Supporting Information

The Chiral Crown Conformation of Rh_2(*S*-PTTL)$_4$: Enantioselective Cyclopropanation with α-Alkyl-α-diazoesters

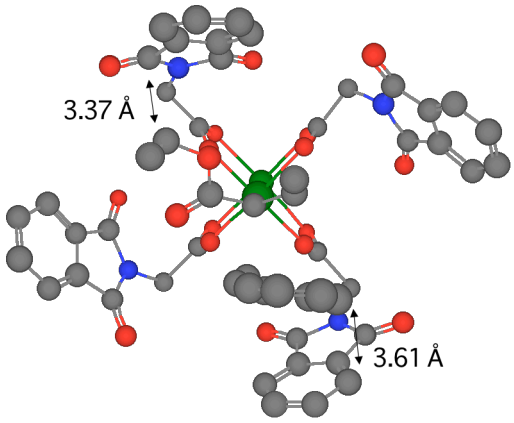
Andrew DeAngelis, Olga Dmitrenko, Glenn P. A. Yap, and Joseph M. Fox*

Brown Laboratories, Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716

Computational Details

Optimizations of large systems were performed using the Amsterdam Density Functional (ADF) program package [1] using the OLYP functional and a TZP (small frozen core) basis set. For small model system optimizations and single-point energy calculations, we applied the B3LYP method with a LANL2DZ basis set and effective core potential on Rh atoms and a 6-31G(d) on the other atoms (Gaussian 03 program [2]). It was previously demonstrated by Davies and Singleton groups [3] for similar Rh-catalyzed cyclopropanation, that this method provides adequate accuracy and geometries. Unfortunately for large transition structures studied in this work, B3LYP Gaussian 03 calculations require too much cpu-time. Thus, we report B3LYP/gen(LANL2DZ, 6-31G(d)) [g03] energy single point calculations using OLYP/TZP(Small)[ADF] optimized geometries.

In preliminary calculations using the OLYP functional and the DZ (large frozen core) basis set, we found a transition state **TS-3** in addition to **TS-1** and **TS-2** (the latter two transition states are described in the main body of the paper). **TS-3** is analogous to **TS-1**, except that the alkene approached the carbenoid from the *Re*-face. We observed close contacts in **TS-3** (3.37 Å from the ethyl ester to a phthalimido group; 3.61 Å from the styrene to a phthalimido group). **TS-3**, shown below, is higher in energy than **TS-1** by 2.96 kcal/mol, and was not considered in higher level calculations.



TS-3

Conformational searching was performed with a 1000 step Monte Carlo multiple minimum search on Rh_2(*S*-PTTL)$_4$. The method was PRCG with 500 maximum iterations, with a convergence threshold of 0.050 kJ/mol. The force field was MMFFS with constant dielectric constant (1.0). For the search, the tetracarboxylate core was frozen. The miminum conformation from the search was the chiral crown

conformation. Within 3 kcal/mol of this conformation were two additional conformations. These three lowest energy conformers were subjected to calculations using the OLYP functional and the TZP (small frozen core) basis set.

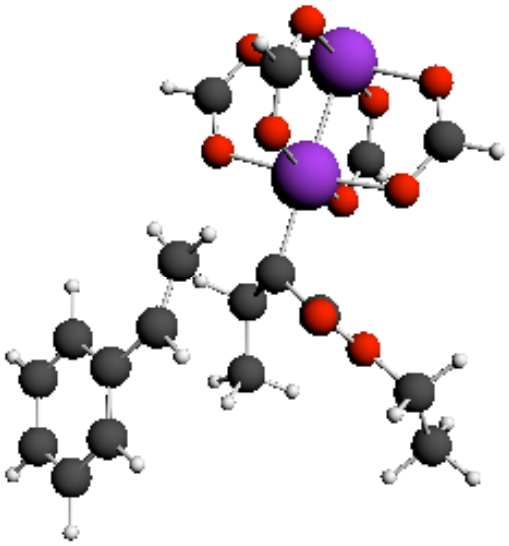
References

[1] ADF2008.01, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com

[2] *Gaussian 03*, revision D.01; M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

[3] Daniel T. Nowlan III, Timothy M. Gregg, Huw M. L. Davies, and Daniel A. Singleton. J. Am. Chem. Soc., 2003, 125 (51), pp 15902–15911

TS-1s (small model):



TS1 OLYP/TZP(Small) Energy: -11.29353 Hartree

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Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

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C	-2.12912	1.31142	7.20977
C	-2.47536	2.04983	6.07316
C	-1.52382	2.32935	5.09828
C	0.81529	1.99889	4.19491
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H	-0.53017	0.31589	8.26713
H	-2.88311	1.07357	7.95726
H	-3.49727	2.40086	5.94563
H	-1.81303	2.90663	4.22412
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C	1.6733	-0.29067	2.09782
O	2.72385	0.25497	2.38646
O	1.51951	-1.63766	1.9835
C	2.68357	-2.47179	2.23696
C	-0.93903	-0.10761	2.2676
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H	1.66772	-3.74551	3.66979
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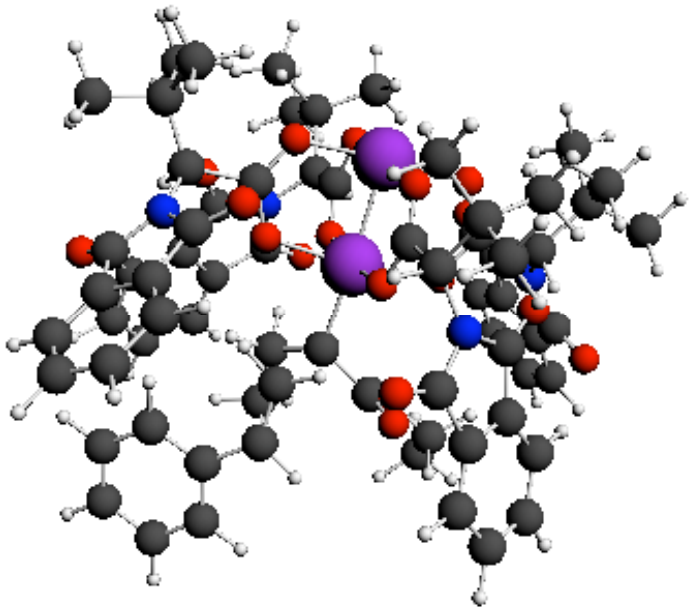

TS-1

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Coordinates in Geometry Cycle 5

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5.C	-2.582693	1.831298	6.001772	
6.C	-1.614182	2.190141	5.070406	
7.C	0.757627	1.994283	4.221070	
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17.O	1.618632	-1.591396	1.994089	
18.C	2.806424	-2.361173	2.322556	

19.C	-0.882082	-0.141864	2.284308
20.C	-0.895252	-1.107952	3.478785
21.C	2.358938	-3.731567	2.793101
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31.C	-1.884422	7.027857	4.821034
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165.H	5.477579	3.749614	4.158979
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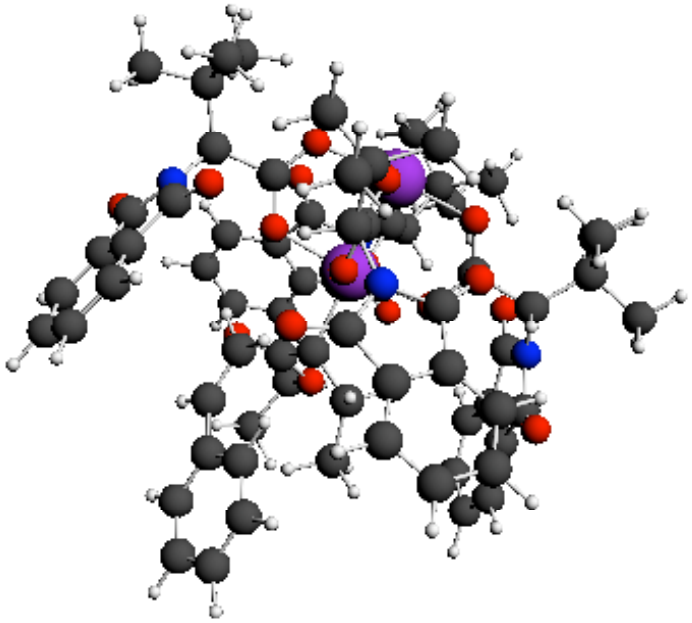

TS-2

E(B3LYP/gen(Lanl2dz,6-31G(d))) = **-4504.3090686 a.u.**
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Coordinates in Geometry Cycle 6

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29.N	3.022054	-3.336829	-1.063617
30.O	1.200965	-4.094218	-2.333792
31.O	4.480924	-3.047065	0.743305
32.C	1.861876	-4.111175	-1.313587
33.C	1.620793	-4.918035	-0.089801
34.C	0.559509	-5.759777	0.213742
35.C	0.546964	-6.329482	1.490988
36.C	1.570287	-6.067700	2.411509
37.C	2.631326	-5.212105	2.089591
38.C	2.630877	-4.633484	0.825738
39.C	3.522669	-3.597656	0.226513
40.N	3.398395	2.987228	0.537956
41.O	4.363085	1.312453	-0.791103
42.O	2.788858	4.199391	2.448337
43.C	4.278812	1.915163	0.260679
44.C	5.062267	1.688490	1.506640
45.C	6.073808	0.773589	1.766296
46.C	6.666888	0.817636	3.033190
47.C	6.249157	1.746721	3.995462
48.C	5.208012	2.645618	3.729306
49.C	4.622517	2.593966	2.469731
50.C	3.501872	3.385088	1.883701
51.N	-3.366456	3.544044	-0.313328
52.O	-1.238081	4.512072	-0.123711
53.O	-5.461519	2.681180	0.287505
54.C	-2.303654	4.178639	0.360738
55.C	-2.729624	4.318277	1.779174
56.C	-2.018067	4.797665	2.870814
57.C	-2.623597	4.696279	4.127271
58.C	-3.901885	4.140300	4.266662
59.C	-4.612146	3.663583	3.158032
60.C	-3.996841	3.758818	1.916186
61.C	-4.425065	3.250133	0.580552
62.O	-1.351767	-1.579684	-1.572703
63.O	-0.880973	-0.893363	-3.686912
64.O	1.488262	-1.161079	-0.824945
65.O	1.917744	-0.554822	-2.967907
66.O	1.005612	1.620670	-0.059811
67.O	1.380588	2.265164	-2.201554
68.O	-1.890633	1.328921	-0.734668
69.O	-1.454643	1.949569	-2.872132
70.C	-1.379911	-1.692720	-2.843677
71.C	-2.043891	-3.015361	-3.369663
72.C	-1.994108	-3.348567	-4.910935
73.C	-2.563329	-4.774906	-5.121376
74.C	-2.796551	-2.366150	-5.788715

75.C	-0.522315	-3.389824	-5.394176
76.C	2.154268	-1.204667	-1.911925
77.C	3.410892	-2.131883	-1.828613
78.C	4.289907	-2.382774	-3.120314
79.C	3.513020	-2.941232	-4.328387
80.C	5.411772	-3.376738	-2.744453
81.C	4.961456	-1.051520	-3.521573
82.C	1.530408	2.366042	-0.954189
83.C	2.386571	3.537132	-0.385556
84.C	2.936339	4.627379	-1.400810
85.C	1.736017	5.301209	-2.093540
86.C	3.670458	5.717575	-0.590263
87.C	3.900156	4.065571	-2.464368
88.C	-2.097548	2.019162	-1.786681
89.C	-3.321886	2.989370	-1.680024
90.C	-3.558449	4.029385	-2.843259
91.C	-3.864964	3.247813	-4.143543
92.C	-4.817242	4.859556	-2.504649
93.C	-2.365476	4.995362	-3.079778
94.C	-3.805546	-3.512158	2.842324
95.H	4.224076	-3.197088	-5.124522
96.H	2.951468	-3.842716	-4.077653
97.H	2.811190	-2.206931	-4.729662
98.H	6.004593	-3.020898	-1.895331
99.H	6.089627	-3.494808	-3.597562
100.H	5.021073	-4.367640	-2.495363
101.H	5.610751	-1.221693	-4.389029
102.H	4.231198	-0.287579	-3.793687
103.H	5.584881	-0.650321	-2.715119
104.H	4.070480	-1.601868	-1.132126
105.H	-0.238620	-5.936878	-0.501616
106.H	-0.280337	-6.974799	1.781296
107.H	1.526305	-6.519743	3.398913
108.H	3.413964	-4.984378	2.808955
109.H	-1.984720	-5.528041	-4.576643
110.H	-2.518205	-5.023725	-6.187130
111.H	-3.609298	-4.861913	-4.813186
112.H	-0.048051	-2.409458	-5.359377
113.H	-0.503880	-3.741793	-6.431526
114.H	0.076776	-4.082727	-4.797996
115.H	-2.500546	-1.329640	-5.616556
116.H	-3.873769	-2.447381	-5.611735
117.H	-2.620568	-2.602964	-6.844742
118.H	-1.463448	-3.798651	-2.871358
119.H	-5.802328	-5.794418	-0.554888
120.H	-7.984523	-4.773973	0.134100
121.H	-8.531733	-2.447297	-0.476331
122.H	-6.928617	-1.074832	-1.831297
123.H	-2.991185	2.714509	-4.518642
124.H	-4.190546	3.955983	-4.914375
125.H	-4.672605	2.520003	-4.000082
126.H	-4.698891	5.428838	-1.577912
127.H	-5.709279	4.231776	-2.407609
128.H	-4.999384	5.581167	-3.309247
129.H	-1.414949	4.571504	-2.758605
130.H	-2.503277	5.942385	-2.544262

131.H	-2.278091	5.231285	-4.148049
132.H	-4.187761	2.315803	-1.698215
133.H	-5.594615	3.211721	3.263039
134.H	-4.338766	4.059238	5.259872
135.H	-2.084983	5.028225	5.011627
136.H	-1.013068	5.196021	2.751425
137.H	-2.076558	0.268524	6.162530
138.H	-0.684646	0.063629	8.196087
139.H	1.733257	0.656621	8.115765
140.H	2.709887	1.565757	6.013388
141.H	1.323750	1.814421	4.001354
142.H	-0.005230	1.713843	2.164774
143.H	-1.765627	1.420787	1.707528
144.H	-2.336466	0.667364	3.880957
145.H	1.331467	-2.097755	3.853838
146.H	0.021032	-3.037134	3.118480
147.H	-0.340557	-1.560786	4.015929
148.H	1.058812	-1.848893	1.295910
149.H	1.276974	-0.408146	2.193333
150.H	2.100363	6.112071	-2.735872
151.H	1.177933	4.607149	-2.721503
152.H	1.041864	5.740267	-1.369855
153.H	3.034432	6.145578	0.191306
154.H	3.958984	6.532331	-1.264700
155.H	4.586295	5.344956	-0.121800
156.H	4.825350	3.686102	-2.022368
157.H	3.444489	3.260767	-3.042901
158.H	4.173710	4.870869	-3.158369
159.H	1.698555	4.069823	0.278736
160.H	4.873551	3.365188	4.472466
161.H	6.741580	1.765721	4.964608
162.H	7.466613	0.121085	3.274947
163.H	6.383380	0.053011	1.014551
164.H	-3.021656	-4.215575	0.946902
165.H	-3.932391	-2.683621	0.852367
166.H	-3.118621	-4.094963	3.464327
167.H	-4.741921	-4.075618	2.746814
168.H	-4.031209	-2.568372	3.345425

<Feb25-2009> <05:21:56> >>>> CORORT

Table Energies (a.u.) of the reactants and transition states. Relative energies ($E_{rel.}$, kcal/mol) are with respect to isolated reactants and styrene.

	OLYP/TZP(Small), E (a.u)	single-point energy refinment: B3LYP/gen (lanl2dz, 6-31G*) //OLYP/TZP(Small), E(a.u)	E_{rel} (kcal/mol)
Styrene	-3.56107742	-309.6480403	
R-1 (Rh-reactant)	-34.1685580	-4194.678305	
TS-1	-37.6863646	-4504.309478	10.6
TS-2	-37.6885425	-4504.309069	10.8
R-1s (Rh-reactant)	-7.75820338	-1360.868602	
TS-1s	-11.2934487	-1670.506744	6.2

Reactants:

Styrene

<Feb12-2009> <13:27:10> Geometry Converged
Coordinates in Geometry Cycle 7

Atom	X	Y	Z (Angstrom)
1.C	-0.160479	2.103625	5.306685
2.C	0.159444	1.402785	6.482746
3.C	-0.788745	1.190719	7.482576
4.C	-2.084928	1.684357	7.333921
5.C	-2.417816	2.396849	6.173436
6.C	-1.470413	2.602996	5.176108
7.C	0.882295	2.282569	4.275970
8.C	0.749683	2.748044	3.033748
9.H	1.168197	1.012395	6.610893
10.H	-0.514444	0.639246	8.380129
11.H	-2.828420	1.525096	8.110303
12.H	-3.422256	2.796809	6.054876
13.H	-1.751590	3.172763	4.293955
14.H	1.614005	2.821723	2.374436
15.H	-0.203837	3.064043	2.611677
16.H	1.880371	1.971388	4.595320

<Feb12-2009> <13:30:51> Bond Energy LDA -3.65721205 a.u.
<Feb12-2009> <13:30:51> Bond Energy LDA -99.51780328 eV
<Feb12-2009> <13:30:51> + GGA-X -3.22011320 a.u.
<Feb12-2009> <13:30:51> + GGA-X -87.62373850 eV
<Feb12-2009> <13:30:51> + GGA-XC -3.56107742 a.u.
<Feb12-2009> <13:30:51> + GGA-XC -96.90184698 eV
<Feb12-2009> <13:30:51> NORMAL TERMINATION
<Feb12-2009> <13:30:51> END

R-1s

<Feb25-2009> <17:00:31> Geometry Converged
Coordinates in Geometry Cycle 16

Atom	X	Y	Z (Angstrom)
1.C	0.334036	0.149391	1.534928
2.C	1.578602	-0.477122	2.034846
3.O	2.360941	0.222559	2.659242
4.O	1.700460	-1.783467	1.757540
5.C	2.894442	-2.489765	2.221913
6.C	-0.859067	0.135472	2.424362
7.C	-0.834226	-0.684136	3.720737
8.C	2.479963	-3.863618	2.711183
9.Rh	0.275961	0.975581	-0.275830
10.Rh	0.103504	1.861275	-2.590801
11.O	-1.395615	2.160612	0.193522
12.O	-1.559481	2.967476	-1.944756
13.O	-1.008981	-0.560256	-0.932574
14.O	-1.127681	0.243913	-3.071511
15.O	1.946478	-0.111812	-0.941231
16.O	1.794521	0.728027	-3.068771
17.O	1.532561	2.602936	0.116989
18.O	1.353490	3.428695	-2.011441

19.C	-1.905115	2.867017	-0.737421
20.C	-1.395630	-0.567027	-2.145036
21.C	2.310169	0.031573	-2.152164
22.C	1.771596	3.428570	-0.821054
23.H	-1.801825	-0.600132	4.228230
24.H	-0.062984	-0.327806	4.411376
25.H	-0.653825	-1.745080	3.520611
26.H	-1.107308	1.189637	2.632981
27.H	-1.697746	-0.180609	1.782570
28.H	3.565462	-2.554643	1.358656
29.H	3.381236	-1.901635	3.002342
30.H	1.876602	-3.798364	3.622607
31.H	3.375154	-4.454263	2.936862
32.H	1.903185	-4.397869	1.949339
33.H	2.442355	4.258825	-0.539116
34.H	-2.774371	3.472796	-0.425211
35.H	-2.059158	-1.409815	-2.406355
36.H	3.210623	-0.544718	-2.429411

<Feb25-2009> <17:00:32> >>>> CORORT

<Feb25-2009> <17:08:22> Bond Energy LDA -8.13678946 a.u.
<Feb25-2009> <17:08:22> Bond Energy LDA -221.41330689 eV
<Feb25-2009> <17:08:22> + GGA-X -6.95024038 a.u.
<Feb25-2009> <17:08:22> + GGA-X -189.12566351 eV
<Feb25-2009> <17:08:22> + GGA-XC -7.75820338 a.u.
<Feb25-2009> <17:08:22> + GGA-XC -211.11145551 eV
<Feb25-2009> <17:08:22> NORMAL TERMINATION
<Feb25-2009> <17:08:24> END

R-1

<Feb19-2009> <17:00:28> Geometry Converged
Coordinates in Geometry Cycle 22

Atom	X	Y	Z (Angstrom)
1.C	0.377438	0.246927	1.521199
2.C	1.612980	-0.309415	2.110985
3.O	2.283040	0.454878	2.787544
4.O	1.851961	-1.605196	1.880869
5.C	3.013792	-2.222991	2.521267
6.C	-0.829880	0.269309	2.391039
7.C	-0.818958	-0.472165	3.732902
8.C	2.616314	-3.612102	2.981389
9.Rh	0.293681	0.986156	-0.323207
10.Rh	0.047164	1.774172	-2.644534
11.N	-2.515596	4.791600	0.903205
12.O	-0.614480	5.868588	0.051174
13.O	-4.088313	3.994604	2.443618
14.C	-1.407295	5.668319	0.949868
15.C	-1.420108	6.277682	2.310062
16.C	-0.583068	7.235359	2.865374
17.C	-0.854748	7.644676	4.175565
18.C	-1.924621	7.098306	4.896320
19.C	-2.751168	6.119725	4.331965
20.C	-2.476161	5.725575	3.029013
21.C	-3.159615	4.730716	2.156222
22.N	-3.513933	-1.747767	-0.850395
23.O	-4.381889	0.418735	-0.645342

24.O	-2.854802	-3.920841	-0.274753
25.C	-4.186396	-0.693580	-0.196447
26.C	-4.575528	-1.207541	1.146153
27.C	-5.213782	-0.559866	2.195559
28.C	-5.394350	-1.283238	3.379536
29.C	-4.947856	-2.606015	3.493390
30.C	-4.301835	-3.246056	2.429473
31.C	-4.123683	-2.518652	1.259814
32.C	-3.419501	-2.876457	-0.004915
33.N	3.064626	-2.564104	-2.214491
34.O	0.889944	-3.018375	-2.968590
35.O	5.048181	-2.760660	-0.981806
36.C	1.897042	-3.343649	-2.371314
37.C	2.156022	-4.628952	-1.663234
38.C	1.347248	-5.747758	-1.522787
39.C	1.873021	-6.834776	-0.815995
40.C	3.164019	-6.788661	-0.274168
41.C	3.962279	-5.646674	-0.405340
42.C	3.428260	-4.572285	-1.104190
43.C	3.996992	-3.224853	-1.389124
44.N	4.157706	3.638449	0.187962
45.O	4.813058	1.746017	-1.026166
46.O	3.857342	5.114351	1.978268
47.C	4.813165	2.403877	-0.003725
48.C	5.482501	2.077404	1.284777
49.C	6.222335	0.959164	1.643142
50.C	6.686905	0.894038	2.961065
51.C	6.412895	1.919419	3.875133
52.C	5.663805	3.040867	3.501349
53.C	5.204751	3.094196	2.192317
54.C	4.336548	4.096353	1.512684
55.O	-1.216727	2.382270	0.180249
56.O	-1.429753	3.097578	-1.958836
57.O	-1.179757	-0.423887	-0.778832
58.O	-1.434060	0.289251	-2.913530
59.O	1.788491	-0.321478	-1.079130
60.O	1.528765	0.423813	-3.205228
61.O	1.760200	2.461191	-0.082054
62.O	1.564774	3.171827	-2.225082
63.C	-1.745372	3.095477	-0.738369
64.C	-2.945098	3.965897	-0.242596
65.C	-3.840175	4.723348	-1.303818
66.C	-5.004571	5.409050	-0.551215
67.C	-3.092661	5.792198	-2.125584
68.C	-4.468606	3.682934	-2.259948
69.C	-1.710409	-0.459932	-1.937860
70.C	-2.725586	-1.636664	-2.098263
71.C	-3.530743	-1.779806	-3.442981
72.C	-4.382329	-0.548902	-3.811815
73.C	-4.457914	-3.009717	-3.321333
74.C	-2.521639	-2.071059	-4.579452
75.C	2.076537	-0.290593	-2.320291
76.C	3.287437	-1.193105	-2.718664
77.C	3.842379	-1.110584	-4.198169
78.C	4.420767	0.306381	-4.421657
79.C	5.017445	-2.106381	-4.337740

80.C	2.805619	-1.424992	-5.295302
81.C	2.083341	3.194513	-1.073059
82.C	3.176461	4.256858	-0.724984
83.C	3.778861	5.150748	-1.876994
84.C	2.652770	6.054178	-2.433481
85.C	4.852637	6.078748	-1.263703
86.C	4.421702	4.354941	-3.029942
87.H	-1.792299	-0.358463	4.220913
88.H	-0.054396	-0.075896	4.407524
89.H	-0.638997	-1.543150	3.596742
90.H	-1.092777	1.330762	2.530896
91.H	-1.651463	-0.093417	1.756693
92.H	3.803879	-2.257332	1.765642
93.H	3.345892	-1.590419	3.346220
94.H	1.872242	-3.568506	3.783288
95.H	3.500549	-4.135463	3.363831
96.H	2.204800	-4.199464	2.155889
97.H	4.961658	-5.598170	0.019390
98.H	3.547536	-7.654310	0.261148
99.H	1.270999	-7.731062	-0.685298
100.H	0.345449	-5.769126	-1.943761
101.H	4.095473	-0.821649	-2.080598
102.H	5.786371	-1.945966	-3.576394
103.H	5.487192	-1.968779	-5.317819
104.H	4.689113	-3.148972	-4.280354
105.H	3.317097	-1.484857	-6.264082
106.H	2.302139	-2.380346	-5.128930
107.H	2.039677	-0.651000	-5.367613
108.H	4.853778	0.364161	-5.427002
109.H	3.659908	1.082763	-4.340806
110.H	5.216013	0.534864	-3.703997
111.H	-1.868984	-1.220850	-4.780463
112.H	-3.070928	-2.302016	-5.499197
113.H	-1.887954	-2.933990	-4.345600
114.H	-3.898783	-3.920222	-3.082647
115.H	-4.970206	-3.172146	-4.275792
116.H	-5.227830	-2.873435	-2.555953
117.H	-3.773519	0.351076	-3.916931
118.H	-5.157726	-0.347949	-3.068319
119.H	-4.880936	-0.732826	-4.771418
120.H	-2.078815	-2.520743	-2.051647
121.H	-3.937766	-4.266391	2.515420
122.H	-5.097007	-3.138527	4.430198
123.H	-5.880767	-0.809661	4.229262
124.H	-5.538403	0.473641	2.101333
125.H	-3.722506	3.181181	-2.876698
126.H	-5.169394	4.193428	-2.930503
127.H	-5.029561	2.917360	-1.714730
128.H	-2.697278	6.594037	-1.496735
129.H	-3.792752	6.247935	-2.836788
130.H	-2.262805	5.366910	-2.692484
131.H	-5.581397	4.697487	0.048325
132.H	-5.687691	5.860368	-1.279279
133.H	-4.661450	6.211650	0.108681
134.H	-3.605899	3.226641	0.222093
135.H	-3.579647	5.685277	4.885082

136.H	-2.112689	7.440347	5.911646
137.H	-0.224524	8.397243	4.643997
138.H	0.249617	7.644689	2.299743
139.H	5.253957	3.736434	-2.685286
140.H	3.700682	3.705413	-3.529032
141.H	4.814458	5.057567	-3.775426
142.H	3.080084	6.763821	-3.151328
143.H	1.877774	5.482973	-2.945457
144.H	2.173333	6.637013	-1.638116
145.H	5.714054	5.521721	-0.883298
146.H	4.452362	6.686543	-0.446275
147.H	5.221039	6.760953	-2.037924
148.H	2.639943	4.953333	-0.068608
149.H	5.433064	3.833141	4.208351
150.H	6.781078	1.835254	4.895369
151.H	7.263915	0.030732	3.285864
152.H	6.413094	0.162562	0.927736

<Feb19-2009> <17:00:32> >>>> CORORT
<Feb19-2009> <19:50:59> Bond Energy LDA -35.54579684 a.u.
<Feb19-2009> <19:50:59> Bond Energy LDA -967.25034603 eV
<Feb19-2009> <19:50:59> + GGA-X -30.62944806 a.u.
<Feb19-2009> <19:50:59> + GGA-X -833.46968894 eV
<Feb19-2009> <19:50:59> + GGA-XC -34.16855803 a.u.
<Feb19-2009> <19:50:59> + GGA-XC -929.77377124 eV
<Feb19-2009> <19:50:59> NORMAL TERMINATION
<Feb19-2009> <19:51:05> END

PRELIMINARY OLYP/DZ(Large) optimizations of TS-1, TS-2 and TS-3

TS-1 Bond Energy LDA + GGA-XC -35.86168368 a.u.

Atom	X	Y	Z (Angstrom)
1.C	-0.251554	1.802520	5.232741
2.C	0.072915	1.018336	6.368893
3.C	-0.925232	0.536438	7.215647
4.C	-2.267995	0.866760	6.978286
5.C	-2.591022	1.741624	5.931227
6.C	-1.596079	2.212231	5.072250
7.C	0.788811	2.054921	4.242805
8.C	0.627102	2.416658	2.919077
9.H	1.110859	0.752523	6.553520
10.H	-0.663297	-0.111492	8.048483
11.H	-3.051287	0.455777	7.610757
12.H	-3.621419	2.050652	5.776891
13.H	-1.856599	2.914563	4.293013
14.C	0.435307	0.465400	1.813395
15.C	1.730241	-0.181260	2.193551
16.O	2.800945	0.378326	2.497970
17.O	1.583986	-1.570416	2.102878
18.C	2.820098	-2.404231	2.296436
19.C	-0.880975	-0.077716	2.295409
20.C	-0.927182	-1.080584	3.467344
21.C	2.353918	-3.773604	2.764234
22.Rh	0.332904	1.103877	-0.209688
23.Rh	0.060800	1.792608	-2.661778
24.N	-2.679150	4.718218	0.846397
25.O	-0.655799	5.595172	-0.049767

26.O	-4.324903	4.042524	2.421999
27.C	-1.483373	5.491378	0.872355
28.C	-1.439210	6.111316	2.222862
29.C	-0.492823	6.965329	2.769958
30.C	-0.716066	7.423544	4.080696
31.C	-1.855105	7.028317	4.798417
32.C	-2.797843	6.146929	4.237109
33.C	-2.563121	5.694459	2.945400
34.C	-3.334706	4.736864	2.101527
35.N	-3.393877	-1.771509	-0.816356
36.O	-4.108957	0.490062	-0.657791
37.O	-2.861966	-4.011417	-0.238622
38.C	-3.990243	-0.652283	-0.180801
39.C	-4.388273	-1.121865	1.171777
40.C	-4.966653	-0.409976	2.212836
41.C	-5.183432	-1.096061	3.420427
42.C	-4.829393	-2.447000	3.555967
43.C	-4.240827	-3.154944	2.491827
44.C	-4.025547	-2.466311	1.305483
45.C	-3.367029	-2.903501	0.038708
46.N	3.123929	-2.462095	-2.144677
47.O	0.862975	-2.730341	-2.843020
48.O	5.161765	-2.798444	-0.970966
49.C	1.890364	-3.154671	-2.286690
50.C	2.093852	-4.472328	-1.625267
51.C	1.222115	-5.545823	-1.512650
52.C	1.693425	-6.695088	-0.853589
53.C	2.994467	-6.743268	-0.329551
54.C	3.863075	-5.641654	-0.440329
55.C	3.386908	-4.512671	-1.093880
56.C	4.046437	-3.201978	-1.364012
57.N	4.151726	3.678112	0.151645
58.O	4.541982	1.702238	-1.107678
59.O	4.009320	5.195120	1.970950
60.C	4.652322	2.361185	-0.060872
61.C	5.292982	1.961875	1.217507
62.C	5.878214	0.754196	1.567785
63.C	6.348626	0.622865	2.884750
64.C	6.231539	1.678205	3.801679
65.C	5.627961	2.894846	3.434778
66.C	5.158387	3.010258	2.133171
67.C	4.399486	4.113876	1.479356
68.O	-1.293527	2.401770	0.222788
69.O	-1.550379	3.041904	-1.992549
70.O	-1.060999	-0.466911	-0.727739
71.O	-1.332826	0.203623	-2.926801
72.O	1.918332	-0.184813	-0.972860
73.O	1.676156	0.534535	-3.168437
74.O	1.710942	2.671317	0.004020
75.O	1.523753	3.307066	-2.213415
76.C	-1.880978	3.055895	-0.751588
77.C	-3.117386	3.852222	-0.272632
78.C	-3.987115	4.593744	-1.344146
79.C	-5.135970	5.305808	-0.584375
80.C	-3.191923	5.631713	-2.175644
81.C	-4.613729	3.537548	-2.286725

82.C	-1.597483	-0.550879	-1.915119
83.C	-2.616122	-1.713907	-2.072541
84.C	-3.475224	-1.769316	-3.384649
85.C	-4.249088	-0.449062	-3.679261
86.C	-4.485572	-2.935040	-3.236052
87.C	-2.523918	-2.105664	-4.563129
88.C	2.227006	-0.177923	-2.240800
89.C	3.415877	-1.092941	-2.629561
90.C	3.911688	-1.055863	-4.121726
91.C	4.427268	0.369956	-4.441325
92.C	5.120830	-2.022253	-4.228377
93.C	2.818519	-1.471424	-5.156647
94.C	2.057676	3.372828	-1.045743
95.C	3.197259	4.377280	-0.738017
96.C	3.836589	5.140658	-1.944999
97.C	2.746209	6.045460	-2.575260
98.C	4.965500	6.039474	-1.385841
99.C	4.418244	4.197473	-3.018632
100.H	1.512927	2.696842	2.361127
101.H	-0.319344	2.770740	2.530494
102.H	1.805896	1.860055	4.580307
103.H	-1.935986	-1.080433	3.892688
104.H	-0.219932	-0.825551	4.258853
105.H	-0.691932	-2.084528	3.105219
106.H	-1.547547	0.772185	2.484084
107.H	-1.319803	-0.559289	1.407865
108.H	3.315905	-2.444174	1.328360
109.H	3.457772	-1.898417	3.025211
110.H	1.827913	-3.694396	3.722158
111.H	3.225246	-4.428513	2.893063
112.H	1.686667	-4.223987	2.022766
113.H	4.872666	-5.669382	-0.040921
114.H	3.336105	-7.647460	0.166631
115.H	1.041321	-7.558357	-0.753425
116.H	0.215692	-5.490709	-1.916494
117.H	4.240197	-0.745052	-1.999089
118.H	5.917636	-1.744709	-3.527690
119.H	5.526237	-1.969342	-5.246927
120.H	4.826775	-3.060458	-4.034358
121.H	3.190307	-2.280767	-5.798936
122.H	1.896317	-1.807963	-4.684160
123.H	2.558153	-0.622053	-5.797983
124.H	4.875147	0.363721	-5.443803
125.H	3.610943	1.092563	-4.428149
126.H	5.189976	0.691522	-3.723877
127.H	-1.796922	-1.306203	-4.723921
128.H	-3.121763	-2.231409	-5.475141
129.H	-1.979751	-3.041223	-4.380514
130.H	-3.976680	-3.891740	-3.065252
131.H	-5.072150	-3.015681	-4.160524
132.H	-5.178525	-2.754398	-2.405909
133.H	-3.866333	0.389664	-3.104217
134.H	-5.315459	-0.559970	-3.446974
135.H	-4.158064	-0.191613	-4.741781
136.H	-1.999408	-2.620937	-2.049170
137.H	-3.950129	-4.196551	2.591406

138.H	-5.002616	-2.951030	4.502608
139.H	-5.622931	-0.569150	4.262353
140.H	-5.218883	0.640429	2.096556
141.H	-3.841628	2.977774	-2.816742
142.H	-5.239718	4.052038	-3.027423
143.H	-5.240875	2.829136	-1.734333
144.H	-2.425661	6.136859	-1.583760
145.H	-3.884236	6.392344	-2.561076
146.H	-2.692844	5.150657	-3.021916
147.H	-5.678766	4.608553	0.065033
148.H	-5.845918	5.715094	-1.313832
149.H	-4.758245	6.134323	0.026818
150.H	-3.755344	3.094938	0.196199
151.H	-3.678840	5.831974	4.788287
152.H	-2.007253	7.403400	5.806527
153.H	0.005812	8.090541	4.543561
154.H	0.388255	7.254633	2.204687
155.H	5.283674	3.646784	-2.639915
156.H	3.671487	3.479138	-3.356922
157.H	4.741317	4.795464	-3.881593
158.H	3.211768	6.697460	-3.325280
159.H	1.970228	5.448872	-3.060399
160.H	2.270479	6.682479	-1.817583
161.H	5.716190	5.445197	-0.852504
162.H	4.569129	6.798743	-0.700393
163.H	5.463355	6.549854	-2.220149
164.H	2.735657	5.131939	-0.087849
165.H	5.519957	3.713489	4.140385
166.H	6.603878	1.549363	4.814561
167.H	6.797290	-0.314767	3.201652
168.H	5.934075	-0.064990	0.857254

TS-2 Bond Energy LDA + GGA-XC= -35.85860588 a.u.

1.C	-0.512585	0.924589	4.849343
2.C	-1.034340	0.422261	6.069623
3.C	-0.198193	0.147666	7.152811
4.C	1.181242	0.381929	7.052050
5.C	1.703402	0.945814	5.878674
6.C	0.868060	1.231495	4.797262
7.C	-1.393978	1.003001	3.689070
8.C	-1.057703	1.289067	2.381689
9.C	-0.642537	-0.638351	1.294419
10.C	-1.998565	-1.253451	1.454634
11.O	-3.088273	-0.649759	1.520784
12.O	-1.909298	-2.649923	1.444235
13.C	-3.231934	-3.367418	1.363606
14.C	0.557214	-1.160485	2.025755
15.C	0.345391	-1.981089	3.312185
16.Rh	-0.272540	0.015834	-0.663952
17.Rh	0.231688	0.719973	-3.054943
18.N	-3.327428	-3.222474	-2.753236
19.O	-4.128239	-1.020561	-3.173198
20.O	-3.086860	-5.372241	-1.771643
21.C	-4.271104	-2.158088	-2.693478
22.C	-5.421087	-2.690585	-1.915261
23.C	-6.601810	-2.060661	-1.552214

24.C	-7.520380	-2.799095	-0.786515
25.C	-7.245973	-4.123819	-0.412952
26.C	-6.038221	-4.747395	-0.780402
27.C	-5.133397	-4.004251	-1.528681
28.C	-3.758995	-4.343635	-2.005355
29.N	3.024001	-3.304748	-1.070618
30.O	1.125912	-3.955508	-2.347234
31.O	4.540357	-3.068102	0.740458
32.C	1.821062	-4.024413	-1.320440
33.C	1.562915	-4.827581	-0.100154
34.C	0.479316	-5.641997	0.199042
35.C	0.452247	-6.232116	1.474158
36.C	1.484159	-6.003808	2.397381
37.C	2.573772	-5.171317	2.080281
38.C	2.588596	-4.586808	0.820144
39.C	3.531348	-3.594206	0.224699
40.N	3.358964	3.007807	0.566719
41.O	4.207676	1.243019	-0.779369
42.O	2.822807	4.312614	2.477377
43.C	4.194734	1.895124	0.277775
44.C	5.010372	1.679949	1.504280
45.C	6.014043	0.752539	1.744488
46.C	6.651445	0.798131	2.997164
47.C	6.273440	1.742400	3.964158
48.C	5.238449	2.663469	3.714897
49.C	4.619172	2.612003	2.472424
50.C	3.511661	3.439413	1.907704
51.N	-3.364147	3.533415	-0.321088
52.O	-1.121495	4.316296	-0.144704
53.O	-5.539229	2.791721	0.275060
54.C	-2.233619	4.065337	0.354128
55.C	-2.635149	4.190478	1.781033
56.C	-1.877093	4.586518	2.874712
57.C	-2.470260	4.483418	4.144627
58.C	-3.785396	4.015096	4.289019
59.C	-4.546575	3.627342	3.170584
60.C	-3.943564	3.716672	1.922339
61.C	-4.436612	3.287109	0.582235
62.O	-1.353330	-1.630642	-1.566414
63.O	-0.846914	-0.977273	-3.732147
64.O	1.508149	-1.153841	-0.822315
65.O	1.964134	-0.535262	-3.008189
66.O	0.987621	1.621210	-0.015751
67.O	1.351591	2.306831	-2.196961
68.O	-1.939296	1.327549	-0.736776
69.O	-1.522961	1.936357	-2.931197
70.C	-1.349939	-1.787975	-2.865895
71.C	-1.980172	-3.123860	-3.355167
72.C	-1.961767	-3.411993	-4.900008
73.C	-2.562607	-4.822017	-5.143789
74.C	-2.777723	-2.366898	-5.700671
75.C	-0.493571	-3.448940	-5.395000
76.C	2.209742	-1.189379	-1.928106
77.C	3.460184	-2.101339	-1.825042
78.C	4.299922	-2.366604	-3.123311
79.C	3.458819	-2.905336	-4.307828

80.C	5.411230	-3.381917	-2.751479
81.C	4.977963	-1.035955	-3.542118
82.C	1.511309	2.404573	-0.926227
83.C	2.344951	3.574224	-0.348260
84.C	2.917576	4.614946	-1.371699
85.C	1.719271	5.288597	-2.088745
86.C	3.669786	5.708908	-0.567035
87.C	3.876576	3.980973	-2.406582
88.C	-2.169752	2.020399	-1.819620
89.C	-3.373932	2.989311	-1.699232
90.C	-3.548359	4.054314	-2.835302
91.C	-3.854148	3.310096	-4.163655
92.C	-4.786102	4.917498	-2.480421
93.C	-2.296052	4.967759	-3.008142
94.C	-3.857154	-3.520020	2.744900
95.H	4.112223	-3.446966	-5.004503
96.H	2.672783	-3.582702	-3.976820
97.H	2.984990	-2.081304	-4.848537
98.H	6.127330	-2.941273	-2.046244
99.H	5.957757	-3.667581	-3.659043
100.H	4.992535	-4.289910	-2.303173
101.H	5.610074	-1.219909	-4.420770
102.H	4.232454	-0.279331	-3.798631
103.H	5.610234	-0.636977	-2.739521
104.H	4.119583	-1.576768	-1.123827
105.H	-0.325686	-5.787187	-0.515880
106.H	-0.385305	-6.866682	1.750935
107.H	1.434046	-6.468300	3.378212
108.H	3.367136	-4.975173	2.795076
109.H	-1.888623	-5.609905	-4.784274
110.H	-2.707387	-4.960318	-6.223574
111.H	-3.536220	-4.945532	-4.657671
112.H	-0.013069	-2.474853	-5.302619
113.H	-0.488634	-3.747253	-6.451540
114.H	0.090588	-4.182024	-4.830759
115.H	-2.646477	-1.360892	-5.300511
116.H	-3.846727	-2.613771	-5.694759
117.H	-2.435093	-2.366142	-6.744078
118.H	-1.388370	-3.901353	-2.860995
119.H	-5.817188	-5.770683	-0.491745
120.H	-7.977199	-4.674319	0.172324
121.H	-8.453867	-2.335892	-0.478228
122.H	-6.791884	-1.030967	-1.841598
123.H	-2.959109	2.828215	-4.561809
124.H	-4.225389	4.038618	-4.896316
125.H	-4.626288	2.541077	-4.026490
126.H	-4.711880	5.325153	-1.465892
127.H	-5.712435	4.334621	-2.557824
128.H	-4.845997	5.758348	-3.182968
129.H	-1.455309	4.631751	-2.407931
130.H	-2.521381	6.000807	-2.715976
131.H	-1.973011	4.972613	-4.055719
132.H	-4.260042	2.340457	-1.716998
133.H	-5.560600	3.251737	3.272039
134.H	-4.217353	3.939862	5.283330
135.H	-1.893789	4.746131	5.027150

136.H	-0.853210	4.927116	2.750839
137.H	-2.099209	0.217587	6.150723
138.H	-0.613703	-0.266586	8.068509
139.H	1.840261	0.132245	7.880201
140.H	2.767831	1.147376	5.797530
141.H	1.292557	1.686308	3.911265
142.H	-0.093299	1.696238	2.109333
143.H	-1.872139	1.449626	1.685166
144.H	-2.439364	0.772556	3.891931
145.H	1.277601	-1.998872	3.890210
146.H	0.056776	-3.002948	3.058245
147.H	-0.432879	-1.545724	3.942139
148.H	1.089814	-1.780200	1.286513
149.H	1.245333	-0.322427	2.190140
150.H	2.103870	6.033528	-2.796514
151.H	1.126657	4.562892	-2.644848
152.H	1.067772	5.798950	-1.369995
153.H	3.113936	6.007241	0.329889
154.H	3.792191	6.597441	-1.199693
155.H	4.666974	5.368722	-0.262523
156.H	4.842271	3.730910	-1.953002
157.H	3.451290	3.076153	-2.842557
158.H	4.059072	4.701545	-3.215163
159.H	1.645706	4.107360	0.305045
160.H	4.940826	3.399740	4.455756
161.H	6.793222	1.764635	4.918153
162.H	7.449174	0.093562	3.215761
163.H	6.286225	0.018116	0.992979
164.H	-2.960695	-4.323130	0.917768
165.H	-3.876525	-2.790948	0.700299
166.H	-3.220415	-4.126910	3.398110
167.H	-4.834956	-4.009787	2.639726
168.H	-4.015521	-2.537705	3.199682

TS-3 Bond Energy LDA + GGA-XC= -35.85696892
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C -2.359433 0.608979 6.874302
C -3.696218 0.663797 6.453021
C -3.996031 1.100830 5.153892
C -2.972243 1.435288 4.269765
C -0.514225 1.498188 3.720218
C -0.581667 1.675671 2.352171
C -0.430613 -0.468317 1.516177
C 0.878668 -0.777446 2.186802
O 1.831986 0.014042 2.325273
O 0.952730 -2.111791 2.593460
C 2.318179 -2.561616 3.038425
C -1.729034 -1.162754 1.832820
C -1.927984 -1.968585 3.133907
C 2.497663 -2.420454 4.544095
Rh -0.169280 -0.139961 -0.532638
Rh 0.178584 0.112757 -3.046233
N -3.641336 -3.386955 -1.824274
O -4.387254 -1.265945 -2.603915
O -3.407381 -5.320928 -0.465670

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C -5.687343 -2.646702 -1.033773
C -6.871595 -1.960503 -0.806005
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C -7.528700 -3.772259 0.697290
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O 4.706051 -4.037660 0.736744
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O -0.865112 4.247065 -0.649350
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C -2.089927 5.319481 3.557109
C -3.438141 5.012071 3.794409
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C -1.066742 -4.291231 -4.578403
C 2.082263 -1.783610 -1.681792

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C 5.013004 -4.352464 -2.470904
C 4.628747 -2.121339 -3.552069
C 1.698260 2.040068 -1.344448
C 2.607819 3.232021 -0.978233
C 3.194669 4.085610 -2.150023
C 2.007184 4.706094 -2.929360
C 4.027874 5.233984 -1.518414
C 4.086987 3.271625 -3.110335
C -2.049758 1.774329 -1.897242
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C -3.458351 3.667360 -3.153569
C -3.915149 2.738640 -4.309186
C -4.620668 4.640844 -2.829290
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H -4.495737 0.369836 7.128315
H -2.121826 0.288900 7.885706
H -0.297974 0.879197 6.318712
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H -2.977071 -2.293982 3.172176
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H -0.694920 -5.855289 0.690770
H -0.363155 -7.028000 2.885496
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H 3.856665 -6.062199 2.817371
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H 4.932936 2.819475 -2.583430
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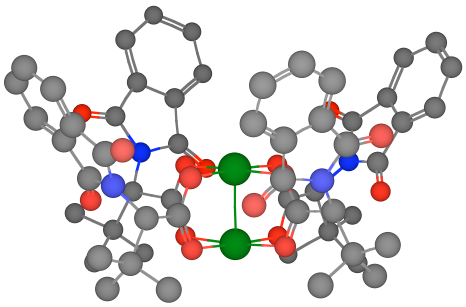
H 4.486641 3.945597 -3.880507
H 1.957153 3.890681 -0.392514
H 5.254908 3.617350 3.772989
H 7.022875 1.971020 4.465442
H 7.559256 0.026649 3.032208
H 6.359070 -0.316957 0.853247

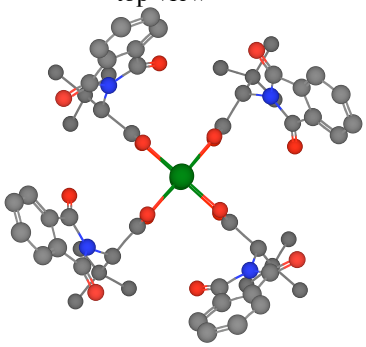
Results from Conformational Searching on Rh_2(*S*-PTTL)$_4$ using MacroModel, followed by optimization at OLYP/TZP (small frozen core)

Lowest energy structure

side view



top view



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Rh	0.60386	-0.885409	-0.729477
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O	-2.7979	3.137411	-3.287994
O	1.644041	2.184	-4.083064
C	-1.590825	3.282756	-3.365393
C	-0.776421	4.455356	-2.936636
C	-1.159662	5.660752	-2.362346
C	-0.144717	6.559243	-2.01393
C	1.20423	6.248861	-2.228664
C	1.58109	5.032889	-2.808498
C	0.56402	4.156019	-3.161003
C	0.645109	2.797358	-3.761269
N	1.619422	-4.074062	2.558969
O	3.237711	-3.237535	4.027694
O	-0.467854	-4.645255	1.670787
C	2.085586	-3.546835	3.784142
C	0.897894	-3.449243	4.678726
C	0.79271	-3.01309	5.993276
C	-0.484612	-2.994927	6.564573
C	-1.611128	-3.394715	5.833851
C	-1.494845	-3.834201	4.510611
C	-0.220928	-3.857675	3.958657
C	0.220479	-4.251302	2.591956
O	-0.278659	0.337697	-2.122748
O	0.107551	-1.135586	-3.792779
O	1.476309	-2.175864	0.628029
O	1.870204	-3.725005	-0.968948
C	-0.332353	-0.035307	-3.33681
C	-1.09297	0.967662	-4.257514
C	-1.206446	0.679669	-5.801631
C	-2.020848	-0.62069	-5.996905
C	0.148219	0.556241	-6.52549
C	-2.013502	1.829125	-6.446379
C	1.878227	-3.313455	0.232145
C	2.485449	-4.191281	1.370244
C	2.996884	-5.64412	1.037937
C	1.921148	-6.578166	0.448422
C	4.182852	-5.523131	0.052516
C	3.539149	-6.27922	2.338391
H	-2.206564	5.887828	-2.180498
H	-0.40432	7.510554	-1.554475
H	1.970053	6.960247	-1.928068
H	2.624753	4.769518	-2.96028
H	1.668983	-2.689004	6.548533
H	-0.608898	-2.653721	7.590064
H	-2.592482	-3.351743	6.300768
H	-2.36422	-4.126336	3.926955
H	-2.118045	0.908289	-3.87491
H	-1.489073	-1.501547	-5.635021
H	-2.221666	-0.763368	-7.064562
H	-2.985713	-0.573689	-5.480782
H	0.766329	-0.237592	-6.101331
H	0.719729	1.486981	-6.486666
H	-0.028523	0.318822	-7.581739

H	-1.492659	2.78894	-6.380676
H	-2.998833	1.945805	-5.983408
H	-2.16629	1.61259	-7.509344
H	3.379363	-3.62737	1.66434
H	1.109057	-6.763313	1.156096
H	2.378101	-7.546216	0.208834
H	1.484527	-6.175976	-0.467579
H	4.959058	-4.850634	0.436821
H	3.874255	-5.155165	-0.926866
H	4.640555	-6.508915	-0.086525
H	2.754377	-6.425201	3.086523
H	4.331566	-5.674677	2.790966
H	3.958872	-7.265412	2.110836
Rh	1.012917	-2.490908	-2.445744
N	5.129348	0.650791	-1.339873
O	5.059642	2.976761	-1.597339
O	5.379757	-1.451353	-0.335382
C	5.357063	1.988219	-0.95
C	6.011784	1.92946	0.386384
C	6.456941	2.949233	1.21689
C	7.000274	2.581267	2.453194
C	7.090803	1.236027	2.832924
C	6.638844	0.216184	1.988321
C	6.103189	0.593078	0.76484
C	5.517424	-0.24347	-0.318383
N	-3.937705	-2.359349	-0.638504
O	-4.605747	-2.857483	1.548939
O	-3.64014	-1.18722	-2.63988
C	-4.652819	-2.147623	0.559971
C	-5.442808	-0.899979	0.361364
C	-6.329736	-0.250109	1.20898
C	-6.889711	0.950166	0.756332
C	-6.560193	1.475202	-0.499605
C	-5.667831	0.811368	-1.348
C	-5.129278	-0.384212	-0.892891
C	-4.157648	-1.302288	-1.545847
O	2.447607	-0.035466	-1.209038
O	2.833538	-1.566486	-2.825969
O	-1.244885	-1.7992	-0.417803
O	-0.846569	-3.326982	-2.034878
C	3.130709	-0.527193	-2.16026
C	4.383565	0.303843	-2.562483
C	5.260876	-0.169565	-3.78638
C	5.902862	-1.558763	-3.605366
C	4.383753	-0.161626	-5.06144
C	6.382823	0.870809	-4.005181
C	-1.56864	-2.795386	-1.136147
C	-2.944436	-3.436831	-0.790136
C	-3.422974	-4.700657	-1.606861
C	-4.798372	-5.141258	-1.057646
C	-3.556476	-4.467059	-3.125378
C	-2.432788	-5.859936	-1.342717
H	6.374871	3.990753	0.917929
H	7.350894	3.351947	3.135982
H	7.509552	0.983162	3.804228
H	6.689294	-0.830289	2.276898

H -6.569418 -0.655628 2.188176
H -7.5826 1.493678 1.394787
H -6.995546 2.420749 -0.81476
H -5.38807 1.219483 -2.315725
H 3.947988 1.261157 -2.868772
H 6.463654 -1.81653 -4.512318
H 5.155683 -2.336821 -3.438522
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H 3.895115 0.806902 -5.209735
H 3.610464 -0.929715 -5.039886
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H 6.964015 0.592257 -4.89128
H 7.078442 0.918243 -3.162184
H -2.800086 -3.788774 0.237332
H -5.572212 -4.385702 -1.222246
H -4.760486 -5.362737 0.013615
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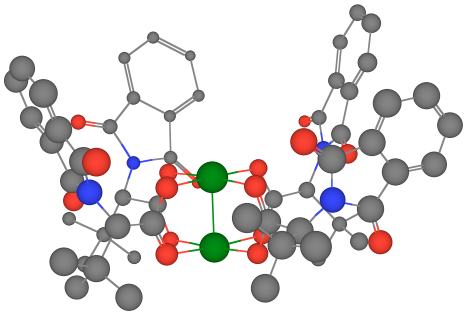
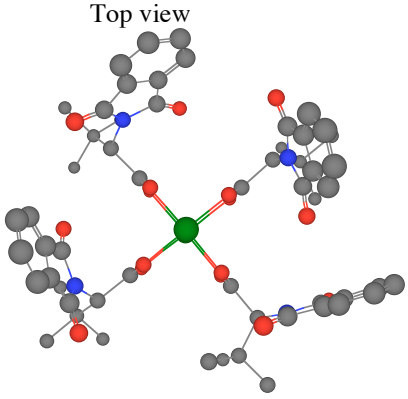
H -4.325302 -3.725975 -3.359675
H -3.847323 -5.408286 -3.60806
H -2.619446 -4.134413 -3.574863
H -2.301329 -6.042107 -0.27058
H -1.448856 -5.674161 -1.774515
H -2.827367 -6.779327 -1.789649

Second lowest Energy Conformation (E = 3.86 kcal/mol)
This conformation differs from the lowest energy (chiral crown) conformation in that one of the ligands is rotated so that the C-C bond to the *t*-Bu group is ~perpindicular to the Rh-Rh bond.

Side view



Top view



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O 1.113303 2.033402 -4.275068
O -3.262076 3.227467 -3.454896
C 0.152357 2.704898 -3.954188
C 0.14788 4.074517 -3.376126
C 1.211271 4.905878 -3.051761
C 0.90216 6.145314 -2.481782
C -0.426347 6.523007 -2.2481
C -1.489195 5.672384 -2.57257
C -1.172675 4.444572 -3.138226

C	-2.051408	3.311905	-3.542604
N	1.769384	-3.624287	2.53653
O	-0.558905	-3.864994	2.587166
O	3.938926	-3.017752	3.171386
C	0.478098	-3.499592	3.097418
C	0.660581	-2.845822	4.423498
C	-0.279939	-2.505134	5.385862
C	0.187342	-1.88247	6.548319
C	1.550737	-1.616255	6.727197
C	2.489359	-1.9679	5.750474
C	2.014998	-2.584963	4.600001
C	2.741143	-3.068845	3.392047
O	-0.953421	0.313989	-2.239685
O	-0.582407	-1.183181	-3.893066
O	0.938033	-2.123552	0.518018
O	1.271434	-3.706088	-1.062359
C	-0.986167	-0.062929	-3.454722
C	-1.683767	0.963499	-4.403511
C	-1.806808	0.653664	-5.943791
C	-2.576319	1.819331	-6.605648
C	-2.662813	-0.621832	-6.121075
C	-0.459346	0.473924	-6.670793
C	1.349683	-3.258263	0.126706
C	2.09429	-4.12029	1.189053
C	2.079094	-5.697357	1.016855
C	0.674341	-6.289794	0.78503
C	2.993209	-6.07377	-0.172964
C	2.688589	-6.339826	2.282578
H	2.238968	4.592189	-3.214664
H	1.706526	6.82168	-2.201931
H	-0.631808	7.490193	-1.794882
H	-2.521772	5.950024	-2.378569
H	-1.334907	-2.711056	5.230615
H	-0.519013	-1.594374	7.324075
H	1.88144	-1.123337	7.638766
H	3.548195	-1.760751	5.8793
H	-2.715482	0.982365	-4.030168
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H	-2.725656	1.59838	-7.668163
H	-2.029447	2.764487	-6.54331
H	-3.626329	-0.536708	-5.60424
H	-2.154795	-1.515843	-5.756619
H	-2.877677	-0.767849	-7.185519
H	0.141643	-0.324202	-6.230766
H	0.135903	1.390091	-6.660188
H	-0.649593	0.21579	-7.71986
H	3.141456	-3.81775	1.062595
H	0.01695	-6.139178	1.642875
H	0.76108	-7.370117	0.615528
H	0.185502	-5.858227	-0.091166
H	4.002246	-5.661033	-0.054964
H	2.59364	-5.727715	-1.126768
H	3.086918	-7.16465	-0.221913
H	2.08303	-6.157792	3.175161
H	3.704506	-5.981143	2.478302
H	2.74075	-7.425183	2.142164

Rh	0.367496	-2.511048	-2.535011
N	4.527368	0.504229	-1.491604
O	4.681627	-1.643133	-0.576583
O	4.516444	2.836776	-1.653849
C	4.859051	-0.443258	-0.498682
C	5.439838	0.329487	0.632888
C	5.929959	-0.114725	1.853047
C	6.397468	0.855348	2.745737
C	6.36595	2.216423	2.417467
C	5.862318	2.651858	1.186296
C	5.400862	1.682488	0.306007
C	4.778831	1.816501	-1.040931
N	-3.769281	-3.712071	0.599979
O	-3.235873	-5.993169	0.64729
O	-4.471025	-1.590947	1.35414
C	-3.559543	-4.969715	1.221462
C	-3.826206	-4.782196	2.670028
C	-3.710282	-5.674872	3.726388
C	-3.998689	-5.193899	5.007376
C	-4.399614	-3.865949	5.2071
C	-4.508514	-2.975296	4.133096
C	-4.203811	-3.460751	2.86851
C	-4.176734	-2.751288	1.555669
O	1.820265	-0.037491	-1.402732
O	2.170124	-1.591441	-3.009438
O	-1.844386	-1.819004	-0.423948
O	-1.457079	-3.364611	-2.038257
C	2.495018	-0.55829	-2.349453
C	3.784634	0.224894	-2.731761
C	4.661856	-0.259693	-3.951843
C	5.821257	0.747532	-4.130423
C	5.254833	-1.673344	-3.79174
C	3.809393	-0.201756	-5.241425
C	-2.156785	-2.839253	-1.106486
C	-3.495368	-3.57815	-0.842283
C	-4.690609	-3.127917	-1.78491
C	-4.39242	-3.668766	-3.204162
C	-5.993815	-3.790736	-1.292904
C	-4.884218	-1.600836	-1.871704
H	5.927479	-1.171055	2.105139
H	6.78103	0.548786	3.716351
H	6.72925	2.945973	3.137771
H	5.822244	3.706856	0.929102
H	-3.390809	-6.700088	3.558943
H	-3.905338	-5.857713	5.864057
H	-4.6219	-3.523318	6.215436
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H	3.397668	1.20778	-3.019646
H	6.409344	0.468396	-5.011714
H	6.502295	0.755608	-3.274445
H	5.454966	1.767931	-4.283399
H	4.479806	-2.428586	-3.649088
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H	5.815969	-1.930618	-4.698783
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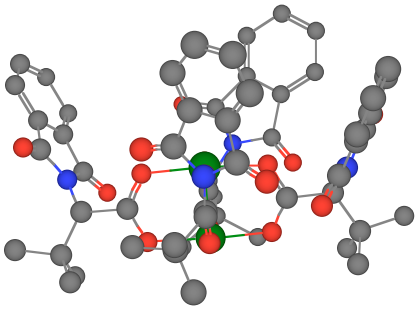
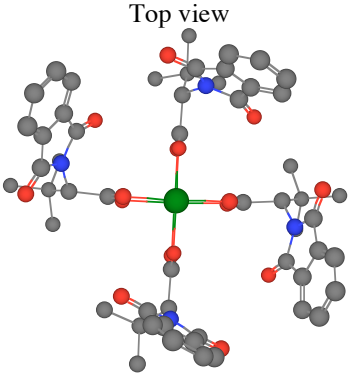
H -5.888917 -4.877609 -1.202159
H -6.793046 -3.596329 -2.017359
H -6.324695 -3.393647 -0.329478
H -3.993193 -1.099952 -2.261103
H -5.112752 -1.158904 -0.901864
H -5.710039 -1.378589 -2.558591

Third lowest Energy Conformation (E = 4.27 kcal/mol)
This conformation differs from the lowest energy (chiral crown) conformation in that one of the ligands is rotated so that the C-N bond is ~parallel to the Rh-Rh bond.

Side view



Top view



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O 1.474407 2.101144 -3.926836
O -2.966035 3.102884 -3.206994
C 0.478678 2.730612 -3.631841
C 0.403709 4.093212 -3.043485
C 1.425835 4.968651 -2.703885
C 1.056234 6.193866 -2.140271
C -0.290832 6.511915 -1.923815
C -1.311433 5.614879 -2.261941
C -0.935728 4.402246 -2.826347
C -1.756722 3.237146 -3.266764
N 2.578325 -3.439524 2.716535
O 0.31415 -3.222358 3.340778
O 4.911344 -3.273495 2.822659
C 1.494006 -2.995809 3.516229
C 2.097212 -2.22733 4.640604
C 1.481527 -1.574906 5.699591
C 2.307882 -0.922768 6.620562
C 3.701604 -0.941396 6.479332
C 4.310347 -1.611512 5.413566
C 3.47968 -2.245669 4.499154
C 3.80527 -3.019604 3.272968
O -0.483804 0.300759 -2.016626

O	-0.113325	-1.201351	-3.664202
O	1.416691	-2.110484	0.734648
O	1.817775	-3.671336	-0.849805
C	-0.538026	-0.087378	-3.225452
C	-1.257801	0.921766	-4.172491
C	-1.301752	0.644129	-5.723
C	-2.098742	-0.657331	-5.973397
C	0.084473	0.52785	-6.384666
C	-2.079783	1.798394	-6.393907
C	1.852297	-3.235164	0.346576
C	2.543675	-4.129667	1.414365
C	2.121024	-5.660175	1.45186
C	2.732716	-6.314302	2.708697
C	0.594644	-5.873315	1.455241
C	2.719649	-6.377288	0.219188
H	2.467987	4.699136	-2.856525
H	1.826474	6.907518	-1.856472
H	-0.544868	7.47022	-1.476165
H	-2.356697	5.851432	-2.083303
H	0.39972	-1.57045	5.797579
H	1.86477	-0.391746	7.459613
H	4.317574	-0.423135	7.210788
H	5.39041	-1.631505	5.296544
H	-2.298993	0.868691	-3.835708
H	-1.578645	-1.538796	-5.596982
H	-2.243463	-0.787288	-7.051902
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H	0.685493	-0.261075	-5.929318
H	0.649365	1.460712	-6.323342
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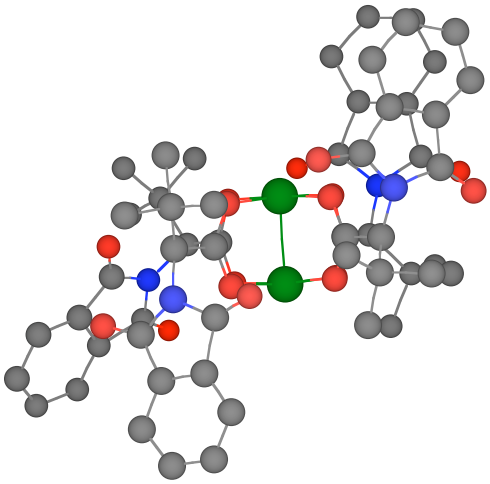
H	-1.57052	2.760242	-6.286462
H	-3.08998	1.902397	-5.984324
H	-2.173471	1.597123	-7.466424
H	3.599022	-4.121567	1.115023
H	3.823038	-6.212851	2.731725
H	2.499031	-7.384727	2.704773
H	2.328943	-5.897372	3.635361
H	0.125964	-5.413042	0.58247
H	0.120639	-5.464341	2.348511
H	0.376467	-6.947428	1.414706
H	3.805445	-6.239296	0.15523
H	2.279345	-6.029701	-0.716036
H	2.527855	-7.453149	0.303029
Rh	0.871005	-2.496446	-2.327295
N	4.998717	0.564308	-1.325241
O	4.927043	2.901347	-1.388621
O	5.247159	-1.611757	-0.510612
C	5.232084	1.863329	-0.828572
C	5.919901	1.68876	0.482636
C	6.385915	2.631176	1.38974
C	6.99191	2.154109	2.557648
C	7.128707	0.78051	2.794525
C	6.649936	-0.161468	1.878827
C	6.042513	0.325098	0.730232
C	5.410204	-0.414855	-0.394594
N	-4.067852	-2.361488	-0.635416

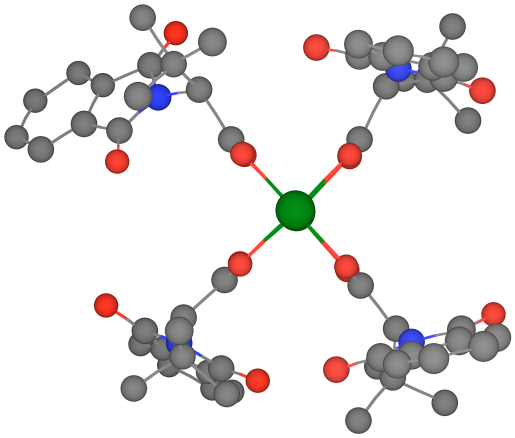
O	-4.87208	-2.816943	1.514351
O	-3.659202	-1.241195	-2.646357
C	-4.839977	-2.112301	0.523886
C	-5.578989	-0.843854	0.267008
C	-6.483603	-0.149107	1.059217
C	-6.989569	1.053559	0.552745
C	-6.594556	1.536588	-0.701339
C	-5.68568	0.828041	-1.492639
C	-5.197555	-0.366624	-0.983082
C	-4.22181	-1.320181	-1.57274
O	2.271374	0.021821	-1.181085
O	2.630817	-1.528095	-2.790604
O	-1.373691	-1.835183	-0.26754
O	-0.929221	-3.399609	-1.83853
C	2.940537	-0.486014	-2.137569
C	4.215473	0.308021	-2.542747
C	5.050305	-0.162814	-3.797185
C	6.199027	0.849577	-4.004351
C	5.653769	-1.576046	-3.671487
C	4.155631	-0.100704	-5.05717
C	-1.67944	-2.843898	-0.978104
C	-3.090264	-3.458624	-0.717288
C	-3.538834	-4.70347	-1.58277
C	-2.587282	-5.888478	-1.294472
C	-4.949279	-5.133837	-1.122836
C	-3.58058	-4.440915	-3.102698
H	6.273975	3.694669	1.199954
H	7.362407	2.861164	3.296424
H	7.610246	0.441689	3.70886
H	6.729534	-1.229192	2.054937
H	-6.775699	-0.523102	2.035635
H	-7.696603	1.630327	1.144095
H	-6.993498	2.481452	-1.060763
H	-5.353764	1.203012	-2.456799
H	3.819776	1.295532	-2.802483
H	6.771162	0.571133	-4.896532
H	6.896007	0.864066	-3.161505
H	5.822174	1.867184	-4.153406
H	4.891631	-2.332183	-3.478698
H	6.395162	-1.638397	-2.87182
H	6.157735	-1.834248	-4.611046
H	3.345753	-0.830182	-5.029434
H	4.768416	-0.316901	-5.939848
H	3.714073	0.890855	-5.195504
H	-3.034546	-3.819097	0.317907
H	-2.537035	-6.119234	-0.223705
H	-1.573858	-5.708003	-1.654339
H	-2.965446	-6.783433	-1.801641
H	-4.972857	-5.394482	-0.059758
H	-5.257365	-6.018336	-1.692005
H	-5.699093	-4.357666	-1.299854
H	-2.62184	-4.090547	-3.486671
H	-4.339379	-3.701911	-3.369316
H	-3.832016	-5.374647	-3.620538

Starting Conformation A (E = 8.18 kcal/mol)
Minimized conformation of Rh_2(*S*-PTTL)$_4$ similar to that in the crystal structure of phenylalanine derived Rh_2(*S*-PTPA)$_4$.

Side view



Top view



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O	1.94046500	-0.18497200	-2.14785100
C	2.08940700	1.07780400	-2.16607300
C	2.56466500	1.69967400	-3.51017500
N	2.81766500	3.13792800	-3.34699300
C	1.85649900	4.07650900	-3.78302500
C	2.31484800	5.40817400	-3.31296700
C	1.71444700	6.65591800	-3.42222400
C	2.38822000	7.74352200	-2.85693400
C	3.62608300	7.57594000	-2.22142900
C	4.21642800	6.31220100	-2.11045300
C	3.52822100	5.23652000	-2.65490800
C	3.85019900	3.78013900	-2.62572700
O	0.85769600	3.81104000	-4.42842400
O	4.80068900	3.24854000	-2.08902200
C	3.59199600	0.88207500	-4.40087300
C	4.08096000	1.79251500	-5.54844900
O	-0.90928300	-0.59979000	-1.64320600
O	-1.06977900	1.42161700	-0.64256000
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C	-2.67450400	0.84444700	-2.39015500
N	-3.61331100	-0.28793400	-2.40210700
C	-4.23483800	-0.88492500	-1.28418900
C	-5.14066800	-1.93725600	-1.82956800
C	-6.02367300	-2.78477200	-1.17332800
C	-6.79294300	-3.64627800	-1.96457300

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C	-5.75995600	-2.81133600	-4.00837500
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C	-3.99598100	-0.93275900	-3.59818900
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O	-3.56812300	-0.67630000	-4.70862000
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C	-0.46268000	-3.87911100	3.08511000
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O	0.63282900	-3.49286000	3.43726800
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H	1.94256600	8.73496300	-2.90235400
H	4.12770200	8.44305500	-1.79754800
H	5.16905700	6.16841200	-1.60805100
H	4.69834000	2.62188600	-5.19300300

H	3.24579400	2.20619400	-6.12465200
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H	-4.90371400	3.34803000	-3.37746200
H	-2.65603100	-1.41054400	2.43230900
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H	0.94453000	-6.42073800	3.06499600
H	-2.52008700	-2.76133700	5.35414100
H	-3.80537500	-1.73996600	4.68513300
H	-2.94259100	-1.24496000	6.14807700
H	5.09194800	-0.58740100	1.17732900
H	3.79424500	3.20014900	5.94619600
H	5.47895900	5.03358500	6.24400400
H	7.44688900	5.18119600	4.76274800
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H	6.80243300	-1.97581000	2.16980500
H	6.42338700	-2.98080500	3.57692700
H	1.97309500	0.02946800	-5.62890200
H	2.50125000	-1.03490400	-4.31550800
H	3.51764700	-0.82056400	-5.74580300
H	4.50081900	-0.34678300	-2.82666000
H	5.40035700	1.13740500	-3.17533400
H	5.45224800	-0.22332500	-4.30853100
H	-1.83953500	3.12622700	-3.65877600
H	-1.51563300	3.43527100	-1.94683400
H	-2.80100200	4.31407500	-2.77961100
H	-3.23734900	2.57642600	-0.13496500
H	-4.79391500	1.94124500	-0.67926500
H	-4.38156000	3.63087200	-0.97868100
H	-3.22433900	0.54797400	3.59184700
H	-1.57825800	1.17587200	3.76218400
H	-2.56711200	0.88925400	5.19778100
H	0.33391100	-0.38348100	4.55606500
H	-0.07698500	-1.91766900	5.33229800
H	-0.58653000	-0.39057800	6.06166600
H	4.83697300	-3.07544400	0.83190000
H	3.31076700	-3.35645600	1.68530700
H	4.80127500	-4.09713500	2.27533000
H	2.80731400	-2.07794600	3.90503000
H	4.18589200	-1.47056700	4.83161000
H	4.06561600	-3.18798800	4.44834300

X-ray structural analysis for compounds **joef082s** and **joef083**: Crystallographic details are reported in tables 1S and 3S. Bond distances and angles are presented in tables 2S and 4S. Crystals were selected and mounted on plastic mesh using Paratone® oil flash-cooled to 120 K. Data were collected on a Brüker-AXS APEX CCD diffractometer with graphite-monochromated Mo-Kα radiation (λ=0.71073 Å). Unit cell parameters were obtained from 60 data frames, 0.3º ω, from three different sections of the Ewald sphere. The systematic absences in the data and the unit cell parameters were consistent to $P2_1$ and $P2_1/m$. The enantiomerically resolved compounds are consistent with the noncentrosymmetrical space group option. The data-sets were treated with SADABS absorption corrections based on redundant multiscan data (Sheldrick, G.M. 2008. Acta Cryst. A64, 112-122). The structures were solved using direct methods and refined with full-matrix, least-squares procedures on F^2. The Flack parameter (Flack, H.D. 1983, Acta Cryst. A39, 876-881: 13930 Friedel pairs) in **joef082s** refined to 0.02(2) indicating that the true hand of the data was determined. The absolute configuration of **joef083** was assigned from the synthetic method. The compound **joef082s** consistently deposits as multiple, cracked crystals and the data presented herein represent the best of several trials. Two symmetry unique but chemically identical molecules are found in the asymmetric unit of **joef082s (**figures 1S and 2S). Common 1,2 and 1,3 atom distances were restrained for equivalent atoms across all the bridging ligands in **joef082s**. Four toluene and two ethyl acetate molecules of solvation per aymmetric unit in **joef082s** were treated as diffused contributions using Squeeze (Spek, A. L. 2003, J. Appl. Cryst. 36, 7-13). The A and B level alerts for **joef082s** in checkCIF (http://checkcif.iucr.org) arise from either Squeeze consequences or from small, unresolvable, apparent disorder causing larger than usual *Ueq* ranges and apparent Hirshfeld failures however the connectivity is corroborated by noncrystallographic information. The n-butyl chain in **joef083** (figure 3S) displayed increasing yet unresolvable disorder toward the methyl end causing a larger than usual *Ueq* range for C, and associated H, resulting in a level B Alert in checkCIF. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. Structure factors are contained in the SHELXTL 6.12 program library (Sheldrick, G. M., *op. cit.*). Structure CIFs are deposited with the Cambridge Crystallographic Data Centre under nos. CCDC 725972 &

726150.

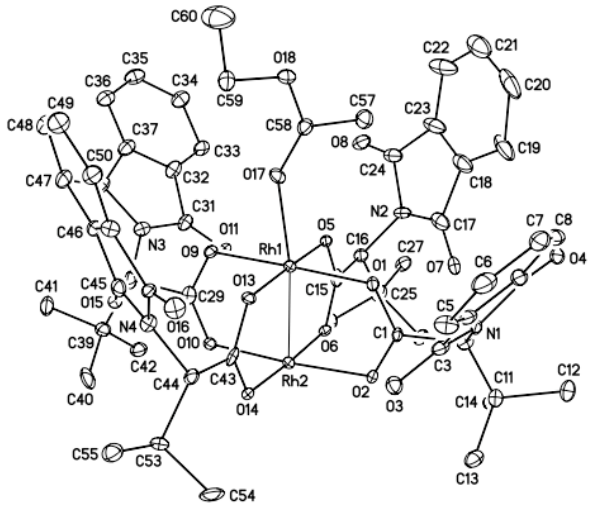

Fig 1S. Molecular diagram and labelling scheme for the first symmetry unique compound molecule in **joef082s** at 30% ellipsoids. Hydrogen atoms omitted for clarity.

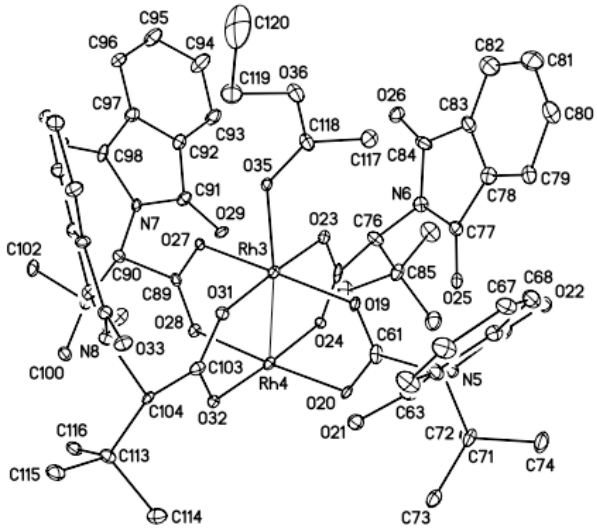

Fig 2S. Molecular diagram and labelling scheme for the second symmetry unique compound molecule in **joef082s** at 30% ellipsoids. Hydrogen atoms omitted for clarity.

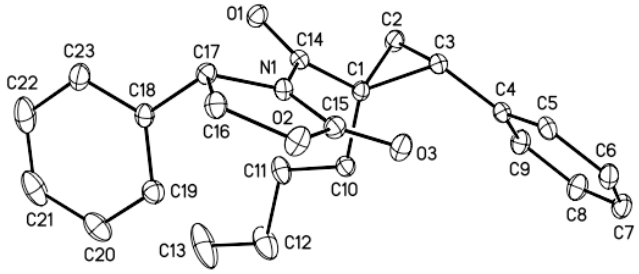

Fig 3S. Molecular diagram and labelling scheme for **joef083** at 30% ellipsoids. Hydrogen atoms omitted for clarity.

Table 1S. Crystal data and structure refinement for **joef082s**.

Identification code	joef082s	
Empirical formula	C_{78} H_{88} N_4 O_{20} Rh_2	
Formula weight	1607.34	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1$	
Unit cell dimensions	a = 14.182(4) Å	alpha = 90 º
	b = 20.088(6) Å	beta = 96.456(6) º
	c = 28.868(9) Å	gamma = 90 º
Volume	8172(4) $Å^3$	
Z, Calculated density	4, 1.306 g/cm^3	
Absorption coefficient	0.473 mm^{-1}	
F(000)	3336	
Crystal size	0.17 x 0.12 x 0.09 mm	
Theta range for data collection	1.45 to 25.00 º	
Limiting indices	-16<=h<=16, -23<=k<=23, -34<=l<=34	
Reflections collected / unique	81795 / 28757 [R(int) = 0.1366]	
Completeness to theta = 25.00	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9587 and 0.9239	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	28757 / 813 / 1513	

Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0718, wR2 = 0.1053
R indices (all data)	R1 = 0.1229, wR2 = 0.1173
Absolute structure parameter	0.02(2)
Largest diff. peak and hole	1.020 and -0.754 e $Å^{-3}$

Table 2S. Selected bond lengths [Å] and angles [°] for **joef082s.**

Rh(1)-O(5)	1.966(6)	Rh(1)-O(13)	1.987(7)	Rh(1)-O(1)	1.997(7)
Rh(1)-O(9)	2.034(7)	Rh(1)-O(17)	2.205(7)	Rh(1)-Rh(2)	2.3786(12)
Rh(2)-O(6)	1.976(7)	Rh(2)-O(10)	2.040(7)	Rh(2)-O(14)	2.028(7)
Rh(2)-O(2)	2.049(7)	Rh(3)-O(31)	1.931(6)	Rh(3)-O(23)	1.985(6)
Rh(3)-O(27)	1.998(7)	Rh(3)-O(19)	2.042(7)	Rh(3)-O(35)	2.237(6)
Rh(3)-Rh(4)	2.3800(12)	Rh(4)-O(32)	1.999(6)	Rh(4)-O(24)	1.994(7)
Rh(4)-O(20)	2.032(7)	Rh(4)-O(28)	2.025(6)		
O(5)-Rh(1)-O(13)	177.3(3)	O(5)-Rh(1)-O(1)	88.1(3)		
O(13)-Rh(1)-O(1)	92.9(3)	O(5)-Rh(1)-O(9)	88.6(3)		
O(13)-Rh(1)-O(9)	90.2(3)	O(1)-Rh(1)-O(9)	176.2(3)		
O(5)-Rh(1)-O(17)	99.1(3)	O(13)-Rh(1)-O(17)	83.3(3)		
O(1)-Rh(1)-O(17)	97.3(3)	O(9)-Rh(1)-O(17)	85.2(3)		
O(5)-Rh(1)-Rh(2)	88.06(17)	O(13)-Rh(1)-Rh(2)	89.49(18)		
O(1)-Rh(1)-Rh(2)	87.88(18)	O(9)-Rh(1)-Rh(2)	89.96(19)		
O(17)-Rh(1)-Rh(2)	171.27(19)	O(6)-Rh(2)-O(10)	91.3(3)		
O(6)-Rh(2)-O(14)	177.5(3)	O(10)-Rh(2)-O(14)	88.4(3)		
O(6)-Rh(2)-O(2)	87.0(3)	O(10)-Rh(2)-O(2)	176.1(3)		
O(14)-Rh(2)-O(2)	93.2(3)	O(6)-Rh(2)-Rh(1)	90.06(19)		
O(10)-Rh(2)-Rh(1)	87.5(2)	O(14)-Rh(2)-Rh(1)	87.48(18)		
O(2)-Rh(2)-Rh(1)	89.05(18)	O(31)-Rh(3)-O(23)	176.9(3)		
O(31)-Rh(3)-O(27)	92.1(3)	O(23)-Rh(3)-O(27)	88.8(3)		
O(31)-Rh(3)-O(19)	90.7(3)	O(23)-Rh(3)-O(19)	88.2(3)		
O(27)-Rh(3)-O(19)	176.1(3)	O(31)-Rh(3)-O(35)	85.1(2)		
O(23)-Rh(3)-O(35)	97.9(2)	O(27)-Rh(3)-O(35)	88.0(2)		
O(19)-Rh(3)-O(35)	94.9(2)	O(31)-Rh(3)-Rh(4)	88.70(18)		
O(23)-Rh(3)-Rh(4)	88.32(19)	O(27)-Rh(3)-Rh(4)	88.51(16)		
O(19)-Rh(3)-Rh(4)	88.90(19)	O(35)-Rh(3)-Rh(4)	172.79(16)		
O(32)-Rh(4)-O(24)	176.9(3)	O(32)-Rh(4)-O(20)	92.1(3)		
O(24)-Rh(4)-O(20)	88.7(3)	O(32)-Rh(4)-O(28)	87.7(2)		

O(24)-Rh(4)-O(28)	91.3(3)	O(20)-Rh(4)-O(28)	176.3(3)
O(32)-Rh(4)-Rh(3)	88.50(17)	O(24)-Rh(4)-Rh(3)	88.54(18)
O(20)-Rh(4)-Rh(3)	87.6(2)	O(28)-Rh(4)-Rh(3)	88.65(17)

Table 3S. Crystal data and structure refinement for **joef083**.

Identification code	joef083	
Empirical formula	C_{23} H_{25} N O_3	
Formula weight	363.44	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1$	
Unit cell dimensions	a = 11.961(4) Å	alpha = 90 °
	b = 5.5326(19) Å	beta = 109.747(5) °
	c = 15.785(5) Å	gamma = 90 °
Volume	983.1(6) $Å^3$	
Z, Calculated density	2, 1.228 g/cm^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	388	
Crystal size	0.24 x 0.14 x 0.10 mm	
Theta range for data collection	1.37 to 28.29 °	
Limiting indices	-15<=h<=15, -7<=k<=7, -21<=l<=21	
Reflections collected / unique	13561 / 2695 [R(int) = 0.0305]	
Completeness to theta = 25.00	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9923 and 0.9807	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2695 / 1 / 245	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0374, wR2 = 0.1015	
R indices (all data)	R1 = 0.0430, wR2 = 0.1123	
Largest diff. peak and hole	0.360 and -0.262 e $Å^{-3}$	

Table 4S. Bond lengths [Å] and angles [°] for **joef083**.

N(1)-C(15)	1.388(2)	N(1)-C(14)	1.406(2)	N(1)-C(17)	1.467(2)
O(1)-C(14)	1.209(2)	O(2)-C(15)	1.353(2)	O(2)-C(16)	1.438(2)
O(3)-C(15)	1.200(2)	C(1)-C(14)	1.505(2)	C(1)-C(2)	1.509(2)
C(1)-C(10)	1.513(2)	C(1)-C(3)	1.533(2)	C(2)-C(3)	1.505(3)
C(3)-C(4)	1.488(2)	C(4)-C(5)	1.398(3)	C(4)-C(9)	1.399(2)
C(5)-C(6)	1.386(3)	C(6)-C(7)	1.395(3)	C(7)-C(8)	1.388(3)
C(8)-C(9)	1.397(3)	C(10)-C(11)	1.533(2)	C(11)-C(12)	1.522(4)
C(12)-C(13)	1.530(4)	C(16)-C(17)	1.541(2)	C(17)-C(18)	1.513(2)
C(18)-C(23)	1.387(3)	C(18)-C(19)	1.393(3)	C(19)-C(20)	1.395(3)
C(20)-C(21)	1.390(4)	C(21)-C(22)	1.373(4)	C(22)-C(23)	1.392(3)

C(15)-N(1)-C(14)	128.39(14)	C(15)-N(1)-C(17)	112.18(14)
C(14)-N(1)-C(17)	118.89(14)	C(15)-O(2)-C(16)	110.97(14)
C(14)-C(1)-C(2)	115.70(15)	C(14)-C(1)-C(10)	111.62(13)
C(2)-C(1)-C(10)	120.34(15)	C(14)-C(1)-C(3)	118.83(14)
C(2)-C(1)-C(3)	59.28(11)	C(10)-C(1)-C(3)	121.82(15)
C(3)-C(2)-C(1)	61.16(11)	C(4)-C(3)-C(2)	124.21(15)
C(4)-C(3)-C(1)	122.60(15)	C(2)-C(3)-C(1)	59.55(11)
C(5)-C(4)-C(9)	117.82(17)	C(5)-C(4)-C(3)	118.62(15)
C(9)-C(4)-C(3)	123.56(16)	C(6)-C(5)-C(4)	121.71(17)
C(5)-C(6)-C(7)	119.89(17)	C(8)-C(7)-C(6)	119.33(19)
C(7)-C(8)-C(9)	120.51(18)	C(8)-C(9)-C(4)	120.68(18)
C(1)-C(10)-C(11)	112.67(16)	C(12)-C(11)-C(10)	111.7(2)
C(11)-C(12)-C(13)	112.2(3)	O(1)-C(14)-N(1)	117.64(16)
O(1)-C(14)-C(1)	123.24(16)	N(1)-C(14)-C(1)	118.70(15)
O(3)-C(15)-O(2)	122.19(17)	O(3)-C(15)-N(1)	128.71(17)
O(2)-C(15)-N(1)	109.10(15)	O(2)-C(16)-C(17)	106.36(14)
N(1)-C(17)-C(18)	112.03(13)	N(1)-C(17)-C(16)	101.14(13)
C(18)-C(17)-C(16)	113.12(15)	C(23)-C(18)-C(19)	119.68(17)
C(23)-C(18)-C(17)	120.24(17)	C(19)-C(18)-C(17)	120.05(16)

C(18)-C(19)-C(20)	119.91(19)	C(21)-C(20)-C(19)	119.7(2)
C(22)-C(21)-C(20)	120.3(2)	C(21)-C(22)-C(23)	120.2(2)
C(18)-C(23)-C(22)	120.1(2)		