4.07291	-0.97303	1.47330
O	4.46903	1.41279	0.66624
C	5.69037	-0.58552	-0.59820
C	6.17429	-1.88194	-0.41016
C	6.28166	0.28316	-1.52242
C	7.26603	-2.31346	-1.16941
C	7.36780	-0.16749	-2.27248
C	7.87757	-1.46851	-2.10907
H	5.71405	-2.53534	0.32597
H	5.90375	1.29457	-1.64513
H	7.64869	-3.32140	-1.02134

TS2(Rh_2(2,4,6-Cl3PhCOO)$_4$)			
C	-1.52234	0.85750	-1.93043
O	-1.47205	0.50171	-0.70759
O	-0.55575	0.91509	-2.74485
Rh	1.32219	0.24262	-2.12132
Rh	0.38182	0.07135	0.14541
C	1.44213	2.70745	-0.56578
O	0.75965	2.11783	0.33681
O	1.86946	2.20427	-1.64334
C	0.31697	-2.40423	-1.42247
O	0.10835	-1.97147	-0.24064
O	0.71975	-1.73241	-2.41619
C	3.24768	-0.54178	-0.09036
O	2.34241	-0.34036	0.78134
O	3.13498	-0.44269	-1.34643
N	-0.86081	1.50086	2.66948
N	-0.66126	2.58651	2.78812
C	-0.57268	-0.19594	2.14396
C	-1.94958	-0.62052	1.88256
N	-2.97930	0.11306	2.11364
H	-2.01492	-1.60905	1.40749
C	1.45455	-0.38578	3.60747
C	2.13348	-0.96573	4.67617
C	0.15222	-0.81290	3.27234
H	3.13135	-0.61848	4.93328
C	1.54268	-2.00569	5.40634
C	-0.44427	-1.84191	4.03466
H	2.08224	-2.46727	6.23051
H	-1.45299	-2.17766	3.80923
C	0.25622	-2.44832	5.07753
H	-0.20703	-3.25290	5.64365
H	1.92513	0.40137	3.02901
S	-4.49325	-0.51275	1.56318
O	-4.35472	-1.91266	1.12337
O	-5.04035	0.49575	0.65042
C	-5.42405	-0.48489	3.09416
C	-5.64348	-1.67718	3.78688
C	-5.93236	0.73202	3.56286
C	-6.37964	-1.64352	4.97508
C	-6.66128	0.74479	4.75164
C	-6.89719	-0.43846	5.47549
H	-5.25726	-2.61483	3.39664
H	-5.76704	1.64827	3.00244
H	-6.55663	-2.57168	5.51490

H	7.82983	0.50478	-2.99319	H	-7.05769	1.68909	5.12049
C	9.07538	-1.92906	-2.90820	C	-7.71420	-0.40841	6.74709
H	9.17041	-3.01854	-2.89909	H	-7.59477	-1.32961	7.32419
H	9.01005	-1.59962	-3.95021	H	-7.42744	0.43435	7.38458
H	10.00092	-1.51184	-2.49284	H	-8.78106	-0.29475	6.51918
C	-3.77947	-2.97800	0.84077	C	4.60573	-0.93864	0.44006
C	-3.26049	-4.14657	0.25994	C	4.80206	-2.14932	1.12729
C	-5.01826	-3.02008	1.50129	C	5.72926	-0.11241	0.26062
C	-3.97452	-5.34471	0.34027	C	6.05449	-2.53215	1.61157
C	-5.73071	-4.21910	1.57797	C	6.99178	-0.46180	0.74366
C	-5.21042	-5.38331	0.99827	C	7.13669	-1.67562	1.41405
H	-2.30082	-4.10567	-0.24613	H	6.17833	-3.47913	2.12666
H	-5.41042	-2.11171	1.94886	H	7.83870	0.20067	0.59761
H	-3.56789	-6.24888	-0.10768	C	1.76430	4.16080	-0.31344
H	-6.68996	-4.24727	2.09017	C	1.34126	5.16812	-1.20149
H	-5.76539	-6.31721	1.06040	C	2.50298	4.56984	0.81133
C	-3.64215	1.67085	-2.86298	C	1.62698	6.51706	-0.98135
C	-4.85344	2.37741	-2.78147	C	2.81551	5.90870	1.05083
C	-3.11675	1.33730	-4.12192	C	2.36588	6.86984	0.14657
C	-5.53082	2.74380	-3.94661	H	1.27731	7.27189	-1.67806
C	-3.79558	1.70587	-5.28587	H	3.39860	6.19022	1.92146
C	-5.00374	2.40914	-5.20048	C	-2.88582	1.24505	-2.44580
H	-5.25211	2.63253	-1.80420	C	-3.56433	2.37137	-1.95200
H	-2.17835	0.79472	-4.18051	C	-3.53479	0.48477	-3.43324
H	-6.46863	3.29063	-3.87825	C	-4.82643	2.73966	-2.41801
H	-3.38339	1.44726	-6.25879	C	-4.80146	0.82028	-3.91307
H	-5.53181	2.69621	-6.10745	C	-5.43058	1.95169	-3.39595
C	0.58759	4.10290	0.54848	H	-5.32419	3.61835	-2.02171
C	-0.00446	5.32181	0.91852	H	-5.28345	0.20804	-4.66810
C	1.94554	4.06336	0.19216	C	0.06982	-3.87505	-1.65924
C	0.75233	6.49546	0.91507	C	-1.18930	-4.46177	-1.43176
C	2.70186	5.23819	0.20411	C	1.09367	-4.71760	-2.13427
C	2.10677	6.45531	0.55858	C	-1.42900	-5.81665	-1.67227
H	-1.05251	5.33814	1.20322	C	0.88544	-6.07794	-2.36871
H	2.40723	3.11538	-0.06631	C	-0.38189	-6.60989	-2.13674
H	0.28954	7.43952	1.19433	H	-2.41462	-6.23680	-1.50055
H	3.75733	5.20183	-0.05612	H	1.69739	-6.70362	-2.72443
H	2.69764	7.36911	0.56366	Cl	-2.53923	-3.50856	-0.86061
C	0.37656	-0.43824	4.12813	Cl	2.70941	-4.10671	-2.42200
C	1.70415	-0.89413	4.08044	Cl	-0.66350	-8.31376	-2.43517
C	-0.27503	-0.31105	5.36650	Cl	3.47257	-3.26037	1.37788
C	2.37065	-1.21998	5.26474	Cl	5.58240	1.42768	-0.55937
C	0.39159	-0.64945	6.54590	Cl	8.71488	-2.13546	2.02181
C	1.71605	-1.10377	6.49709	Cl	3.11812	3.39798	1.96241
H	2.21847	-0.97191	3.12771	Cl	0.39529	4.77822	-2.62038
H	-1.29884	0.05020	5.39246	Cl	2.73970	8.55681	0.43398
H	3.40318	-1.55964	5.22431	Cl	-2.78235	-0.95648	-4.08475
H	-0.11831	-0.55597	7.50229	Cl	-2.82419	3.39868	-0.74206
H	2.23708	-1.36132	7.41709	Cl	-7.01989	2.39353	-3.98984
TS2(Rh_2(p-OMePhCOO)$_4$)				TS2(Rh_2(p-NMe_2PhCOO)$_4$)			
C	0.65562	-1.96689	-1.96416	C	-0.91762	1.90665	-1.81264
O	0.72386	-1.51436	-0.76339	O	-0.87413	1.47990	-0.59946
O	-0.23540	-1.64977	-2.81946	O	-0.10975	1.56017	-2.73924
Rh	-1.66976	-0.21194	-2.34762	Rh	1.37458	0.14545	-2.35798
Rh	-0.63261	-0.07042	-0.14167	Rh	0.53885	0.05538	-0.06893
C	-2.79380	-2.06664	-0.37150	C	2.66105	2.05554	-0.53618
O	-1.95213	-1.57788	0.46958	O	1.89700	1.58136	0.38643
O	-2.91235	-1.70150	-1.58495	O	2.66867	1.66320	-1.74915
C	0.49675	1.75016	-2.16276	C	-0.75587	-1.82411	-1.93365
O	0.61498	1.40663	-0.93007	O	-0.76535	-1.44758	-0.70321
O	-0.36538	1.27944	-2.97610	O	0.03365	-1.37109	-2.83000
C	-2.92430	1.74115	-0.57185	C	2.80777	-1.74803	-0.65214
O	-2.05724	1.39650	0.30813	O	2.01222	-1.38888	0.28982
O	-3.02654	1.24523	-1.74242	O	2.79829	-1.28167	-1.84160
N	0.50470	-1.66332	2.23541	N	-0.39766	1.71002	2.34719
N	0.21781	-2.73526	2.28211	N	-0.10931	2.78266	2.32688
C	0.30511	0.07058	1.87320	C	-0.21841	-0.03283	2.02078

C	1.68533	0.47728	1.66817	C	-1.60636	-0.45618	1.95331
N	2.70594	-0.29792	1.81184	N	-2.62097	0.31018	2.17277
H	1.77325	1.50914	1.30376	H	-1.71363	-1.49880	1.62665
C	-1.83086	0.37006	3.14710	C	2.02413	-0.28714	3.10829
C	-2.54019	0.87909	4.23392	C	2.83045	-0.76101	4.14230
C	-0.44552	0.60909	3.02699	C	0.63492	-0.53242	3.12045
H	-3.60665	0.68432	4.32055	H	3.89963	-0.56259	4.12557
C	-1.88724	1.65325	5.20250	C	2.27099	-1.50571	5.18912
C	0.20539	1.37249	4.02110	C	0.07966	-1.26577	4.19209
H	-2.44665	2.05778	6.04352	H	2.90573	-1.88357	5.98807
H	1.27608	1.55070	3.95760	H	-0.99151	-1.44814	4.23016
C	-0.51406	1.90520	5.09109	C	0.89446	-1.76330	5.20943
H	-0.00480	2.50337	5.84307	H	0.45738	-2.33898	6.02203
H	-2.33712	-0.21215	2.38492	H	2.45690	0.27134	2.28556
S	4.21705	0.36010	1.31966	S	-4.16096	-0.38511	1.85828
O	4.07988	1.77478	0.92324	O	-4.04376	-1.81067	1.49617
O	4.79338	-0.61246	0.38397	O	-4.85490	0.54635	0.96175
C	5.12798	0.29327	2.86321	C	-4.90481	-0.28023	3.48865
C	5.32978	1.46618	3.59345	C	-5.02526	-1.43391	4.26549
C	5.63426	-0.93362	3.30702	C	-5.36637	0.95698	3.95240
C	6.04619	1.40261	4.79253	C	-5.61272	-1.34065	5.53129
C	6.34338	-0.97684	4.50726	C	-5.94566	1.03037	5.21895
C	6.56160	0.18647	5.26783	C	-6.07902	-0.11338	6.02746
H	4.94477	2.41257	3.22363	H	-4.67710	-2.38877	3.88112
H	5.48214	-1.83489	2.71933	H	-5.27959	1.84311	3.32942
H	6.20929	2.31609	5.36111	H	-5.71224	-2.23962	6.13654
H	6.73754	-1.92954	4.85643	H	-6.30389	1.99151	5.58359
C	7.35837	0.12520	6.55116	C	-6.73458	-0.01873	7.38667
H	8.43091	0.04100	6.33734	H	-7.82124	0.09192	7.28662
H	7.21146	1.02219	7.15931	H	-6.54627	-0.91302	7.98736
H	7.07841	-0.74572	7.15273	H	-6.37050	0.85038	7.94453
C	-3.89202	2.80828	-0.19071	C	3.81950	-2.78470	-0.32635
C	-3.81604	3.43161	1.06172	C	3.86955	-3.37867	0.94586
C	-4.89804	3.21084	-1.09025	C	4.75180	-3.20727	-1.28906
C	-4.71671	4.43740	1.42302	C	4.81267	-4.35341	1.25210
C	-5.80120	4.20674	-0.74281	C	5.70270	-4.17833	-0.99773
C	-5.71671	4.82931	0.51745	C	5.76793	-4.77667	0.28932
H	-3.04022	3.12693	1.75767	H	3.14995	-3.07239	1.69956
H	-4.96033	2.73287	-2.06332	H	4.72161	-2.76548	-2.28104
H	-4.62777	4.90354	2.39884	H	4.80242	-4.78943	2.24501
H	-6.58125	4.52421	-1.43030	H	6.39573	-4.47379	-1.77766
C	-3.70069	-3.14318	0.11594	C	3.60254	3.13606	-0.15236
C	-4.66373	-3.70182	-0.74719	C	4.48390	3.68611	-1.09940
C	-3.61547	-3.62172	1.42995	C	3.64160	3.64604	1.15633
C	-5.51374	-4.70640	-0.30510	C	5.37301	4.69801	-0.75875
C	-4.46362	-4.63328	1.88831	C	4.52411	4.65884	1.51383
C	-5.42024	-5.18129	1.01747	C	5.42672	5.21135	0.56546
H	-4.73454	-3.33705	-1.76747	H	4.46261	3.31021	-2.11831
H	-2.87355	-3.20065	2.10150	H	2.96204	3.24422	1.90212
H	-6.25959	-5.14307	-0.96455	H	6.02791	5.09176	-1.52814
H	-4.36850	-4.98261	2.91116	H	4.50835	5.02324	2.53509
C	1.70407	-2.93622	-2.38042	C	-1.98878	2.87430	-2.14878
C	1.54827	-3.68897	-3.56042	C	-1.98593	3.54878	-3.38149
C	2.86964	-3.09797	-1.61923	C	-3.04632	3.12540	-1.25795
C	2.52602	-4.59181	-3.95661	C	-2.98651	4.45549	-3.71075
C	3.86671	-3.99296	-2.01587	C	-4.05950	4.02143	-1.57865
C	3.69474	-4.74932	-3.18665	C	-4.05264	4.72668	-2.81151
H	0.65175	-3.55814	-4.15941	H	-1.18461	3.35306	-4.08856
H	3.01303	-2.50102	-0.72377	H	-3.08740	2.58905	-0.31473
H	2.41308	-5.18322	-4.86182	H	-2.93969	4.94969	-4.67485
H	4.76591	-4.07978	-1.41508	H	-4.86710	4.16027	-0.86868
C	1.43976	2.77964	-2.67731	C	-1.73429	-2.86263	-2.33675
C	2.56506	3.16145	-1.93426	C	-2.77611	-3.25884	-1.48052
C	1.21796	3.37561	-3.93425	C	-1.65590	-3.46198	-3.60573
C	3.45706	4.11928	-2.42399	C	-3.70068	-4.22103	-1.87068
C	2.09085	4.33717	-4.42536	C	-2.56729	-4.43253	-4.00448
C	3.21932	4.71603	-3.67274	C	-3.61618	-4.84927	-3.14147

H	2.76588	2.69405	-0.97538
H	0.35235	3.07653	-4.51788
H	4.32682	4.37968	-1.82999
H	1.92496	4.80751	-5.39138
O	4.02038	5.66450	-4.24274
C	5.18942	6.07944	-3.53387
H	4.93126	6.53234	-2.56888
H	5.87778	5.24088	-3.37405
H	5.67049	6.82699	-4.16700
O	-6.64722	5.79805	0.76290
C	-6.60815	6.47594	2.01972
H	-6.76451	5.78056	2.85344
H	-5.65900	7.00809	2.15676
H	-7.42640	7.19750	1.99317
O	-6.29778	-6.17022	1.35484
C	-6.24949	-6.70061	2.68092
H	-5.27522	-7.15762	2.89225
H	-6.46408	-5.92686	3.42798
H	-7.02487	-7.46730	2.72185
O	4.59998	-5.65471	-3.66328
C	5.81480	-5.84627	-2.93606
H	6.39850	-4.91941	-2.88311
H	5.61895	-6.21614	-1.92220
H	6.37814	-6.59749	-3.49232

H	-2.88428	-2.78885	-0.50785
H	-0.86631	-3.15558	-4.28605
H	-4.49960	-4.47285	-1.18221
H	-2.46407	-4.86316	-4.99438
N	-4.51636	-5.83114	-3.52257
N	6.72726	-5.72680	0.59462
N	6.32403	6.20203	0.91763
N	-5.04226	5.64473	-3.12320
C	6.64749	-6.45316	1.85645
H	7.48882	-7.14463	1.92699
H	6.71259	-5.76992	2.71131
H	5.71758	-7.03426	1.95092
C	7.56664	-6.27179	-0.46640
H	8.15871	-5.48411	-0.94650
H	8.26690	-6.99042	-0.03723
H	6.98227	-6.78542	-1.24472
C	7.12245	6.85677	-0.11242
H	7.77688	7.59445	0.35470
H	7.76093	6.13648	-0.63740
H	6.50179	7.37423	-0.85901
C	6.24318	6.81777	2.23686
H	5.27833	7.31795	2.40850
H	6.39078	6.07623	3.03112
H	7.03364	7.56356	2.33490
C	-6.22183	5.74724	-2.27135
H	-6.79465	4.80851	-2.22706
H	-5.94612	6.02836	-1.24857
H	-6.87752	6.52901	-2.65894
C	-5.12163	6.18574	-4.47527
H	-5.94895	6.89553	-4.52994
H	-4.20674	6.72916	-4.73785
H	-5.28793	5.40567	-5.23381
C	-4.53139	-6.29581	-4.90488
H	-5.29071	-7.07217	-5.01444
H	-4.75855	-5.49011	-5.61967
H	-3.56836	-6.73887	-5.18322
C	-5.69403	-6.08459	-2.70005
H	-6.27226	-6.89786	-3.14234
H	-5.40882	-6.39740	-1.68926
H	-6.34845	-5.20375	-2.61504

Rh_2(p-OMePhCOO)$_4$

C	-1.82418	-2.07845	0.14741
O	-1.33492	-1.64368	1.24886
O	-1.49851	-1.65048	-1.01574
Rh	-0.08123	-0.14569	-1.18204
Rh	0.08927	-0.13721	1.20148
C	-1.92720	1.69367	0.14077
O	-1.41589	1.28901	1.24370
O	-1.57851	1.28044	-1.02107
C	1.93520	-1.97660	-0.12131
O	1.58682	-1.56304	1.04052
O	1.42365	-1.57222	-1.22421
C	1.83206	1.79570	-0.12796
O	1.50625	1.36785	1.03517
O	1.34318	1.36056	-1.22946
C	-3.00200	2.71639	0.21522
C	-3.59814	3.20823	-0.95409
C	-3.43817	3.20786	1.46119
C	-4.60882	4.17035	-0.89761
C	-4.44217	4.16397	1.53100
C	-5.03604	4.65331	0.35107
H	-3.26506	2.83256	-1.91709
H	-2.98046	2.83079	2.37087
H	-5.04939	4.53088	-1.82119
H	-4.78670	4.54998	2.48707
C	-2.84255	-3.15713	0.22536
C	-3.42374	-3.67251	-0.94137

Rh_2(p-NMe$_2$PhCOO)$_4$

C	1.89735	-1.87900	-0.00030
O	1.49612	-1.43549	1.13531
O	1.44990	-1.48233	-1.13594
Rh	-0.00005	0.00005	-1.19415
Rh	0.00000	0.00011	1.19340
C	-1.88194	-1.89446	-0.00017
O	-1.43650	-1.49521	1.13536
O	-1.48325	-1.44902	-1.13588
C	1.88191	1.89461	-0.00038
O	1.43651	1.49542	1.13520
O	1.48316	1.44911	-1.13605
C	-1.89739	1.87917	-0.00031
O	-1.49611	1.43571	1.13530
O	-1.45000	1.48243	-1.13595
C	-2.94892	2.92041	-0.00017
C	-3.49455	3.39708	1.20448
C	-3.43489	3.45772	-1.20484
C	-4.48364	4.37258	1.21308
C	-4.42262	4.43463	-1.21326
C	-4.97415	4.92883	0.00023
H	-3.13518	2.98929	2.14504
H	-3.02908	3.09715	-2.14580
H	-4.87677	4.70306	2.16812
H	-4.76760	4.81401	-2.16873
C	-2.92854	-2.94071	0.00004
C	-3.47284	-3.41938	-1.20439

C	-3.23960	-3.67858	1.47220
C	-4.38217	-4.68650	-0.88138
C	-4.19083	-4.68696	1.54545
C	-4.77012	-5.19950	0.36814
H	-3.12068	-3.27381	-1.90502
H	-2.79334	-3.28340	2.37988
H	-4.81285	-5.06373	-1.80296
H	-4.50445	-5.09689	2.50219
C	3.00984	-2.99948	-0.19572
C	3.60576	-3.49151	0.97362
C	3.44607	-3.49096	-1.44168
C	4.61626	-4.45384	0.91719
C	4.44989	-4.44724	-1.51145
C	5.04353	-4.93677	-0.33146
H	3.27265	-3.11585	1.93661
H	2.98852	-3.11375	-2.35139
H	5.05668	-4.81446	1.84080
H	4.79449	-4.83327	-2.46748
C	2.85026	2.87452	-0.20593
C	3.43140	3.38999	0.96078
C	3.24721	3.39606	-1.45278
C	4.38960	4.40420	0.90081
C	4.19817	4.40467	-1.52601
C	4.77736	4.91738	-0.34870
H	3.12846	2.99122	1.92444
H	2.80106	3.00074	-2.36046
H	4.82034	4.78137	1.82239
H	4.51171	4.81466	-2.48275
O	6.01957	-5.87338	-0.50502
C	6.66295	-6.40983	0.65349
H	7.17902	-5.62638	1.22124
H	5.94665	-6.92626	1.30365
H	7.39495	-7.12757	0.27980
O	-5.69355	-6.18748	0.54506
C	-6.31687	-6.75270	-0.61072
H	-6.87939	-5.99571	-1.17022
H	-5.57935	-7.22667	-1.26939
H	-7.00593	-7.51054	-0.23455
O	-6.01225	5.58973	0.52464
C	-6.65561	6.12621	-0.63386
H	-5.93946	6.64323	-1.28370
H	-7.17113	5.34266	-1.20196
H	-7.38813	6.84340	-0.26012
O	5.70042	5.90564	-0.52572
C	6.32389	6.47097	0.62991
H	5.58637	6.94443	1.28898
H	6.88705	5.71421	1.18907
H	7.01236	7.22929	0.25361

C	-3.41245	-3.47943	1.20487
C	-4.45888	-4.39800	-1.21258
C	-4.39712	-4.45944	1.21364
C	-4.94736	-4.95563	0.00041
H	-3.11530	-3.01033	-2.14510
H	-3.00788	-3.11715	2.14570
H	-4.85139	-4.72951	-2.16751
H	-4.74091	-4.83940	2.16929
C	2.94888	-2.92025	-0.00016
C	3.43477	-3.45765	-1.20482
C	3.49460	-3.39682	1.20448
C	4.42249	-4.43455	-1.21323
C	4.48370	-4.37231	1.21309
C	4.97410	-4.92868	0.00026
H	3.02889	-3.09715	-2.14578
H	3.13532	-2.98894	2.14504
H	4.76741	-4.81401	-2.16869
H	4.87692	-4.70267	2.16813
C	2.92850	2.94085	-0.00027
C	3.41247	3.47963	1.20452
C	3.47276	3.41947	-1.20474
C	4.39714	4.45964	1.21320
C	4.45881	4.39808	-1.21302
C	4.94734	4.95577	-0.00008
H	3.00794	3.11741	2.14539
H	3.11518	3.01037	-2.14541
H	4.74097	4.83964	2.16882
H	4.85128	4.72954	-2.16798
N	5.91290	5.94345	-0.00067
N	-5.94281	5.91312	0.00116
N	-5.91292	-5.94333	-0.00010
N	5.94268	-5.91307	0.00115
C	-6.58741	6.29834	1.25116
H	-7.31089	7.09084	1.05374
H	-7.12041	5.45956	1.72259
H	-5.85861	6.68936	1.97143
C	-6.52105	6.36617	-1.25852
H	-7.03051	5.55575	-1.80040
H	-7.25220	7.15066	-1.05739
H	-5.75503	6.79098	-1.91845
C	-6.56191	-6.32470	-1.24914
H	-7.28134	-7.12104	-1.05228
H	-7.10010	-5.48570	-1.71445
H	-5.83478	-6.70971	-1.97413
C	-6.49494	-6.39158	1.25964
H	-7.22239	-7.17981	1.05960
H	-5.73009	-6.81048	1.92450
H	-7.00932	-5.58019	1.79555
C	6.58776	-6.29781	1.25108
H	7.12137	-5.45898	1.72179
H	5.85913	-6.68810	1.97187
H	7.31077	-7.09077	1.05377
C	6.52152	-6.36538	-1.25853
H	7.25268	-7.14989	-1.05750
H	5.75583	-6.78995	-1.91897
H	7.03109	-5.55461	-1.79980
C	6.56183	6.32479	-1.24976
H	7.28127	7.12113	-1.05296
H	7.09997	5.48577	-1.71508
H	5.83465	6.70979	-1.97471
C	6.49495	6.39180	1.25903
H	7.22239	7.18002	1.05891
H	5.73011	6.81075	1.92386
H	7.00933	5.58045	1.79499

$Rh_2(C6F5COO)_4$			
C	-1.87626	-1.86279	-0.11121
O	-1.47504	-1.52465	1.04693

TS2($Rh_2(C6F5COO)_4$)			
C	-0.22648	2.85000	0.55116
O	0.26208	1.84012	-0.07164

O	-1.46289	-1.40061	-1.22187
Rh	-0.00005	0.07304	-1.19967
Rh	-0.00003	-0.07307	1.19965
C	-1.87766	1.86136	0.11127
O	-1.46392	1.39951	1.22194
O	-1.47620	1.52350	-1.04686
C	1.87760	-1.86138	-0.11128
O	1.47590	-1.52377	1.04683
O	1.46409	-1.39930	-1.22194
C	1.87620	1.86275	0.11120
O	1.46302	1.40037	1.22185
O	1.47479	1.52482	-1.04693
C	-2.94840	2.91017	0.17450
C	-2.86787	4.07620	-0.59826
C	-4.06476	2.75555	1.00693
C	-3.85550	5.05748	-0.53973
C	-5.06869	3.71982	1.06527
C	-4.96042	4.87566	0.29195
C	-2.94621	-2.91241	-0.17443
C	-4.06302	-2.75840	-1.00634
C	-2.86432	-4.07872	0.59777
C	-5.06612	-3.72352	-1.06471
C	-3.85110	-5.06086	0.53918
C	-4.95652	-4.87962	-0.29197
C	2.94841	-2.91012	-0.17451
C	2.86737	-4.07670	0.59738
C	4.06534	-2.75492	-1.00607
C	3.85506	-5.05792	0.53884
C	5.06933	-3.71912	-1.06438
C	4.96055	-4.87550	-0.29195
C	2.94617	2.91236	0.17443
C	4.06302	2.75828	1.00627
C	2.86427	4.07873	-0.59769
C	5.06614	3.72339	1.06466
C	3.85107	5.06084	-0.53908
C	4.95652	4.87954	0.29201
F	-6.13525	-3.54545	-1.85135
F	-4.21725	-1.65143	-1.74466
F	-5.90980	-5.81275	-0.34800
F	-3.74191	-6.17774	1.26971
F	-1.80782	-4.30056	1.38932
F	1.81085	-4.29970	1.38858
F	3.74666	-6.17508	1.26908
F	5.91468	-5.80775	-0.34792
F	6.13853	-3.53989	-1.85067
F	4.21887	-1.64761	-1.74405
F	4.21729	1.65126	1.74451
F	6.13531	3.54524	1.85124
F	5.90982	5.81265	0.34805
F	3.74185	6.17778	-1.26953
F	1.80773	4.30064	-1.38918
F	-1.81190	4.29858	-1.39036
F	-3.74759	6.17412	-1.27083
F	-5.91450	5.80796	0.34793
F	-6.13734	3.54115	1.85242
F	-4.21775	1.64877	1.74580

O	-1.34196	2.86878	1.16549
Rh	-2.49320	1.13449	1.28768
Rh	-0.76140	0.03265	-0.03992
C	-2.92389	1.28150	-1.60909
O	-1.83419	0.61459	-1.74122
O	-3.43984	1.63438	-0.50224
C	-0.34922	-0.07781	2.87190
O	0.17898	-0.44741	1.76248
O	-1.44181	0.56629	2.98854
C	-3.01852	-1.69123	0.76067
O	-1.91199	-1.70982	0.11601
O	-3.52491	-0.67296	1.33476
N	1.07395	0.25877	-2.49904
N	0.79698	1.02899	-3.24948
C	0.81179	-0.97985	-1.24531
C	2.04982	-0.88105	-0.48812
N	3.03189	-0.10358	-0.79168
H	2.03885	-1.49156	0.42430
C	-0.74366	-2.40411	-2.59767
C	-1.02115	-3.57434	-3.30228
C	0.51892	-2.21840	-1.99571
H	-1.99516	-3.70542	-3.76789
C	-0.05647	-4.58650	-3.39643
C	1.49061	-3.23621	-2.11708
H	-0.28112	-5.50341	-3.93731
H	2.47654	-3.10423	-1.67819
C	1.19804	-4.41862	-2.79700
H	1.94898	-5.20164	-2.87114
H	-1.49571	-1.62802	-2.50633
S	4.29672	-0.01473	0.37427
O	4.07291	-0.97303	1.47330
O	4.46903	1.41279	0.66624
C	5.69037	-0.58552	-0.59820
C	6.17429	-1.88194	-0.41016
C	6.28166	0.28316	-1.52242
C	7.26603	-2.31346	-1.16941
C	7.36780	-0.16749	-2.27248
C	7.87757	-1.46851	-2.10907
H	5.71405	-2.53534	0.32597
H	5.90375	1.29457	-1.64513
H	7.64869	-3.32140	-1.02134
H	7.82983	0.50478	-2.99319
C	9.07538	-1.92906	-2.90820
H	9.17041	-3.01854	-2.89909
H	9.01005	-1.59962	-3.95021
H	10.00092	-1.51184	-2.49284
C	-3.77947	-2.97800	0.84077
C	-3.26049	-4.14657	0.25994
C	-5.01826	-3.02008	1.50129
C	-3.97452	-5.34471	0.34027
C	-5.73071	-4.21910	1.57797
C	-5.21042	-5.38331	0.99827
H	-2.30082	-4.10567	-0.24613
H	-5.41042	-2.11171	1.94886
H	-3.56789	-6.24888	-0.10768
H	-6.68996	-4.24727	2.09017
H	-5.76539	-6.31721	1.06040
C	-3.64215	1.67085	-2.86298
C	-4.85344	2.37741	-2.78147
C	-3.11675	1.33730	-4.12192
C	-5.53082	2.74380	-3.94661
C	-3.79558	1.70587	-5.28587
C	-5.00374	2.40914	-5.20048
H	-5.25211	2.63253	-1.80420
H	-2.17835	0.79472	-4.18051
H	-6.46863	3.29063	-3.87825
H	-3.38339	1.44726	-6.25879

	H -5.53181 2.69621 -6.10745 C 0.58759 4.10290 0.54848 C -0.00446 5.32181 0.91852 C 1.94554 4.06336 0.19216 C 0.75233 6.49546 0.91507 C 2.70186 5.23819 0.20411 C 2.10677 6.45531 0.55858 H -1.05251 5.33814 1.20322 H 2.40723 3.11538 -0.06631 H 0.28954 7.43952 1.19433 H 3.75733 5.20183 -0.05612 H 2.69764 7.36911 0.56366 C 0.37656 -0.43824 4.12813 C 1.70415 -0.89413 4.08044 C -0.27503 -0.31105 5.36650 C 2.37065 -1.21998 5.26474 C 0.39159 -0.64945 6.54590 C 1.71605 -1.10377 6.49709 H 2.21847 -0.97191 3.12771 H -1.29884 0.05020 5.39246 H 3.40318 -1.55964 5.22431 H -0.11831 -0.55597 7.50229 H 2.23708 -1.36132 7.41709
$Rh_2(p\text{-}NO_2PhCOO)_4$ C 1.88498 -1.87478 0.00004 O 1.46930 -1.46144 1.13470 O 1.46929 -1.46151 -1.13463 Rh -0.00001 -0.00004 -1.19760 Rh -0.00006 -0.00002 1.19763 C -1.87474 -1.88506 0.00000 O -1.46147 -1.46938 1.13467 O -1.46148 -1.46934 -1.13466 C 1.87468 1.88498 0.00002 O 1.46140 1.46929 1.13468 O 1.46142 1.46929 -1.13464 C -1.88509 1.87468 -0.00002 O -1.46939 1.46142 1.13467 O -1.46934 1.46140 -1.13468 C -2.93009 -2.94665 -0.00001 C -3.42308 -3.44319 -1.21710 C -3.42352 -3.44277 1.21709 C -4.40547 -4.43174 -1.22374 C -4.40594 -4.43129 1.22372 C -4.88094 -4.90980 -0.00002 H -3.03428 -3.05231 -2.15201 H -3.03504 -3.05157 2.15200 H -4.80036 -4.82949 -2.15240 H -4.80120 -4.82869 2.15236 C 2.94676 -2.92995 0.00006 C 3.44322 -3.42307 -1.21703 C 3.44309 -3.42313 1.21718 C 4.43185 -4.40538 -1.22365 C 4.43175 -4.40542 1.22384 C 4.91011 -4.88056 0.00010 H 3.05217 -3.03447 -2.15194 H 3.05194 -3.03458 2.15207 H 4.82948 -4.80044 -2.15229 H 4.82932 -4.80048 2.15250 C 2.93000 2.94658 0.00003 C 3.42294 3.44319 1.21711 C 3.42349 3.44264 -1.21707 C 4.40533 4.43173 1.22373 C 4.40592 4.43115 -1.22372 C 4.88087 4.90974 -0.00001 H 3.03409 3.05235 2.15202 H 3.03506 3.05139 -2.15198 H 4.80018 4.82953 2.15238	$Rh_2(tBuCOO)_4$ C -1.87750 -1.89585 0.02103 O -1.46011 -1.48700 -1.11504 O -1.45785 -1.46799 1.14763 Rh -0.00024 0.01173 1.19554 Rh 0.00023 -0.01116 -1.19551 C 1.89894 -1.87420 0.02321 O 1.47900 -1.46849 -1.11312 O 1.47770 -1.44747 1.14958 C -1.89910 1.87460 -0.02314 O -1.47733 1.44843 -1.14952 O -1.47945 1.46860 1.11319 C 1.87756 1.89633 -0.02102 O 1.45835 1.46804 -1.14761 O 1.45961 1.48805 1.11505 C -2.98018 -2.96729 0.01133 C 2.98987 -2.95764 0.01226 C -2.99071 2.95736 -0.01213 C 2.98101 2.96696 -0.01145 C -3.40794 3.33354 -1.44435 H -3.80801 2.47143 -1.98623 H -4.18522 4.10528 -1.40645 H -2.56397 3.72587 -2.01928 C -2.42481 4.19773 0.71804 H -1.55462 4.60620 0.19142 H -3.18998 4.98111 0.75869 H -2.12416 3.95306 1.74033 C -4.20715 2.40519 0.76674 H -4.99335 3.16735 0.80898 H -4.62538 1.51966 0.27440 H -3.93285 2.13264 1.78935 C -4.25279 -2.31665 -0.58270 H -4.07344 -1.95045 -1.59754 H -5.06082 -3.05597 -0.61888 H -4.59408 -1.47685 0.03336 C -2.52579 -4.13752 -0.88933 H -3.31300 -4.89885 -0.92746 H -2.32072 -3.79862 -1.90801 H -1.61897 -4.61216 -0.49725 C -3.26592 -3.47513 1.43536 H -3.59799 -2.66645 2.09239 H -4.05480 -4.23510 1.39970 H -2.37700 -3.92720 1.88612 C 2.42096 -4.19943 -0.71324

H	4.80124	4.82847	-2.15238
C	-2.94679	2.92994	-0.00004
C	-3.44340	3.42293	1.21705
C	-3.44290	3.42334	-1.21715
C	-4.43193	4.40534	1.22367
C	-4.43149	4.40570	-1.22380
C	-4.90998	4.88074	-0.00007
H	-3.05253	3.03415	2.15196
H	-3.05163	3.03491	-2.15205
H	-4.82964	4.80031	2.15231
H	-4.82890	4.80092	-2.15247
N	5.92135	5.95667	-0.00008
O	6.32796	6.36628	1.09266
O	6.32854	6.36551	-1.09290
N	-5.95690	5.92121	-0.00002
O	-6.36605	6.32799	1.09281
O	-6.36635	6.32783	-1.09279
N	-5.92137	-5.95672	-0.00009
O	-6.32839	-6.36591	1.09269
O	-6.32791	-6.36616	-1.09294
N	5.95711	-5.92092	0.00008
O	6.36680	-6.32727	1.09292
O	6.36621	-6.32777	-1.09278

TS2[Rh_2(p-NO_2PhCOO)$_4$]			
C	-0.89679	1.83312	-1.85109
O	-0.88273	1.43070	-0.63557
O	-0.05992	1.51321	-2.75264
Rh	1.44975	0.13941	-2.32237
Rh	0.56087	0.06092	-0.03757
C	2.63806	2.09630	-0.49504
O	1.86974	1.63043	0.41916
O	2.69078	1.69503	-1.69753
C	-0.62819	-1.87466	-1.90445
O	-0.68362	-1.48828	-0.68493
O	0.15375	-1.41586	-2.79555
C	2.87495	-1.68822	-0.54673
O	2.06244	-1.33788	0.37585
O	2.88798	-1.25033	-1.74028
N	-0.48529	1.72911	2.32316
N	-0.24583	2.81293	2.33594
C	-0.25438	-0.00862	2.03717
C	-1.63500	-0.45650	1.91318
N	-2.66091	0.31100	2.03691
H	-1.71631	-1.51161	1.62109
C	1.94956	-0.21114	3.21332
C	2.72015	-0.65659	4.28576
C	0.56399	-0.47648	3.17338
H	3.78558	-0.44032	4.31278
C	2.12799	-1.39261	5.32123
C	-0.02507	-1.19891	4.23500
H	2.73472	-1.74768	6.15145
H	-1.09452	-1.39497	4.23474
C	0.75532	-1.66852	5.29128
H	0.29404	-2.23603	6.09587
H	2.40935	0.34388	2.40294
S	-4.17270	-0.39599	1.59420
O	-4.00735	-1.82939	1.28645
O	-4.73839	0.51019	0.58780
C	-5.09356	-0.23931	3.11941
C	-5.27405	-1.36244	3.93018
C	-5.62994	1.00536	3.46881
C	-5.99968	-1.22802	5.11701
C	-6.34809	1.11821	4.65887
C	-6.54523	0.00788	5.50014
H	-4.86839	-2.32502	3.63117
H	-5.49652	1.86504	2.81780
H	-6.14783	-2.10168	5.74855

TS2[Rh_2(tBuCOO)$_4$]			
C	0.67182	-2.65641	-1.09302
O	0.02807	-1.55093	-1.02812
O	1.84278	-2.84681	-0.63685
Rh	2.85438	-1.29935	0.33130
Rh	0.88525	0.09027	-0.07134
C	2.90877	0.16751	-2.21480
O	1.76587	0.65004	-1.88779
O	3.59229	-0.63252	-1.50712
C	0.86583	-1.39858	2.47791
O	0.16954	-0.58132	1.77882
O	1.99571	-1.87048	2.13868
C	3.08592	1.41858	1.38714
O	1.91194	1.62818	0.92359
O	3.73464	0.33038	1.28521
N	-1.24786	0.93679	-2.12339
N	-0.99981	0.74369	-3.18870
C	-0.92841	1.33366	-0.41676
C	-2.03442	0.65551	0.24263
N	-2.97382	0.02259	-0.37230
H	-1.95381	0.67436	1.33740
C	0.26470	3.47925	-0.90463
C	0.32492	4.87154	-0.88652
C	-0.86380	2.80959	-0.38686
H	1.19260	5.38068	-1.29967
C	-0.72080	5.61588	-0.32408
C	-1.92181	3.57117	0.15593
H	-0.66375	6.70209	-0.29995
H	-2.80895	3.07522	0.54210
C	-1.84097	4.96313	0.20492
H	-2.65476	5.53871	0.63969
H	1.08121	2.89805	-1.31958
S	-4.04952	-0.86979	0.63551
O	-3.82182	-0.56079	2.05946
O	-3.98178	-2.25972	0.16872
C	-5.62317	-0.16622	0.14343
C	-6.26331	0.74351	0.98713
C	-6.19514	-0.55420	-1.07369
C	-7.49510	1.27789	0.59653
C	-7.42239	-0.00716	-1.44691
C	-8.09160	0.91470	-0.62100
H	-5.81287	1.01743	1.93726
H	-5.69249	-1.27704	-1.71065
H	-7.99897	1.98316	1.25450

H	-6.76735	2.08388	4.93506
C	-7.35418	0.14196	6.76974
H	-7.12487	1.07636	7.29181
H	-8.42743	0.15081	6.54352
H	-7.16759	-0.68903	7.45568
C	3.91106	-2.71090	-0.17985
C	3.92788	-3.26487	1.10990
C	4.86241	-3.11273	-1.13070
C	4.88849	-4.21431	1.45376
C	5.82991	-4.05984	-0.79940
C	5.82699	-4.59561	0.49121
H	3.18515	-2.94963	1.83550
H	4.83799	-2.67934	-2.12551
H	4.91746	-4.65637	2.44382
H	6.57428	-4.38251	-1.51940
C	3.55889	3.21527	-0.10365
C	4.43515	3.75738	-1.05734
C	3.54929	3.71916	1.20646
C	5.29857	4.79474	-0.70953
C	4.40688	4.75655	1.56818
C	5.27011	5.27782	0.60123
H	4.43416	3.36119	-2.06777
H	2.86754	3.29818	1.93783
H	5.98270	5.22617	-1.43237
H	4.41313	5.16024	2.57493
C	-2.00419	2.76681	-2.23536
C	-1.88616	3.54202	-3.40019
C	-3.15822	2.85262	-1.44079
C	-2.90546	4.41943	-3.76403
C	-4.19106	3.71627	-1.80368
C	-4.04363	4.49287	-2.95560
H	-0.99439	3.45499	-4.01318
H	-3.26087	2.22782	-0.55938
H	-2.83066	5.03478	-4.65407
H	-5.09742	3.78637	-1.21216
C	-1.56839	-2.96847	-2.31478
C	-2.64814	-3.32255	-1.49067
C	-1.36539	-3.63004	-3.53706
C	-3.52134	-4.33705	-1.88208
C	-2.22482	-4.65250	-3.93303
C	-3.29135	-4.99057	-3.09503
H	-2.82235	-2.79657	-0.55769
H	-0.53275	-3.33973	-4.16996
H	-4.36769	-4.61682	-1.26416
H	-2.08120	-5.18036	-4.86960
N	-4.20575	-6.07097	-3.50801
O	-3.99310	-6.62664	-4.59219
O	-5.13523	-6.36554	-2.74788
N	-5.12685	5.41832	-3.33503
O	-6.11943	5.48081	-2.60040
O	-4.98405	6.08516	-4.36670
N	6.18146	6.37488	0.97776
O	6.93589	6.82365	0.10790
O	6.14105	6.78495	2.14341
N	6.84843	-5.59680	0.85032
O	6.83129	-6.05391	1.99921
O	7.66721	-5.92425	-0.01573

H	-7.87019	-0.30548	-2.39319
C	-9.43480	1.47497	-1.03020
H	-9.70890	2.34477	-0.42666
H	-9.43662	1.77517	-2.08324
H	-10.22280	0.72222	-0.90603
C	3.45964	0.56630	-3.59682
C	-0.05746	-3.84891	-1.73669
C	0.26869	-1.83227	3.82889
C	3.74918	2.59366	2.13166
C	3.19949	2.06440	-3.85627
H	3.58434	2.33978	-4.84476
H	2.13185	2.29687	-3.82759
H	3.70707	2.69082	-3.11358
C	4.96837	0.27128	-3.68194
H	5.17989	-0.78830	-3.51850
H	5.34048	0.55005	-4.67454
H	5.52998	0.84227	-2.93521
C	2.70071	-0.28468	-4.64498
H	3.06066	-0.03843	-5.65051
H	2.86645	-1.35495	-4.48024
H	1.62415	-0.09152	-4.60997
C	-0.88159	-3.37287	-2.95010
H	-1.40757	-4.22630	-3.39312
H	-1.62329	-2.62570	-2.65833
H	-0.23824	-2.93688	-3.72333
C	-1.00751	-4.42599	-0.65710
H	-1.53475	-5.29677	-1.06421
H	-0.44676	-4.75584	0.22473
H	-1.75495	-3.69118	-0.34434
C	0.95382	-4.92478	-2.17390
H	1.65637	-4.53565	-2.91883
H	1.53702	-5.29596	-1.32744
H	0.41726	-5.76934	-2.62145
C	1.24493	-2.75327	4.58187
H	2.19742	-2.25348	4.78300
H	0.80185	-3.04667	5.54064
H	1.46032	-3.66162	4.01188
C	-0.01316	-0.56555	4.66838
H	-0.71423	0.10012	4.15815
H	-0.44929	-0.85261	5.63196
H	0.90842	-0.00700	4.86992
C	-1.05682	-2.57999	3.55422
H	-0.88989	-3.46822	2.93416
H	-1.49051	-2.91338	4.50428
H	-1.78628	-1.94052	3.05150
C	3.82627	3.80100	1.17036
H	2.83095	4.10025	0.83201
H	4.28888	4.65239	1.68293
H	4.43685	3.56910	0.28972
C	2.86208	2.95290	3.34599
H	2.78494	2.11118	4.04375
H	3.30186	3.79808	3.88801
H	1.85276	3.23024	3.03002
C	5.16168	2.21232	2.60781
H	5.81107	1.94822	1.76785
H	5.61108	3.06158	3.13569
H	5.13838	1.35767	3.29002