

## Supporting Information

### Redox-neutral Depolymerization of Lignin-Derived Aryl Ethers Catalyzed by Rh(III)-complexes: A Mechanistic Insight

Yan Zhang,<sup>a,b</sup> Yafei Luo,<sup>a,b</sup> Changwei Hu,<sup>a</sup> Dianyong Tang<sup>\*b</sup>, and Zhishan Su<sup>\*a</sup>

<sup>1</sup>Key Laboratory of Green Chemistry and Technology, Ministry of Education, College of Chemistry, Sichuan University, Chengdu, Sichuan, 610064, P.R. China

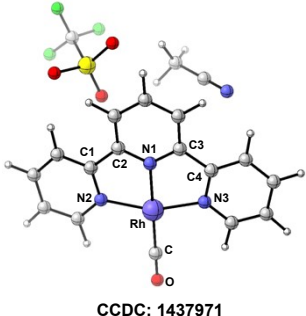
<sup>2</sup> College of Pharmacy & International Academy of Targeted Therapeutics and Innovation, Chongqing University of Arts and Sciences, Chongqing 402160, China.

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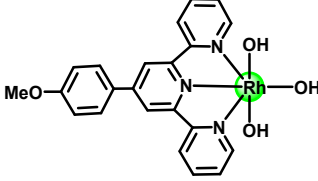
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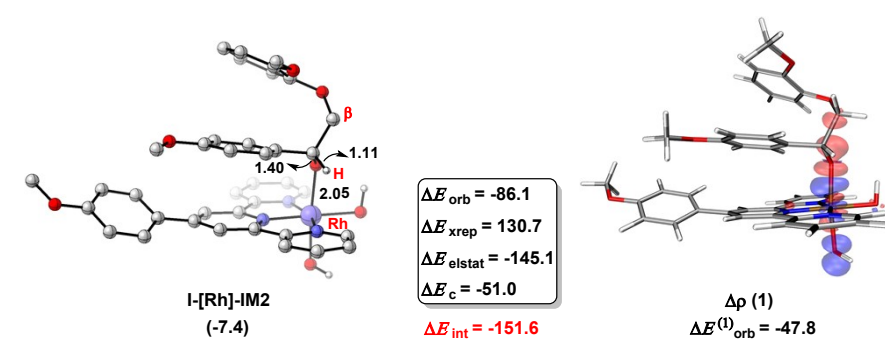
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**Table S1** Comparison of key geometric parameters obtained by experiments and theoretical calculations at the TPSSh-D3(BJ)/def2-SVP (SMD, water) theoretical level.

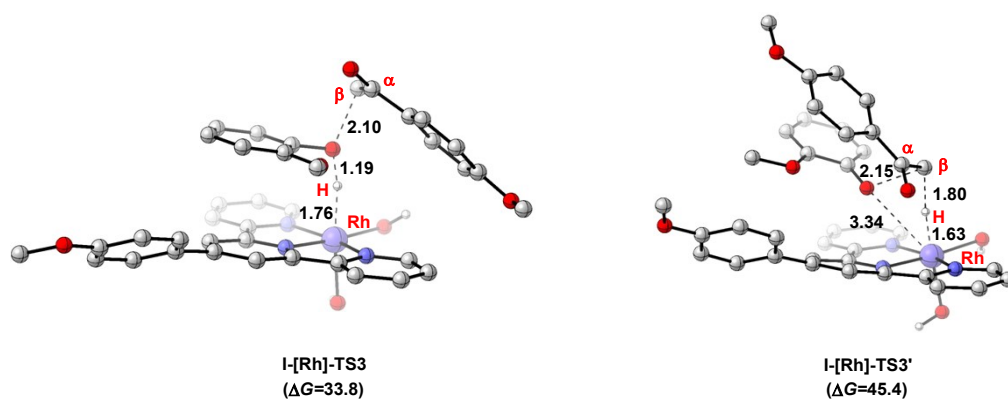
Rh complex	Parameters	Exp.	Calc.	$ \Delta $	
 CCDC: 1437971	<b>Bond (Å)</b>	Rh-N1	1.981	1.994	0.013
		Rh-N2	2.051	2.054	0.003
		Rh-N3	2.051	2.052	0.001
		Rh-C	1.839	1.857	0.018
		C-O	1.166	1.156	0.010
	<b>Angle (°)</b>	N1-Rh-N2	79.006	79.506	0.500
		N1-Rh-N3	79.304	79.410	0.106
		N2-Rh-N3	158.286	158.784	0.498
	<b>Dihedral (°)</b>	Rh-N2-C1-C2	-0.920	-5.445	4.525
		Rh-N3-C4-C3	-1.851	3.026	4.877

**Table S2** Comparison of relative Gibbs free energy ( $\Delta G$ ) of [Rh]-OH species with different spin states.

[Rh]-OH species	Spin state	$\Delta G(\text{kcal mol}^{-1})$
	Singlet	0.0
	Triplet	33.4
	Quintet	92.1



**Figure S1** Results of energy decomposition analysis (EDA). Dominating contributions to the deformation density  $\Delta\rho(1)$  associated with the interaction between Rh-complex and lignin moiety in the I-[Rh]-IM2, determined by the extended transition state- natural orbitals for chemical valence (ETS-NOCV) analysis. The contour value  $|\Delta\rho| = 0.003$  au. The blue/red contours correspond to accumulation/depletion of electron density.

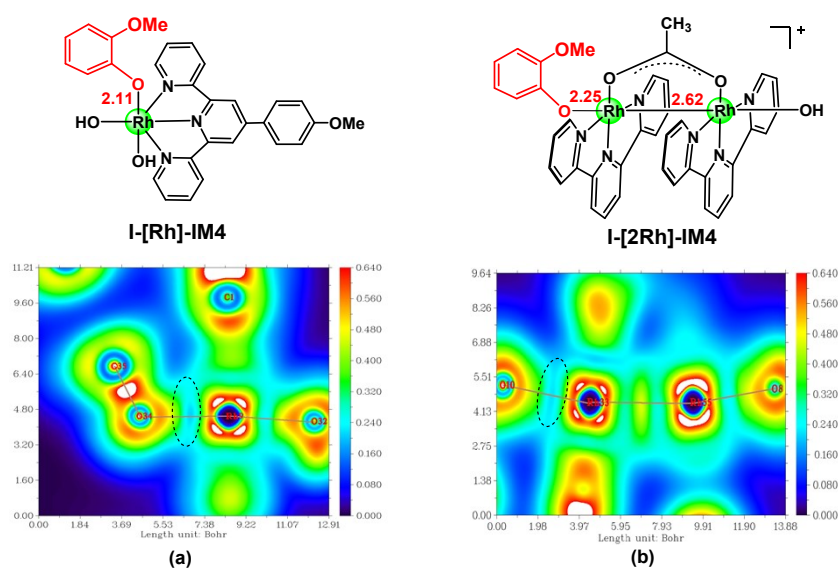


**Figure S2** Optimized geometries of I-[Rh]-TS3 and I-[Rh]-TS3'.

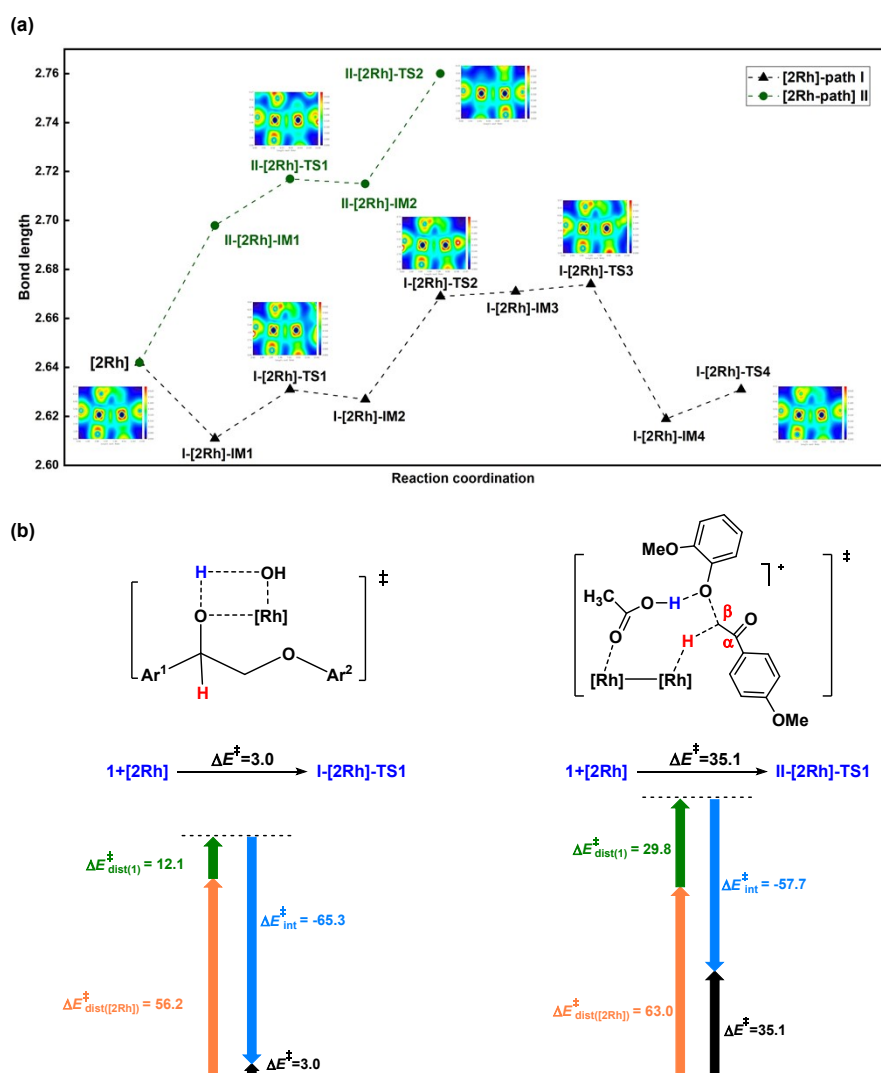
**Table S3** Selected parameters for  $C_{\beta}$ -O,  $C_{\alpha}$ - $C_{\beta}$  and O-Ar<sup>2</sup> bond in species 2, 1a and 1b.

Species	structure	Bond	Bond length(Å)	Wiberg bond index	$E_{BDE}$ (kcal mol <sup>-1</sup> ) <sup>a</sup>	$\Delta G^{\ddagger}$ (kcal mol <sup>-1</sup> )
2		$C_{\beta}$ -O	1.43	1.41	41.1	40.9
		$C_{\alpha}$ - $C_{\beta}$	1.53	1.16	76.6	55.0
		O-Ar <sup>2</sup>	1.37	1.53	87.5	44.6
1a		$C_{\alpha}$ -O	1.46	1.34	40.2	38.0
1b		C-O	1.39	1.45	66.2	39.9

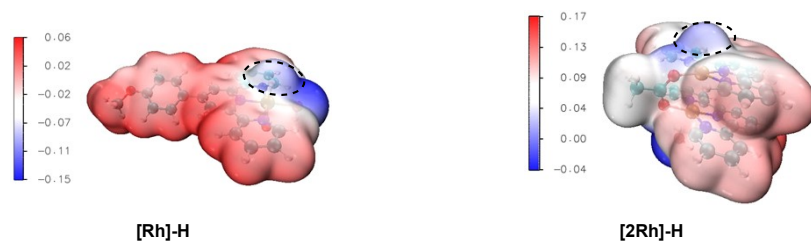
<sup>a</sup> Bond dissociation energy was calculated at the TPSSh-D3(BJ)/def2-TZVP (SMD, water) level of theory



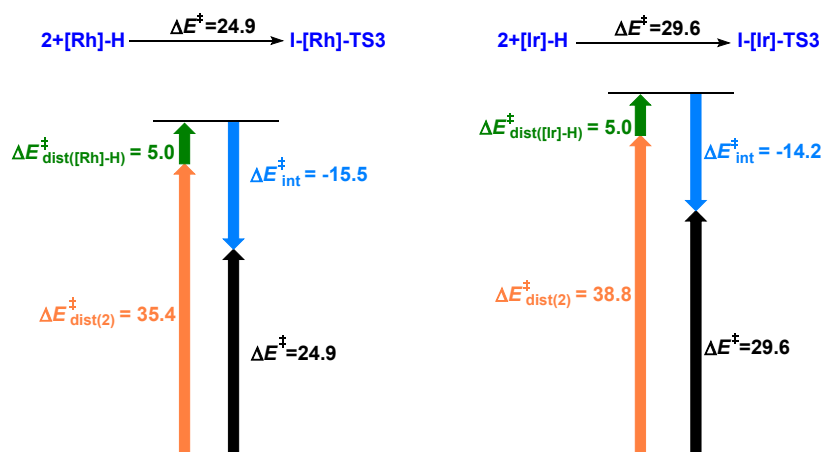
**Figure S3** Results of Localized orbital locator (LOL) calculation for I-[Rh]-IM4 and I-[2Rh]-IM4.



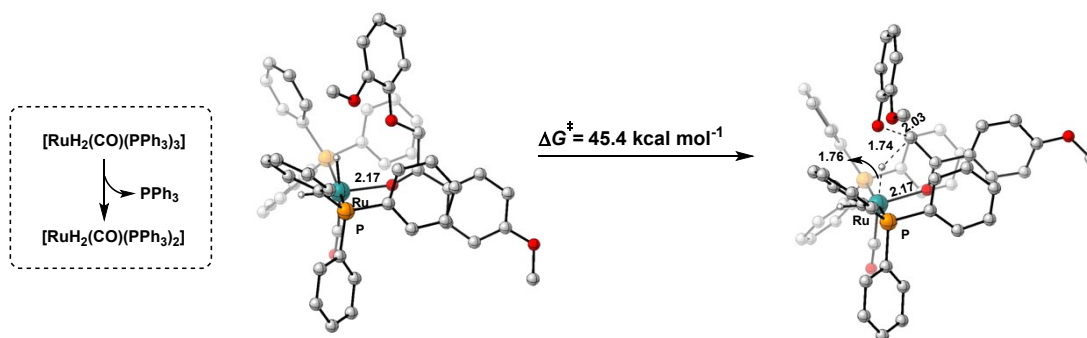
**Figure S4** (a) The bond length and the corresponding Localized orbital locator (LOL) analysis for the stationary points on the potential energy surface along path I-[2Rh] and II-[2Rh]. (b) Distortion-interaction analysis for I-[2Rh]-TS1 and II-[2Rh]-TS1.



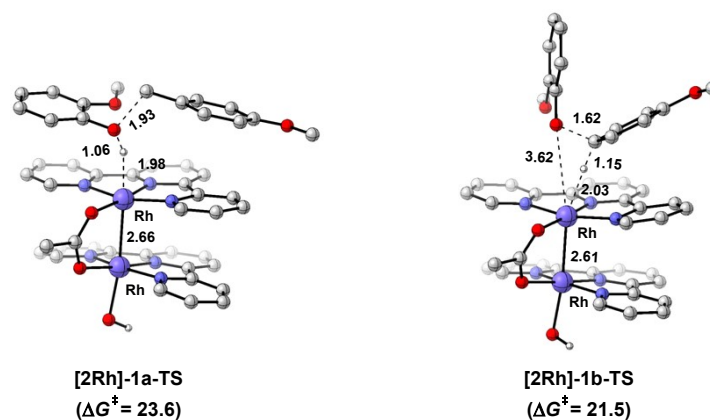
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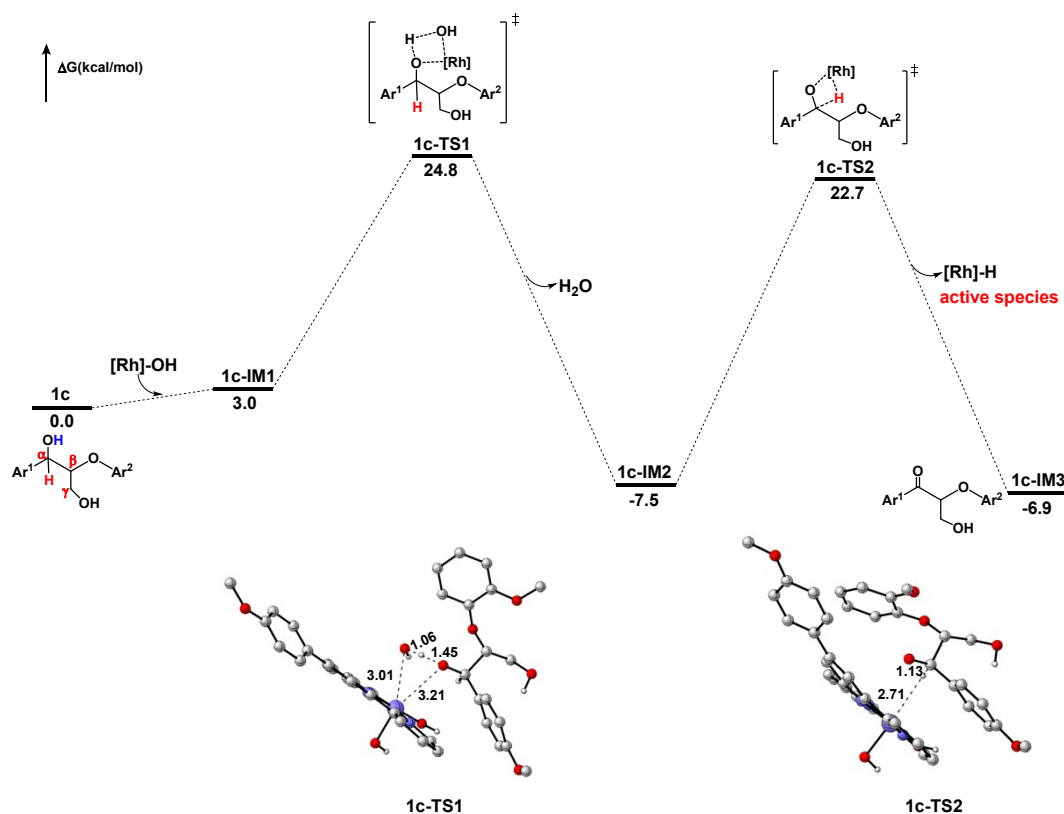
**Figure S6** Distortion interaction analysis for the formation of I-[Rh]-TS3 and I-[Ir]-TS3. The energy is in kcal mol<sup>-1</sup>.



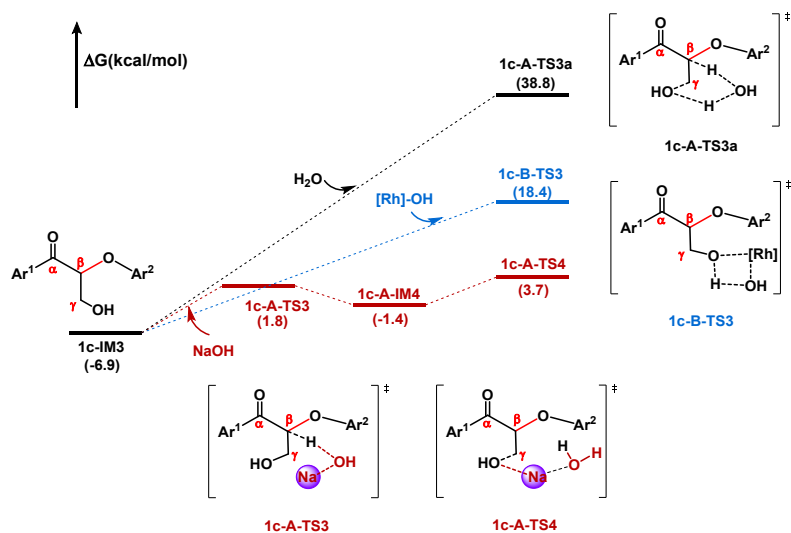
**Figure S7** Activation barrier associated with the C<sub>β</sub>-O bond cleavage in ketone intermediate 2 catalyzed by RuH<sub>2</sub>(CO)PPh<sub>3</sub>.



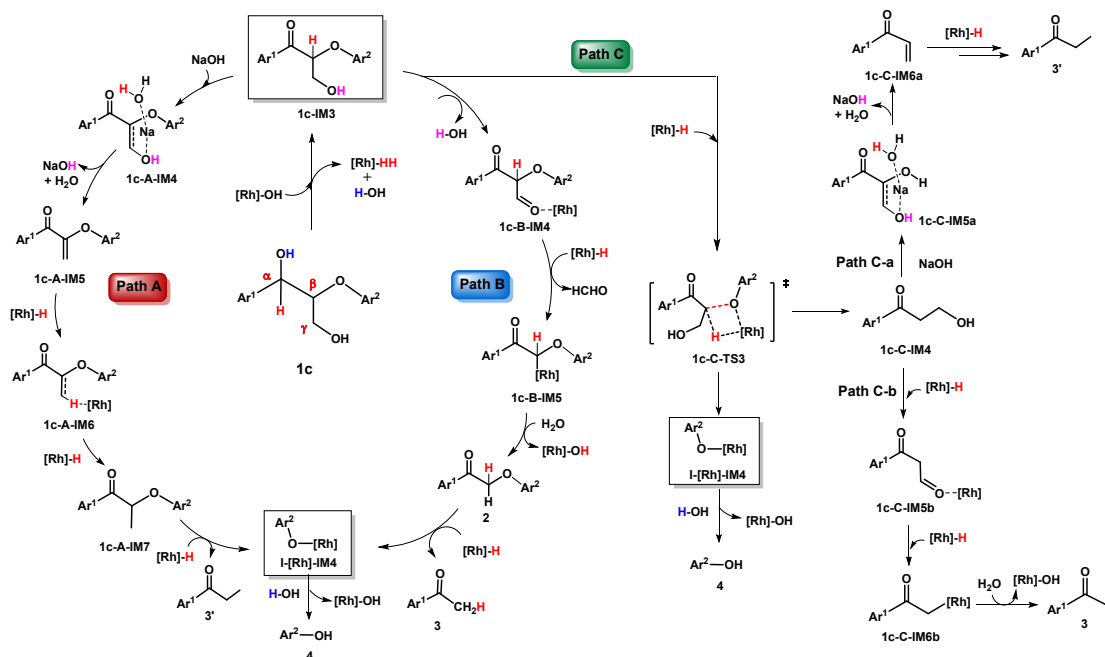
**Figure S8** Optimized geometries of [2Rh]-1a-TS and [2Rh]-1b-TS in the C-O bond cleavage catalyzed by [2Rh]-H species. Relative Gibbs free energy was in kcal mol<sup>-1</sup>.



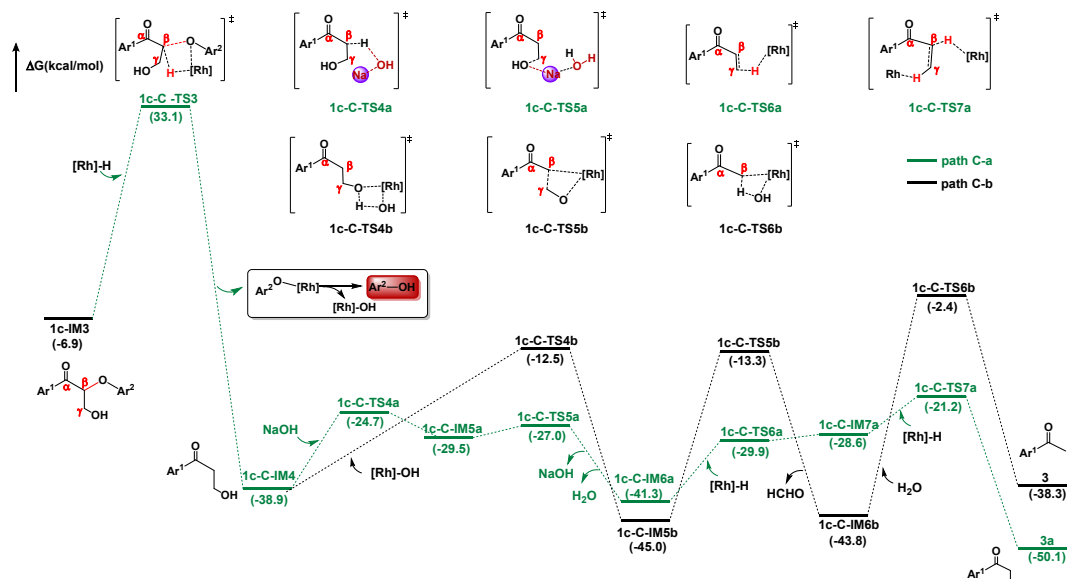
**Figure S9** Energy profile for the formation of C=O group at the C<sub>α</sub> atom of 1c catalyzed by rhodium-terpyridine complex.



**Figure S10** Energy profiles for the elimination of hydroxyl group in 1c-IM3 along three pathways.



**Scheme S1** Depolymerization mechanism for the  $\beta$ -O-4 model compound with  $\gamma$ -OH functionality (1c), catalyzed by rhodium-terpyridine complex.



**Figure S11** Energy profiles associated with the depolymerization of  $\beta$ -O-4 model compounds with  $\gamma$ -OH functionality, catalyzed by rhodium-terpyridine complex along path C.

**Table S4** Comparison of relative Gibbs free energy ( $\Delta G$ ) and activation barrier ( $\Delta G^\ddagger$ ), obtained by using different functionals.

Energy (kcal mol <sup>-1</sup> )	<sup>a</sup> TPSSH-D3(BJ)	<sup>b</sup> PBE0-D3(BJ)	<sup>c</sup> M06-D3(BJ)	<sup>d</sup> B3LYP-D3(BJ)
$\Delta G(\text{I-}[\text{Rh}]\text{-IM3})$	-7.1	-10.0	-11.1	-10.1
$\Delta G(\text{I-}[\text{Rh}]\text{-TS3})$	33.8	42.8	38.1	33.0



$\Delta G^\ddagger$	40.9	52.8	49.2	43.1
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<sup>a</sup> Gibbs free energy obtained at the TPSSh-D3(BJ)/def2-TZVP (SMD, water)//TPSSh-D3(BJ)/def2-SVP (SMD, water) theoretical level.

<sup>b</sup> Gibbs free energy obtained at the PBE0-D3(BJ)/def2-TZVP (SMD, water)//PBE0-D3(BJ)/def2-SVP (SMD, water) theoretical level.

<sup>d</sup> Gibbs free energy obtained at the M06-D3/def2-TZVP (SMD, water)//M06-D3/def2-SVP (SMD, water) theoretical level.

<sup>e</sup> Gibbs free energy obtained at the B3LYP-D3(BJ)/def2-TZVP (SMD, water)//B3LYP-D3(BJ)/def2-SVP (SMD, water) theoretical level.

**Table S5** Comparison of relative Gibbs free energy ( $\Delta G$ ) for key species (I-[2Rh]-IM3 and I-[2Rh]-TS3) in binuclear Rh-complex system with or without counterion (Cl<sup>-</sup>).

$\Delta G(\text{kcal mol}^{-1})$	I-[2Rh]-IM3	I-[2Rh]-TS3
with Cl anion	-3.6	26.1
without Cl anion	-2.7	27.6

**Table S6** Electronic energies ( $E_Z$ ), enthalpies ( $H$ ), and Gibbs free energies ( $G$ ) for all stationary points (in Hartree), obtained at the TPSSh-D3(BJ)/def2-SVP (SMD, water) theoretical level. Single-point energy calculations were run at the TPSSh-D3(BJ)/def2-TZVP (SMD, water) level of theory.

Structures	<sup>a</sup> ZPE	<sup>b</sup> H <sub>c</sub>	<sup>c</sup> G <sub>c</sub>	$E_{ZPE}$	$H$	$G$	$G^d$
<b>1</b>	0.31186	0.34265	0.24503	-920.54448	-920.51370	-920.61132	-921.60924
<b>1a</b>	0.27884	0.30606	0.21517	-806.11732	-806.09009	-806.18098	-807.04978
<b>1b</b>	0.24974	0.27513	0.18804	-766.85275	-766.82735	-766.91444	-767.74217
<b>1c</b>	0.34385	0.37898	0.27122	-1034.96765	-1034.93252	-1035.04028	-1036.17082
<b>2</b>	0.28851	0.31853	0.22096	-919.36153	-919.33150	-919.42907	-920.42471
<b>2a</b>	0.31630	0.34885	0.24498	-958.62946	-958.59691	-958.70078	-959.74063
<b>3</b>	0.17004	0.18757	0.11969	-498.95545	-498.93791	-499.00580	-499.54864
<b>3a</b>	0.19879	0.21837	0.14512	-538.21832	-538.19874	-538.27199	-538.85533
<b>4</b>	0.13691	0.13691	0.09202	-421.59926	-421.58529	-421.64415	-422.10799
<b>[Rh]-Cl</b>	0.34821	0.39156	0.26311	-2578.09582	-2578.05247	-2578.18091	-2579.82180
<b>[Rh]-OH</b>	0.38315	0.42791	0.29930	-1425.01295	-1424.96819	-1425.09680	-1426.55287
<b>[2Rh]-OH</b>	0.54036	0.60289	0.44053	-2084.69030	-2084.62777	-2084.79013	-2086.83108
<b>I-[Rh]-IM1</b>	0.69699	0.77281	0.57707	-2345.60121	-2345.52540	-2345.72114	-2348.16158
<b>I-[Rh]-TS1</b>	0.69418	0.76978	0.57208	-2345.55798	-2345.48239	-2345.68008	-2348.12673
<b>I-[Rh]-IM2</b>	0.67210	0.74438	0.55620	-2269.24029	-2269.16801	-2269.35619	-2271.70216
<b>I-[Rh]-TS2</b>	0.66937	0.74181	0.55118	-2269.18618	-2269.11374	-2269.30437	-2271.65604
<b>I-[Rh]-IM3</b>	0.66838	0.74209	0.54712	-2269.22692	-2269.15321	-2269.34818	-2271.70166
<b>I-[Rh]-TS3</b>	0.66099	0.73500	0.54198	-2269.16424	-2269.09023	-2269.28325	-2271.63651
<b>I-[Rh]-IM4</b>	0.49734	0.55281	0.40162	-1770.29832	-1770.24285	-1770.39404	-1772.20683
<b>I-[Rh]-TS4</b>	0.52248	0.58052	0.42263	-1846.63441	-1846.57637	-1846.73426	-1848.64166
<b>II-[Rh]-IM1</b>	0.69760	0.77357	0.57626	-2345.55003	-2345.47405	-2345.67137	-2348.11607
<b>II-[Rh]-TS1</b>	0.68947	0.76601	0.56593	-2345.53499	-2345.45845	-2345.65853	-2348.09974
<b>I-[Rh]-TS3'</b>	0.66240	0.73631	0.54351	-2269.14880	-2269.07488	-2269.26769	-2271.61809
<b>I-[Rh]-TS3-Cl</b>	0.65081	0.72430	0.52896	-2653.52687	-2653.45337	-2653.64871	-2656.06484
<b>I-[Rh]-TS3-2Cl</b>	0.63913	0.71248	0.51535	-3037.89319	-3037.81984	-3038.01697	-3040.49315
<b>I-[Rh]-TS3a</b>	0.66801	0.74114	0.54808	-2269.15813	-2269.08500	-2269.27806	-2271.63066
<b>I-[Rh]-TS3b</b>	0.66588	0.73883	0.54981	-2269.14989	-2269.07694	-2269.26596	-2271.61401

<b>I-[2Rh]-IM1</b>	0.85493	0.94816	0.71707	-3005.26322	-3005.16999	-3005.40108	-3008.42777
<b>I-[2Rh]-TS1</b>	0.85406	0.94648	0.71656	-3005.20441	-3005.11198	-3005.34191	-3008.40458
<b>I-[2Rh]-IM2</b>	0.82970	0.91963	0.69599	-2928.91355	-2928.82363	-2929.04726	-2931.98095
<b>I-[2Rh]-TS2</b>	0.82420	0.91411	0.69109	-2928.89896	-2928.80905	-2929.03206	-2931.97007
<b>I-[2Rh]-IM3</b>	0.82457	0.91561	0.68844	-2928.89859	-2928.80755	-2929.03472	-2931.97297
<b>I-[2Rh]-TS3</b>	0.82109	0.82109	0.68746	-2928.85763	-2928.76673	-2928.99126	-2931.92465
<b>I-[2Rh]-IM4</b>	0.65556	0.72746	0.54562	-2429.97754	-2429.90564	-2430.08747	-2432.48644
<b>I-[2Rh]-TS4</b>	0.67505	0.75127	0.55765	-2506.33569	-2506.25948	-2506.45309	-2508.94706
<b>I-[2Rh]-IM5</b>	0.67711	0.75379	0.55933	-2506.33372	-2506.25704	-2506.45150	-2508.94546
<b>II-[2Rh]-IM1</b>	0.85288	0.94658	0.71442	-3005.09555	-3005.00185	-3005.23401	-3008.38002
<b>II-[2Rh]-TS1</b>	0.84599	0.93952	0.70791	-3005.09299	-3004.99945	-3005.23107	-3008.36214
<b>II-[2Rh]-IM2</b>	0.85103	0.94539	0.71041	-3005.09978	-3005.00541	-3005.24040	-3008.36936
<b>II-[2Rh]-TS2</b>	0.84713	0.94172	0.70783	-3005.16868	-3005.07409	-3005.30798	-3008.34183
<b>b-TS1</b>	0.54420	0.60290	0.44218	-1810.71227	-1810.65357	-1810.81429	-1812.67717
<b>b-IM1</b>	0.52096	0.57700	0.42398	-1734.39984	-1734.34380	-1734.49682	-1736.26237
<b>b-TS2</b>	0.51988	0.57524	0.42317	-1734.34232	-1734.28697	-1734.43903	-1736.21460
<b>acetophenone</b>	0.13754	0.15119	0.09221	-384.53618	-384.52253	-384.58150	-384.99410
<b>c-TS1</b>	0.39924	0.44460	0.31582	-1426.12399	-1426.07863	-1426.20741	-1427.66322
<b>I-[Ir]-IM1</b>	0.69757	0.77300	0.57826	-2339.43375	-2339.35832	-2339.55306	-2341.98087
<b>I-[Ir]-TS1</b>	0.69471	0.76997	0.57368	-2339.39587	-2339.32062	-2339.51690	-2341.94705
<b>I-[Ir]-IM2</b>	0.67150	0.74411	0.55332	-2263.07247	-2262.99986	-2263.19064	-2265.52497
<b>I-[Ir]-TS2</b>	0.66877	0.74102	0.55126	-2263.02628	-2262.95403	-2263.14379	-2265.48027
<b>I-[Ir]-IM3</b>	0.66794	0.74189	0.54620	-2263.06104	-2262.98710	-2263.18279	-2265.52630
<b>I-[Ir]-TS3</b>	0.66126	0.73520	0.54242	-2262.99162	-2262.91769	-2263.11046	-2265.45222
<b>I-[Ir]-IM4</b>	0.49747	0.55276	0.40263	-1764.13052	-1764.07523	-1764.22535	-1766.02509
<b>I-[Ir]-TS4</b>	0.52224	0.57986	0.42396	-1840.46977	-1840.41216	-1840.56806	-1842.46000
<b>1a-TS</b>	0.65417	0.72541	0.53790	-2155.91844	-2155.84720	-2156.03471	-2158.26357
<b>1b-TS</b>	0.62714	0.69562	0.51559	-2116.66045	-2116.59197	-2116.77200	-2118.95295
<b>[2Rh]-1a-TS</b>	0.81094	0.89947	0.67895	-2815.61435	-2815.52582	-2815.74634	-2818.55044
<b>[2Rh]-1b-TS</b>	0.78589	0.87199	0.65561	-2776.35178	-2776.26568	-2776.48206	-2779.24915
<b>1c-IM1</b>	0.72911	0.80946	0.59706	-2460.01222	-2459.93187	-2460.14427	-2462.71890
<b>1c-TS1</b>	0.72590	0.80599	0.59478	-2459.97673	-2459.89664	-2460.10785	-2462.68414

<b>1c-IM2</b>	0.70482	0.78116	0.58335	-2383.66299	-2383.58665	-2383.78446	-2386.26395
<b>1c-TS2</b>	0.70264	0.77853	0.58135	-2383.61234	-2383.53644	-2383.73362	-2386.21575
<b>1c-IM3</b>	0.32153	0.35548	0.24907	-1033.78784	-1033.75388	-1033.86029	-1034.98852
<b>1c-A-TS3</b>	0.32902	0.36836	0.24930	-1271.84511	-1271.80576	-1271.92483	-1273.19932
<b>1c-A-IM4</b>	0.33432	0.37399	0.25510	-1271.84809	-1271.80841	-1271.92731	-1273.20440
<b>1c-A-TS4</b>	0.33044	0.37131	0.24980	-1271.83273	-1271.79185	-1271.91336	-1273.19627
<b>1c-A-IM5</b>	0.29281	0.32442	0.22182	-957.42116	-957.38955	-957.49215	-958.53087
<b>1c-A-TS5</b>	0.67076	0.74461	0.55447	-2307.27787	-2307.20402	-2307.39416	-2309.78527
<b>1c-A-IM6</b>	0.67509	0.74919	0.55839	-2307.27936	-2307.20526	-2307.39606	-2309.78448
<b>1c-A-TS6</b>	1.05119	1.16850	0.88494	-3657.14336	-3657.02605	-3657.30961	-3661.04700
<b>1c-A-IM7</b>	0.31630	0.34885	0.24498	-958.62946	-958.59691	-958.70078	-959.74063
<b>1c-A-TS7</b>	0.68821	0.76478	0.56639	-2308.44097	-2308.36440	-2308.56279	-2310.95420
<b>1c-A-TS3a</b>	0.34217	0.37823	0.26680	-1110.09261	-1110.05655	-1110.16797	-1111.38752
<b>1c-B-TS3</b>	0.70566	0.78366	0.57914	-2458.79988	-2458.72188	-2458.92641	-2461.50116
<b>1c-B-IM4</b>	0.68191	0.75746	0.55713	-2382.47598	-2382.40043	-2382.60076	-2385.07954
<b>1c-B-TS4</b>	0.67802	0.75386	0.55612	-2382.41976	-2382.34391	-2382.54166	-2385.01730
<b>1c-B-IM5</b>	0.64875	0.72062	0.53262	-2268.06762	-2267.99575	-2268.18376	-2270.52768
<b>1c-B-TS5</b>	0.67192	0.74734	0.54916	-2344.35891	-2344.28349	-2344.48167	-2346.92204
<b>1c-C-TS3</b>	0.69400	0.77185	0.56913	-2383.59244	-2383.51458	-2383.71730	-2386.19931
<b>1c-C-IM4</b>	0.20398	0.22476	0.14829	-613.37736	-613.35658	-613.43304	-614.10711
<b>1c-C-TS4a</b>	0.21132	0.23784	0.14787	-851.41940	-851.39288	-851.48285	-852.30909
<b>1c-C-IM5a</b>	0.21549	0.24290	0.15079	-851.42333	-851.39593	-851.48803	-852.31675
<b>1c-C-TS5a</b>	0.21189	0.24046	0.14559	-851.41367	-851.38509	-851.47996	-852.31277
<b>1c-C-IM6a</b>	0.17531	0.19400	0.12324	-537.00334	-536.98465	-537.05541	-537.63924
<b>1c-C-TS6a</b>	0.55329	0.61448	0.44773	-1886.84808	-1886.78689	-1886.95364	-1888.89550
<b>1c-C-IM7a</b>	0.55610	0.61732	0.45290	-1886.85339	-1886.79216	-1886.95659	-1888.89342
<b>1c-C-TS7a</b>	0.93277	1.03748	0.77842	-3236.71265	-3236.60794	-3236.86700	-3240.15612
<b>1c-C-TS4b</b>	0.58776	0.65217	0.48261	-2038.39660	-2038.33218	-2038.50175	-2040.61797
<b>1c-C-IM5b</b>	0.56453	0.62666	0.46124	-1962.07311	-1962.01099	-1962.17640	-1964.19813
<b>1c-C-TS5b</b>	0.56025	0.62309	0.45420	-1962.01028	-1961.94745	-1962.11634	-1964.14750
<b>1c-C-IM6b</b>	0.53154	0.59004	0.43151	-1847.64324	-1847.58473	-1847.74327	-1849.63869
<b>1c-C-TS6b</b>	0.55400	0.61606	0.44930	-1923.94798	-1923.88592	-1924.05268	-1926.04432

<sup>a</sup> Zero-point correction energy;

<sup>b</sup> Thermal correction to enthalpy;

<sup>c</sup> Thermal correction to Gibbs free energy;

<sup>d</sup> Gibbs free energy obtained at the TPSSh-D3(BJ)/def2-TZVP (SMD, water)//TPSSh-D3(BJ)/def2-SVP (SMD, water) theoretical level.

### Cartesian coordinates of all stationary points

<b>1</b>				C	2.21741	0.52721	0.15340
C	-1.71873	-0.97145	-1.03352	C	3.18924	0.36502	-0.83429
C	-0.37384	-1.35444	-1.09314	C	1.61804	-0.60538	0.75301
C	0.35026	-1.66647	0.06198	C	3.58237	-0.91673	-1.24174
C	-0.31944	-1.62790	1.29793	H	3.63046	1.25903	-1.28068
C	-1.65583	-1.24544	1.37810	C	2.01168	-1.88712	0.34097
C	-2.35993	-0.89677	0.21174	C	2.98827	-2.03580	-0.65289
H	0.12629	-1.38692	-2.06233	H	4.34558	-1.03462	-2.01368
H	0.21729	-1.88487	2.21508	H	1.55739	-2.77090	0.78988
H	-2.17474	-1.20375	2.33783	H	3.28266	-3.04132	-0.96215
C	1.83495	-1.99703	0.01290	O	0.68208	-0.35784	1.70671
H	2.00079	-2.90556	0.62415	C	-0.11864	-1.44520	2.16106
C	2.71738	-0.93074	0.66637	H	-0.61611	-1.94798	1.31603
H	3.74668	-1.31021	0.72098	H	0.48243	-2.17684	2.72538
O	2.83975	0.28460	-0.08876	H	-0.87465	-1.00567	2.82316
C	1.71249	1.00177	-0.42731	C	0.88112	2.43576	-0.33969
C	1.51855	1.30747	-1.77491	H	0.76868	3.44958	0.06531
C	0.80520	1.49141	0.54298	H	1.33089	2.49510	-1.34401
C	0.41270	2.06016	-2.18725	C	-1.79132	-0.13480	-1.23703
H	2.23983	0.91319	-2.49319	C	-0.64586	0.66821	-1.29403
C	-0.31444	2.22339	0.12402	C	-0.42874	1.70124	-0.37274
C	-0.50800	2.50433	-1.23564	C	-1.40474	1.93091	0.61467
H	0.26827	2.28190	-3.24663	C	-2.55288	1.14880	0.68389
H	-1.03373	2.58711	0.85790	C	-2.74641	0.10047	-0.23586
H	-1.38551	3.07889	-1.54045	H	0.09899	0.47352	-2.07003
O	1.09243	1.20711	1.84245	H	-1.25248	2.72736	1.34786
C	0.16841	1.62556	2.84329	H	-3.31245	1.32204	1.44894
H	0.09073	2.72448	2.87349	H	-1.92562	-0.93441	-1.96541
H	-0.82785	1.18819	2.67084	O	-3.88791	-0.62974	-0.08013
H	0.57104	1.25915	3.79532	C	-4.11602	-1.72005	-0.96900
H	2.35484	-0.72867	1.68395	H	-5.06693	-2.16957	-0.65759
O	2.31694	-2.19208	-1.30902	H	-4.19772	-1.37382	-2.01230
H	1.81287	-2.92648	-1.69753	H	-3.31189	-2.47024	-0.89229
H	-2.24575	-0.71951	-1.95365				
O	-3.65776	-0.50365	0.38467	<b>1b</b>			
C	-4.38850	-0.09011	-0.76580	O	-0.74594	-1.11382	1.14154
H	-5.38040	0.20765	-0.40372	C	-1.82711	-0.76774	0.34582
H	-3.90329	0.76945	-1.25709	C	-2.58431	-1.77013	-0.25224
H	-4.49562	-0.91433	-1.49025	C	-2.18176	0.59291	0.20253
				C	-3.71685	-1.43640	-1.00774
<b>1a</b>				H	-2.27421	-2.80775	-0.11549
O	1.82577	1.78802	0.56132	C	-3.30756	0.92127	-0.56467

C	-4.06813	-0.09361	-1.16253	C	-1.00299	2.21920	0.23873
H	-4.31223	-2.22378	-1.47384	C	-1.41082	2.53097	-1.06575
H	-3.59920	1.96420	-0.69035	H	-0.90023	2.47623	-3.17108
H	-4.94564	0.17973	-1.75268	H	-1.64692	2.47276	1.08090
O	-1.38019	1.48743	0.83552	H	-2.37663	3.01738	-1.21947
C	-1.64993	2.87659	0.65739	O	0.72754	1.30097	1.69731
H	-1.58987	3.15625	-0.40671	C	-0.08657	1.57489	2.83422
H	-2.64269	3.14138	1.05532	H	-0.27718	2.65597	2.93140
H	-0.87393	3.40682	1.22235	H	-1.04419	1.03345	2.77540
C	2.13613	-0.05919	-0.95308	H	0.48280	1.22228	3.70267
C	0.81880	-0.37387	-0.59187	H	2.07722	-0.47459	1.25384
C	0.52772	-0.76015	0.71717	O	1.85243	-1.77918	-1.79901
C	1.54977	-0.84106	1.67237	H	1.41445	-2.56348	-2.16910
C	2.85922	-0.53411	1.31339	H	-2.88791	-0.84420	-1.74789
C	3.16314	-0.13855	-0.00169	O	-3.97797	-0.88091	0.76585
H	0.02585	-0.31621	-1.33983	C	-4.90605	-0.53107	-0.25622
H	1.30539	-1.14456	2.69204	H	-5.86647	-0.36992	0.24901
H	3.66610	-0.59284	2.04657	H	-4.60126	0.39556	-0.77006
H	2.34203	0.24244	-1.98015	H	-5.01245	-1.34237	-0.99523
O	4.47726	0.14686	-0.25904	C	3.86854	-0.94276	0.17632
C	4.82714	0.53637	-1.58236	H	4.00337	-1.94549	0.62089
H	5.90990	0.71308	-1.57056	H	4.20839	-0.98339	-0.87343
H	4.59378	-0.26016	-2.30859	O	4.56669	0.05109	0.91241
H	4.30808	1.46367	-1.87730	H	5.51492	-0.13205	0.81763

**1c**

C	-2.21425	-1.06669	-0.92053
C	-0.85675	-1.28960	-1.17914
C	0.04960	-1.55604	-0.14842
C	-0.44203	-1.63993	1.16636
C	-1.78804	-1.41771	1.44395
C	-2.68115	-1.11233	0.40136
H	-0.49422	-1.23032	-2.20648
H	0.24113	-1.86616	1.98935
H	-2.17023	-1.47143	2.46525
C	1.53766	-1.72602	-0.41532
H	1.86515	-2.65398	0.09046
C	2.38972	-0.60670	0.20784
O	2.27044	0.64609	-0.49701
C	1.04277	1.24879	-0.64299
C	0.63421	1.58555	-1.93419
C	0.23402	1.60007	0.46477
C	-0.58926	2.22900	-2.15399
H	1.28569	1.30151	-2.76268

**2**

C	-2.22496	0.07100	-0.93736
C	-0.97561	-0.46845	-1.24222
C	-0.37597	-1.43030	-0.40874
C	-1.07051	-1.84909	0.74789
C	-2.30230	-1.30610	1.07462
C	-2.88890	-0.33692	0.23316
H	-0.47159	-0.14424	-2.15265
H	-0.61214	-2.60031	1.39374
H	-2.83637	-1.60913	1.97703
C	0.94324	-2.03703	-0.68213
C	1.96127	-1.36438	-1.59827
H	1.84646	-1.80360	-2.60181
O	1.85894	0.04213	-1.81824
C	1.67996	0.96894	-0.82108
C	1.26671	2.23445	-1.25291
C	1.86990	0.74081	0.56222
C	1.02584	3.26704	-0.34187
H	1.12343	2.38209	-2.32529

C	1.60659	1.77365	1.47215	H	5.79840	2.19776	0.53946
C	1.18877	3.03285	1.02556	H	5.50512	2.31745	-1.23270
H	0.70062	4.24402	-0.70517	H	4.75252	3.50381	-0.11376
H	1.73980	1.59274	2.53913	H	-4.09039	-2.40760	-0.15016
H	0.99539	3.82380	1.75309	O	-6.05438	-0.80583	-0.32967
O	2.29631	-0.49977	0.93289	C	-7.10871	0.15375	-0.43278
C	2.16856	-0.88867	2.29769	H	-8.03359	-0.42846	-0.51995
H	2.88792	-0.34619	2.93178	H	-7.15283	0.78750	0.46687
H	1.14413	-0.71287	2.66263	H	-6.98074	0.78333	-1.32725
H	2.39392	-1.96182	2.32355	O	-0.35799	1.99543	0.09540
H	2.95625	-1.63508	-1.21829	C	0.36068	-0.66240	1.95176
O	1.26575	-3.12359	-0.19780	H	-0.60093	-1.13837	2.18913
H	-2.66960	0.80673	-1.60678	H	1.16620	-1.38033	2.16396
O	-4.09038	0.14385	0.62990	H	0.49062	0.22030	2.59524
C	-4.72751	1.13970	-0.17200	H	0.26333	-1.10218	-0.17995
H	-5.66633	1.38028	0.34082				
H	-4.10277	2.04387	-0.24547	<b>3</b>			
H	-4.94464	0.75381	-1.18055	H	-3.33508	1.52761	-0.88627
				C	1.14202	-0.99558	-0.00001
<b>2a</b>				C	-0.24083	-1.15487	-0.00000
C	-3.78774	-1.35967	-0.11714	C	-1.11103	-0.04902	0.00001
C	-2.45301	-1.00274	0.01089	C	-0.54920	1.24638	-0.00007
C	-2.06949	0.35716	0.04845	C	0.82797	1.42302	-0.00015
C	-3.07535	1.33756	-0.05386	C	1.68483	0.30422	-0.00011
C	-4.41763	0.99570	-0.18141	H	-0.67163	-2.15798	0.00003
C	-4.78175	-0.36489	-0.21149	H	-1.19225	2.12802	-0.00001
H	-1.70711	-1.79631	0.07350	H	1.26990	2.42102	-0.00022
H	-2.78337	2.38901	-0.02730	C	-2.57621	-0.28851	-0.00002
H	-5.17140	1.77924	-0.25459	C	-3.50948	0.89753	0.00026
C	-0.66693	0.80868	0.18266	H	-4.54712	0.54077	0.00030
C	0.41128	-0.23587	0.48274	H	-3.33491	1.52718	0.88709
O	1.66025	0.38788	0.18460	O	-3.02709	-1.43752	-0.00021
C	2.76164	-0.39115	-0.03247	H	1.78794	-1.87337	0.00007
C	2.76918	-1.78543	-0.11664	O	3.01213	0.57153	-0.00020
C	3.97576	0.32840	-0.19317	C	3.93195	-0.52149	0.00027
C	3.96924	-2.47206	-0.36606	H	4.93142	-0.07067	0.00038
H	1.84509	-2.34973	0.01128	H	3.80542	-1.14216	0.90137
C	5.16364	-0.36425	-0.44177	H	3.80584	-1.14261	-0.90058
C	5.15920	-1.76620	-0.52804				
H	3.95682	-3.56222	-0.42825	<b>3a</b>			
H	6.09787	0.18333	-0.56808	C	1.07248	-1.35094	-0.31636
H	6.09590	-2.29361	-0.72060	C	-0.28148	-1.05067	-0.38319
O	3.87004	1.68441	-0.09008	C	-0.74041	0.27026	-0.18444
C	5.05751	2.45706	-0.23481	C	0.21144	1.27306	0.08118



C	1.57213	0.98967	0.15040	C	-1.61478	-1.30586	-0.00907
C	2.01039	-0.33398	-0.04934	C	-0.22308	-1.23258	0.00116
H	-0.98600	-1.85622	-0.59547	N	0.37111	-0.02350	-0.02434
H	-0.13853	2.29553	0.23547	H	-2.25178	2.05415	-0.13082
H	2.28264	1.78950	0.35782	H	-2.10253	-2.27817	0.03743
C	-2.17501	0.64757	-0.24240	Rh	2.30818	0.04567	0.01331
C	-3.22719	-0.42759	-0.42825	C	0.57847	2.32387	-0.08217
H	1.43334	-2.36944	-0.47004	C	0.12993	3.64487	-0.12419
O	3.30796	-0.71707	-0.00414	C	1.06636	4.68134	-0.14437
C	4.30624	0.27143	0.25558	C	2.42801	4.37459	-0.12184
H	5.26400	-0.26222	0.24620	C	2.81813	3.03604	-0.07802
H	4.30617	1.04628	-0.52732	N	1.91779	2.04606	-0.05833
H	4.15174	0.73788	1.24140	H	0.73088	5.71900	-0.17773
O	-2.52050	1.82491	-0.10106	H	-0.93895	3.85706	-0.14144
C	-3.53487	-1.14967	0.89300	H	3.18858	5.15591	-0.13690
H	-3.86635	-0.43184	1.65925	H	3.86312	2.72036	-0.05549
H	-4.33790	-1.88704	0.74262	C	3.02612	-2.89981	0.11258
H	-4.13267	0.07592	-0.79661	C	2.73214	-4.26325	0.13942
H	-2.65110	-1.67983	1.27972	C	1.39600	-4.66658	0.12003
H	-2.90739	-1.15614	-1.18858	C	0.38852	-3.69996	0.07437
<b>4</b>				C	0.74157	-2.34977	0.04992
O	0.08192	2.26622	-0.00003	N	2.05782	-1.97710	0.06946
C	0.51809	0.96952	-0.00002	H	1.13487	-5.72579	0.13967
C	1.86798	0.61503	-0.00002	H	4.04597	-2.50990	0.12472
C	-0.47508	-0.04061	-0.00001	H	3.54611	-4.98804	0.17459
C	2.24906	-0.73527	-0.00000	H	-0.66211	-3.98927	0.05785
H	2.61763	1.41139	-0.00002	C	-3.85405	-0.16867	-0.06304
C	-0.08915	-1.38506	0.00000	C	-4.62101	0.89506	0.44848
C	1.27212	-1.73108	0.00001	C	-4.54294	-1.28451	-0.58880
H	3.30949	-0.99626	0.00000	C	-6.01566	0.86045	0.44649
H	-0.84710	-2.16905	0.00001	H	-4.12528	1.76418	0.88498
H	1.55549	-2.78579	0.00002	C	-5.93050	-1.32908	-0.60633
O	-1.76616	0.40494	-0.00002	H	-3.98646	-2.12007	-1.01718
C	-2.80367	-0.56995	0.00006	C	-6.68094	-0.25682	-0.08690
H	-2.75456	-1.20519	0.90004	H	-6.57196	1.69861	0.86531
H	-3.74603	-0.00827	0.00009	H	-6.45939	-2.18593	-1.02747
H	-2.75466	-1.20525	-0.89987	O	-8.03043	-0.38669	-0.14276
H	0.85768	2.85359	-0.00005	C	-8.83799	0.67825	0.35882
				H	-8.65087	1.61117	-0.19660
				H	-9.87731	0.36257	0.20837
				H	-8.65366	0.84223	1.43262
<b>[Rh]-Cl</b>				Cl	2.18551	0.12049	2.37903
C	-0.30525	1.14151	-0.05931	Cl	2.30530	-0.04309	-2.35563
C	-1.69807	1.11818	-0.07701	Cl	4.69200	0.13802	0.07265
C	-2.37908	-0.11891	-0.05005				

				C	6.39520	-0.26796	0.08054
				H	6.28575	1.66908	-0.90809
<b>[Rh]-OH</b>				H	6.17336	-2.17774	1.05923
C	0.02087	1.14695	0.05976	O	7.74573	-0.40079	0.13070
C	1.41401	1.12020	0.07444	C	8.55174	0.65209	-0.39705
C	2.09132	-0.11895	0.06267	H	8.37085	1.59638	0.14111
C	1.32332	-1.30397	0.03693	H	9.59162	0.33741	-0.24800
C	-0.06873	-1.22551	0.02503	H	8.36042	0.79593	-1.47261
N	-0.66651	-0.01522	0.03874				
H	1.97221	2.05454	0.11282	<b>[2Rh]-OH</b>			
H	1.81062	-2.27732	0.00239	C	0.55600	2.01582	1.62627
Rh	-2.60942	0.06339	0.03623	C	0.30758	3.38699	1.71193
C	-0.85845	2.33385	0.05562	C	-1.01328	3.84351	1.62687
C	-0.40774	3.65566	0.05691	C	-2.06738	2.93760	1.48258
C	-1.34078	4.69493	0.03329	C	-1.78034	1.57098	1.40463
C	-2.70441	4.39256	0.00722	N	-0.48595	1.15812	1.44863
C	-3.09647	3.05471	0.00964	H	1.13145	4.08795	1.84060
N	-2.20011	2.05939	0.03532	H	-3.09833	3.28625	1.43079
H	-1.00206	5.73212	0.03370	Rh	-0.12072	-0.71777	1.31330
H	0.66160	3.86626	0.07404	C	1.84539	1.32409	1.73130
H	-3.46172	5.17699	-0.01403	C	3.06818	1.95308	1.98705
H	-4.14221	2.74200	-0.00929	C	4.21548	1.17697	2.13941
C	-3.32322	-2.88506	-0.13211	C	4.11366	-0.21627	2.05210
C	-3.03387	-4.24687	-0.20786	C	2.87451	-0.78714	1.77970
C	-1.69796	-4.65321	-0.18593	N	1.77200	-0.03915	1.59771
C	-0.68958	-3.69059	-0.09978	H	5.17733	1.65298	2.33557
C	-1.03774	-2.33992	-0.03255	H	3.11090	3.03861	2.07130
N	-2.35526	-1.96294	-0.03695	H	4.98445	-0.85956	2.17910
H	-1.43827	-5.71161	-0.24034	H	2.73910	-1.86551	1.69113
H	-4.34325	-2.49653	-0.14445	C	-2.93591	-1.87605	1.18094
H	-3.84831	-4.96823	-0.28176	C	-4.32643	-1.79264	1.21175
H	0.36020	-3.98340	-0.09184	C	-4.92931	-0.53392	1.27451
O	-2.77715	0.11675	-1.99253	C	-4.12173	0.60253	1.32146
H	-3.05260	-0.78671	-2.22471	C	-2.73167	0.45862	1.30131
O	-4.63995	0.16377	0.02476	N	-2.15380	-0.78410	1.21219
H	-4.74390	0.21156	-0.94452	H	-6.01565	-0.43553	1.28800
O	-2.58779	0.02458	2.07412	H	-2.42345	-2.83696	1.13267
H	-3.46839	0.37202	2.29608	H	-4.91828	-2.70765	1.17947
C	3.56734	-0.17231	0.07080	H	-4.56076	1.59766	1.38195
C	4.33485	0.87853	-0.46549	H	-1.22100	4.91267	1.67974
C	4.25667	-1.27893	0.61458	Rh	0.11739	-0.70781	-1.31746
C	5.72985	0.84047	-0.47005	O	0.21662	-2.77138	1.08577
H	3.83902	1.74037	-0.91628	C	1.05528	3.84553	-1.60316
C	5.64465	-1.32742	0.62471	C	-0.27013	3.40283	-1.69049
H	3.70013	-2.10454	1.06201				

C	2.10042	2.92843	-1.46425	C	1.35412	0.93409	-0.49797
C	-0.53236	2.03378	-1.61168	C	1.78990	0.95718	0.83634
H	-1.08683	4.11268	-1.81630	C	3.07023	0.52975	1.18340
C	1.79961	1.56439	-1.39365	C	3.95430	0.07019	0.19221
H	3.13495	3.26620	-1.41146	H	1.90941	0.36937	-2.51096
N	0.50110	1.16511	-1.43818	H	1.11618	1.32643	1.60968
H	1.27360	4.91283	-1.65084	H	3.41005	0.55681	2.22056
C	-1.82843	1.35510	-1.72185	C	-0.02295	1.43693	-0.90046
C	-3.04494	1.99715	-1.97497	C	0.03014	2.58375	-1.92665
C	-4.19937	1.23293	-2.13377	H	-0.98135	2.74957	-2.32286
C	-4.11102	-0.16169	-2.05472	O	0.38927	3.85429	-1.35520
C	-2.87771	-0.74594	-1.78443	C	1.54357	3.93657	-0.60618
N	-1.76826	-0.00962	-1.59710	C	1.44178	4.33385	0.72707
H	-5.15634	1.71926	-2.32842	C	2.81686	3.69056	-1.17332
H	-3.07737	3.08350	-2.05254	C	2.58492	4.45220	1.52683
H	-4.98776	-0.79587	-2.18664	H	0.44349	4.51360	1.12969
H	-2.75286	-1.82608	-1.70199	C	3.95717	3.78582	-0.36418
C	2.92077	-1.89539	-1.18813	C	3.83753	4.16349	0.98074
C	4.31207	-1.82567	-1.22074	H	2.49049	4.75241	2.57245
C	4.92738	-0.57286	-1.28042	H	4.94227	3.57530	-0.78088
C	4.13115	0.57186	-1.32108	H	4.73772	4.23366	1.59536
C	2.73983	0.44170	-1.29866	O	2.83704	3.36558	-2.49449
N	2.14976	-0.79562	-1.21506	C	4.09495	3.06699	-3.09384
H	6.01462	-0.48535	-1.29575	H	4.76136	3.94447	-3.06879
H	2.39859	-2.85112	-1.14044	H	4.58323	2.21724	-2.59058
H	4.89496	-2.74654	-1.19191	H	3.87599	2.80102	-4.13504
H	4.57987	1.56286	-1.37822	H	0.70005	2.32885	-2.76201
O	-0.24370	-2.76007	-1.11260	H	4.17977	-0.37337	-1.92357
C	-0.02318	-3.36011	-0.01448	O	5.19978	-0.30923	0.61440
C	-0.08607	-4.86315	-0.00974	C	6.16661	-0.63921	-0.37835
H	-1.14011	-5.16298	0.11134	H	7.09621	-0.85505	0.16245
H	0.27769	-5.26758	-0.96335	H	5.86716	-1.52735	-0.95617
H	0.49068	-5.27001	0.83034	H	6.32716	0.20845	-1.06539
O	0.20677	-1.10231	-3.40602	H	-0.53354	0.61149	-1.43616
H	1.13231	-1.36046	-3.55342	O	-0.77077	1.82212	0.23131
O	-0.21144	-1.13282	3.39789	C	-1.71503	-1.77026	-0.79952
H	-1.13007	-1.41959	3.53535	C	-0.46221	-2.38083	-0.77594
				C	0.35559	-2.26400	0.36964
				C	-0.15171	-1.54578	1.47591
				C	-1.40842	-0.95415	1.40360
				N	-2.14109	-1.08272	0.27902
				H	-0.12434	-2.93663	-1.64846
				H	0.44834	-1.40622	2.37203
				Rh	-3.89425	-0.24209	0.21680
<b>I-[Rh]-IM1</b>							
O	-3.21892	1.54679	-0.52672				
H	-3.10110	1.40559	-1.48230				
H	-1.75299	1.74911	-0.03642				
C	3.52548	0.01077	-1.14143				
C	2.22987	0.42864	-1.46761				

C	-2.68035	-1.72974	-1.91764	C	-3.08123	-0.69821	0.89456
C	-2.46232	-2.30150	-3.17263	C	-2.03890	-0.56251	-0.03024
C	-3.43366	-2.16080	-4.16629	C	-1.06378	-1.55572	-0.19400
C	-4.60156	-1.44772	-3.88713	C	-1.14593	-2.69685	0.61787
C	-4.76751	-0.90115	-2.61551	C	-2.17974	-2.85934	1.53679
N	-3.83943	-1.04538	-1.65920	C	-3.15688	-1.86033	1.67937
H	-3.27413	-2.60188	-5.15151	H	-1.99264	0.34677	-0.63617
H	-1.53778	-2.84440	-3.36894	H	-0.37805	-3.46406	0.51354
H	-5.37975	-1.31116	-4.63864	H	-2.24459	-3.75130	2.16351
H	-5.65350	-0.33159	-2.32930	C	0.06353	-1.40205	-1.21583
C	-3.97829	1.16946	2.90213	C	-0.47761	-1.33193	-2.66210
C	-3.45397	1.56005	4.13335	H	0.34257	-1.01341	-3.32103
C	-2.19479	1.08683	4.50958	O	-0.87025	-2.60895	-3.20740
C	-1.49315	0.24318	3.64552	C	-1.77285	-3.37490	-2.50740
C	-2.06580	-0.11037	2.42235	C	-1.37771	-4.64735	-2.09369
N	-3.30531	0.35689	2.07639	C	-3.09499	-2.93334	-2.25859
H	-1.75674	1.37386	5.46686	C	-2.26412	-5.48439	-1.40528
H	-4.95469	1.49990	2.54309	H	-0.34644	-4.94469	-2.29172
H	-4.02964	2.22397	4.77900	C	-3.97345	-3.76369	-1.54942
H	-0.50558	-0.13274	3.91230	C	-3.55607	-5.03349	-1.12522
O	-5.75564	0.56557	0.19325	H	-1.93782	-6.47359	-1.07728
H	-5.55836	1.45988	-0.13714	H	-4.98803	-3.42868	-1.33289
O	-4.67774	-1.94623	0.98149	H	-4.25570	-5.66725	-0.57566
H	-5.63210	-1.76453	0.94048	O	-3.42070	-1.69987	-2.73545
C	1.72758	-2.80828	0.39155	C	-4.71620	-1.18625	-2.44102
C	2.46696	-2.88354	1.58813	H	-5.50213	-1.80756	-2.90069
C	2.37961	-3.19797	-0.79947	H	-4.88154	-1.12579	-1.35331
C	3.79879	-3.29408	1.60823	H	-4.74547	-0.17850	-2.87300
H	2.00307	-2.62089	2.53937	H	-1.30379	-0.60826	-2.74680
C	3.70538	-3.60920	-0.79777	H	-3.81843	0.09882	0.99606
H	1.85977	-3.14171	-1.75641	O	-4.13522	-2.09594	2.60992
C	4.43384	-3.64292	0.40531	C	-5.15790	-1.11868	2.76193
H	4.33389	-3.32729	2.55657	H	-5.83783	-1.50651	3.53084
H	4.20812	-3.88369	-1.72670	H	-4.74365	-0.15207	3.09445
O	5.73798	-4.00614	0.30984	H	-5.71422	-0.97242	1.82085
C	6.54372	-3.94604	1.48706	H	0.44916	-0.36073	-1.07120
H	6.19455	-4.66859	2.24184	O	1.05040	-2.36065	-1.07673
H	7.55974	-4.20882	1.16919	C	2.09178	2.04912	-0.29503
H	6.53854	-2.93100	1.91456	C	1.09646	3.01637	-0.42395
				C	-0.08586	2.91040	0.34158
				C	-0.20238	1.83663	1.24931
				C	0.80863	0.88223	1.32271
				N	1.90080	1.00647	0.53986
				H	1.22248	3.83262	-1.13365
<b>I-[Rh]-TS1</b>							
O	3.05722	-1.39304	-2.21738				
H	2.81022	-0.45778	-2.28630				
H	2.20648	-1.82867	-1.75934				

H	-1.07813	1.74336	1.88897	C	0.14444	1.68562	-1.80094
Rh	3.25726	-0.40141	0.63643	C	-0.61038	1.40564	-0.65674
C	3.39447	1.99476	-0.98837	C	0.07872	1.13800	0.53788
C	3.83959	2.95504	-1.89973	C	1.46701	1.16524	0.59425
C	5.09740	2.81022	-2.48735	C	2.21245	1.44258	-0.56504
C	5.88544	1.70848	-2.15043	H	-0.36656	1.88297	-2.74769
C	5.38725	0.78061	-1.23756	H	-0.49142	0.89554	1.43498
N	4.18022	0.91804	-0.67272	H	1.99788	0.95174	1.52375
H	5.45613	3.55383	-3.20062	C	-2.13587	1.40424	-0.69693
H	3.20756	3.80802	-2.14484	C	-2.73105	2.81699	-0.59076
H	6.87401	1.55817	-2.58501	H	-3.82192	2.73175	-0.69284
H	5.96248	-0.09927	-0.94717	O	-2.55991	3.46849	0.68188
C	1.98419	-2.31811	2.63082	C	-1.31144	3.79856	1.15283
C	1.03142	-2.68832	3.57968	C	-1.04834	3.50688	2.49448
C	-0.04132	-1.83079	3.83085	C	-0.32639	4.46708	0.38255
C	-0.14438	-0.63773	3.11427	C	0.18635	3.81562	3.07483
C	0.82871	-0.32840	2.16372	H	-1.82974	2.99804	3.06272
N	1.89137	-1.16679	1.95405	C	0.91911	4.74938	0.96075
H	-0.80082	-2.09057	4.56941	C	1.17585	4.42353	2.29913
H	2.85152	-2.93816	2.39943	H	0.37388	3.56528	4.12107
H	1.14105	-3.63483	4.10948	H	1.69242	5.23877	0.36852
H	-0.98049	0.04155	3.27575	H	2.15268	4.65719	2.72807
O	4.55569	-1.91043	0.85008	O	-0.65485	4.79398	-0.89895
H	5.34637	-1.71897	0.32016	C	0.35498	5.35252	-1.73410
O	4.06900	0.53653	2.14432	H	0.68446	6.33381	-1.35564
H	4.70129	-0.15174	2.43043	H	1.22118	4.67605	-1.81452
C	-1.18374	3.88382	0.18676	H	-0.10742	5.47670	-2.72087
C	-2.51552	3.51556	0.45722	H	-2.33964	3.44540	-1.40154
C	-0.94123	5.20409	-0.25283	H	2.10306	1.90902	-2.68687
C	-3.57097	4.41416	0.29783	O	3.57212	1.41492	-0.42384
H	-2.74700	2.49703	0.77461	C	4.37288	1.49904	-1.59698
C	-1.98037	6.11208	-0.40694	H	5.41117	1.37338	-1.26540
H	0.07945	5.53473	-0.45417	H	4.11571	0.69907	-2.31049
C	-3.30663	5.72479	-0.13494	H	4.26118	2.47947	-2.08916
H	-4.58897	4.08445	0.50364	H	-2.42606	1.11567	-1.72865
H	-1.78814	7.13587	-0.73292	O	-2.71326	0.57066	0.26425
O	-4.25842	6.67507	-0.31741	C	-0.17627	-1.67891	-1.21402
C	-5.61784	6.33785	-0.04231	C	1.21105	-1.79168	-1.21798
H	-5.74799	6.05123	1.01360	C	1.90025	-1.98117	-0.00039
H	-6.19942	7.24355	-0.25205	C	1.14661	-2.10804	1.18559
H	-5.96216	5.51913	-0.69427	C	-0.23996	-1.96663	1.13887
				N	-0.84615	-1.74825	-0.04473
<b>I-[Rh]-IM2</b>				H	1.75872	-1.67522	-2.15165
C	1.54675	1.70396	-1.77191	H	1.64039	-2.28376	2.14006

Rh	-2.77018	-1.45246	-0.06881	C	3.83085	-2.93799	0.93346
C	-1.06073	-1.42370	-2.36884	C	2.66215	-2.21546	1.20163
C	-0.62294	-1.29434	-3.68864	C	2.69607	-0.87244	1.59318
C	-1.55457	-1.03808	-4.69622	C	3.95358	-0.25745	1.72177
C	-2.90644	-0.91634	-4.36521	C	5.13127	-0.95193	1.44230
C	-3.28573	-1.04849	-3.03091	C	5.07444	-2.29719	1.03803
N	-2.38943	-1.29304	-2.06419	H	1.68771	-2.69075	1.06819
H	-1.22449	-0.93344	-5.73095	H	4.01084	0.79517	2.01307
H	0.43760	-1.38854	-3.92014	H	6.10686	-0.46565	1.51490
H	-3.66341	-0.71586	-5.12389	C	1.37747	-0.11197	1.80911
H	-4.32002	-0.94541	-2.69815	C	1.04191	-0.12971	3.31282
C	-3.43045	-1.62853	2.89024	H	1.89706	0.19051	3.92683
C	-3.12358	-1.79421	4.24029	O	0.01106	0.82352	3.65944
C	-1.79929	-2.05053	4.60272	C	-1.21198	0.85238	3.04030
C	-0.81911	-2.12784	3.61074	C	-1.70369	2.11227	2.67933
C	-1.18415	-1.94997	2.27446	C	-2.03809	-0.28457	2.85257
N	-2.49019	-1.70872	1.93962	C	-2.98523	2.26400	2.13337
H	-1.52677	-2.18613	5.65060	H	-1.04789	2.97378	2.82432
H	-4.44263	-1.42685	2.53430	C	-3.29705	-0.13342	2.26040
H	-3.91525	-1.72159	4.98668	C	-3.77914	1.13746	1.91375
H	0.22240	-2.31909	3.86909	H	-3.34484	3.25942	1.86587
O	-4.78332	-1.16708	-0.10716	H	-3.91705	-1.01348	2.08328
H	-4.78435	-0.19836	0.00240	H	-4.77126	1.23156	1.46691
O	-3.06203	-3.45240	-0.26683	O	-1.55002	-1.49143	3.26861
H	-3.60448	-3.52592	-1.07034	C	-1.96278	-2.64659	2.54043
C	3.37521	-1.94958	0.02512	H	-3.01842	-2.89749	2.73294
C	4.06607	-1.49492	1.16356	H	-1.80434	-2.49390	1.46139
C	4.13698	-2.28164	-1.11676	H	-1.32899	-3.47052	2.89277
C	5.45443	-1.35630	1.17202	H	0.74118	-1.14688	3.60666
H	3.51238	-1.19821	2.05600	H	3.76095	-3.97850	0.61496
C	5.52018	-2.15875	-1.12073	O	6.27395	-2.89399	0.74692
H	3.64150	-2.65662	-2.01392	C	6.25465	-4.24814	0.30956
C	6.19161	-1.68459	0.02201	H	7.30100	-4.52285	0.12596
H	5.94829	-0.97773	2.06651	H	5.83242	-4.91303	1.08144
H	6.10540	-2.42299	-2.00332	H	5.67781	-4.36009	-0.62363
O	7.54175	-1.57462	-0.07691	O	0.35393	-0.58712	1.04612
C	8.26924	-1.10373	1.05699	H	1.62946	0.96903	1.59014
H	8.13339	-1.77432	1.92063	C	-3.74858	-0.98411	-1.31156
H	9.32388	-1.10055	0.75650	C	-4.93978	-0.25388	-1.47668
H	7.96009	-0.08165	1.32883	C	-3.85405	-2.34149	-0.93450
				C	-6.19142	-0.83832	-1.27831
				H	-4.89986	0.79225	-1.78597
<b>I-[Rh]-TS2</b>				C	-5.09205	-2.93420	-0.72307
O	3.58032	2.32767	-0.39816	H	-2.95289	-2.93383	-0.76669
H	4.23306	1.61000	-0.34370				







H	1.49132	1.31453	0.49822	N	0.73160	0.07390	-0.74925
C	4.37485	-3.14660	1.01687	H	-1.88673	-2.00773	-1.01639
C	3.62251	-2.56900	2.04052	H	-1.76308	2.31402	-0.70737
C	3.58682	-1.17950	2.24073	Rh	2.65206	-0.00219	-0.42671
C	4.35510	-0.36673	1.37853	C	0.93942	-2.27126	-0.84574
C	5.11973	-0.92498	0.36233	C	0.48967	-3.58673	-0.97525
C	5.12681	-2.31913	0.16575	C	1.40768	-4.63354	-0.88117
H	3.02581	-3.20409	2.69773	C	2.75572	-4.34261	-0.65906
H	4.34258	0.71928	1.48077	C	3.14692	-3.00903	-0.54874
H	5.70516	-0.29643	-0.31105	N	2.26706	-2.00361	-0.64775
C	2.67668	-0.63019	3.28858	H	1.07031	-5.66701	-0.97423
C	2.57199	0.79104	3.43746	H	-0.57005	-3.78483	-1.13352
H	3.35500	1.46622	3.09866	H	3.50258	-5.13203	-0.56997
O	1.49413	1.11876	1.67052	H	4.18407	-2.72368	-0.36734
C	0.17653	0.84651	2.00234	C	3.32073	2.95023	-0.12064
C	-0.63649	1.83008	2.56669	C	3.01620	4.31076	-0.08304
C	-0.33403	-0.45220	1.76798	C	1.69285	4.71032	-0.27931
C	-1.95674	1.53445	2.92387	C	0.71156	3.74186	-0.50180
H	-0.21525	2.82631	2.71631	C	1.07458	2.39405	-0.52063
C	-1.65156	-0.75105	2.14096	N	2.37875	2.02261	-0.33230
C	-2.45403	0.24420	2.71236	H	1.42261	5.76727	-0.25980
H	-2.59110	2.30783	3.36105	H	4.33518	2.57348	0.01882
H	-2.06215	-1.74596	1.96863	H	3.81087	5.03594	0.09449
H	-3.48330	0.00177	2.98597	H	-0.32887	4.02749	-0.65479
O	0.51121	-1.31842	1.16045	O	4.64593	0.00236	-0.06772
C	0.14940	-2.69421	1.10398	H	5.02526	-0.69422	-0.62996
H	-0.00496	-3.09056	2.12023	O	3.07441	0.16031	-2.39030
H	-0.76137	-2.84508	0.50298	H	4.04750	0.15751	-2.33631
H	0.99252	-3.20769	0.62830	O	2.35502	-0.20635	1.64786
H	1.87623	1.16536	4.19019	C	1.16188	-0.66637	2.03362
H	4.36652	-4.22834	0.88437	C	0.88681	-2.04062	2.17008
O	5.87407	-2.77265	-0.87464	C	0.09872	0.24462	2.32600
C	5.83948	-4.16684	-1.17674	C	-0.39213	-2.50782	2.50525
H	6.47136	-4.29778	-2.06332	H	1.70153	-2.74273	1.97656
H	6.24538	-4.76235	-0.34342	C	-1.17924	-0.21865	2.65125
H	4.81220	-4.49574	-1.40197	C	-1.42962	-1.59972	2.72618
O	1.95128	-1.40612	3.96706	H	-0.57337	-3.58293	2.57876
				H	-1.98865	0.48759	2.84020
				H	-2.43475	-1.95003	2.97183
				O	0.43688	1.56642	2.24610
				C	-0.56631	2.53337	2.52214
				H	-0.95141	2.42275	3.54953
				H	-0.08350	3.51250	2.41649
				H	-1.40508	2.45688	1.81010
<b>I-[Rh]-IM4</b>							
C	0.05571	-1.08916	-0.86379				
C	-1.33540	-1.07337	-0.92410				
C	-2.01991	0.15952	-0.85428				
C	-1.26458	1.34841	-0.77610				
C	0.12656	1.27873	-0.71235				

C	-3.49433	0.20168	-0.81179	H	3.79031	5.07453	-0.15837
C	-4.22362	-0.84320	-0.21462	H	-0.36313	3.92954	-0.55525
C	-4.21483	1.29932	-1.33118	O	4.76945	0.17670	-0.44628
C	-5.61639	-0.80739	-0.12924	H	5.17254	-0.68427	-0.64731
H	-3.69567	-1.69139	0.22618	O	2.76655	0.11626	-2.51845
C	-5.60135	1.34360	-1.26252	H	3.70452	0.33551	-2.67670
H	-3.68395	2.12011	-1.81759	O	3.70157	-0.72867	1.88546
C	-6.31512	0.29147	-0.65746	H	4.27463	-0.25750	1.23222
H	-6.14356	-1.62814	0.35641	H	2.91868	-0.11526	2.08970
H	-6.15789	2.18624	-1.67684	O	1.56180	0.69398	2.30537
O	-7.66660	0.42368	-0.62679	C	0.50127	-0.06541	2.37224
C	-8.43722	-0.61433	-0.02236	C	0.53888	-1.48368	2.43072
H	-8.17600	-0.73232	1.04162	C	-0.81208	0.52823	2.36684
H	-9.48438	-0.30093	-0.11096	C	-0.62749	-2.25978	2.48776
H	-8.29247	-1.57184	-0.54795	H	1.51928	-1.96548	2.42184
				C	-1.96907	-0.24469	2.43415
				C	-1.88400	-1.65115	2.48722
<b>I-[Rh]-TS4</b>				H	-0.54414	-3.34988	2.52399
C	0.14483	-1.16762	-0.75501	H	-2.95011	0.23323	2.42373
C	-1.24460	-1.17768	-0.85664	H	-2.79860	-2.24665	2.53379
C	-1.94894	0.04571	-0.87920	O	-0.80413	1.90190	2.27863
C	-1.21095	1.24671	-0.83371	C	-2.05673	2.56404	2.21826
C	0.17696	1.20220	-0.71587	H	-2.62996	2.42351	3.15110
N	0.79907	0.00763	-0.67955	H	-1.83592	3.63098	2.08426
H	-1.77612	-2.12466	-0.92799	H	-2.66527	2.20742	1.36969
H	-1.71987	2.20874	-0.84415	C	-3.42382	0.06899	-0.90797
Rh	2.75267	0.00097	-0.56248	C	-4.17077	-1.01168	-0.40266
C	1.04968	-2.33247	-0.71240	C	-4.13399	1.18563	-1.40151
C	0.61453	-3.65954	-0.69628	C	-5.56578	-0.99193	-0.37812
C	1.55684	-4.68607	-0.62117	H	-3.65794	-1.87994	0.01402
C	2.91479	-4.36452	-0.56709	C	-5.52227	1.21635	-1.39253
C	3.28901	-3.02229	-0.59150	H	-3.59385	2.03661	-1.81995
N	2.38466	-2.03639	-0.66783	C	-6.25220	0.12839	-0.87650
H	1.23085	-5.72711	-0.60078	H	-6.10488	-1.84334	0.03652
H	-0.45173	-3.88106	-0.72698	H	-6.06761	2.07612	-1.78591
H	3.68251	-5.13610	-0.50356	O	-7.60445	0.24801	-0.89950
H	4.33566	-2.71978	-0.54708	C	-8.39053	-0.82769	-0.38765
C	3.35337	2.97491	-0.34709	H	-8.17537	-1.00191	0.67884
C	3.00826	4.32405	-0.27616	H	-9.43586	-0.51802	-0.50575
C	1.65989	4.67835	-0.35313	H	-8.21288	-1.75368	-0.95764
C	0.69601	3.67941	-0.50292				
C	1.09956	2.34484	-0.57399				
N	2.42639	2.01946	-0.49007	<b>II-[Rh]-IM1</b>			
H	1.35626	5.72474	-0.29480	C	5.13967	-0.84915	-0.13685
H	4.38661	2.63027	-0.28389	C	5.43366	-2.06526	0.50768

C	6.21111	0.02952	-0.41050	H	-1.16508	0.99143	-3.78011
C	6.73823	-2.40506	0.86938	H	-2.90635	1.77948	-1.42949
H	4.62718	-2.75658	0.76054	O	-3.33898	3.01344	-0.50535
C	7.51521	-0.29934	-0.06511	H	-4.29228	2.84291	-0.42532
H	6.02446	0.97318	-0.92689	H	-3.00936	0.32533	3.44737
C	7.79099	-1.52054	0.57909	C	-6.59075	-1.56135	2.37942
H	6.92289	-3.35003	1.37979	C	-5.44187	-0.78512	2.53546
H	8.34371	0.37383	-0.29266	C	-4.72836	-0.32300	1.41992
O	9.09334	-1.75803	0.88052	C	-5.20660	-0.64683	0.14111
C	9.43010	-2.98909	1.51901	C	-6.35589	-1.42342	-0.03400
H	10.51760	-2.96678	1.65841	C	-7.05261	-1.88922	1.09397
H	8.93433	-3.07552	2.49916	H	-5.10078	-0.52699	3.54034
H	9.15635	-3.84972	0.88783	H	-4.66796	-0.27702	-0.73637
C	2.01488	1.15049	-0.86472	H	-6.70051	-1.65300	-1.04240
C	3.33567	0.84791	-0.53747	C	-3.46179	0.50650	1.55344
C	3.75382	-0.49938	-0.50427	C	-2.25701	-0.32342	1.11079
C	2.81121	-1.50623	-0.80586	H	-2.52387	-0.97542	0.27511
C	1.49847	-1.15129	-1.10793	O	-1.17066	0.48953	0.60098
N	1.15136	0.15156	-1.13135	C	-0.43100	1.26399	1.48876
H	4.03022	1.64723	-0.28420	C	-0.75110	2.60673	1.66957
H	3.10557	-2.55445	-0.80815	C	0.69359	0.67989	2.10516
Rh	-0.71663	0.60798	-1.52117	C	0.07919	3.41001	2.45786
C	1.38955	2.48650	-0.94310	H	-1.63938	2.99760	1.16481
C	2.06865	3.67907	-0.69210	C	1.51940	1.49319	2.89688
C	1.38041	4.89096	-0.78887	C	1.21152	2.84936	3.05895
C	0.02783	4.87950	-1.12725	H	-0.15432	4.46758	2.59370
C	-0.60653	3.65707	-1.35721	H	2.40447	1.07571	3.37679
N	0.05791	2.49642	-1.27082	H	1.87043	3.47060	3.66966
H	1.89938	5.83067	-0.59314	O	0.89845	-0.63925	1.86638
H	3.12403	3.65751	-0.42254	C	2.01033	-1.27639	2.49506
H	-0.54924	5.80197	-1.19859	H	2.95803	-0.79435	2.21183
H	-1.68399	3.58144	-1.53729	H	1.89753	-1.26079	3.59096
C	-1.91211	-2.15761	-1.96773	H	2.00236	-2.31218	2.13639
C	-1.87844	-3.55038	-2.01582	H	-1.87104	-0.93988	1.93887
C	-0.67464	-4.20314	-1.74336	H	-7.14784	-1.92290	3.24637
C	0.46144	-3.44910	-1.44140	O	-8.18316	-2.65523	1.03418
C	0.36999	-2.05580	-1.41089	C	-8.68346	-3.01355	-0.25025
N	-0.82381	-1.43640	-1.66691	H	-9.57806	-3.62167	-0.06725
H	-0.61506	-5.29235	-1.76815	H	-8.96054	-2.12070	-0.83471
H	-2.81927	-1.58454	-2.16778	H	-7.94567	-3.60723	-0.81507
H	-2.78554	-4.10321	-2.26166	O	-3.27993	1.04916	2.85615
H	1.41282	-3.93729	-1.23119	H	-3.52618	1.37229	0.86682
O	-2.62068	0.98235	-2.00625				
O	-0.29282	0.70942	-3.44494				

**II-[Rh]-TS1**

C	5.15819	-0.43588	-0.19104	O	-2.71020	1.19320	-1.79176
C	5.49957	-1.72452	0.26045	O	-0.41968	1.35082	-3.34835
C	6.17605	0.54281	-0.22619	H	-1.30952	1.66329	-3.59631
C	6.79744	-2.03781	0.66738	H	-3.00701	1.67833	-0.97870
H	4.73263	-2.49894	0.32990	O	-3.48687	2.46260	0.56609
C	7.47394	0.24271	0.16532	H	-4.44546	2.54481	0.43038
H	5.95552	1.54830	-0.58991	H	-2.90212	-0.73525	3.49167
C	7.79659	-1.05059	0.61915	C	-6.86515	-1.23128	2.36994
H	7.01624	-3.04305	1.02678	C	-5.56326	-0.77593	2.58717
H	8.26204	0.99674	0.12334	C	-4.68960	-0.47289	1.51492
O	9.08761	-1.25004	0.98824	C	-5.21879	-0.62820	0.20956
C	9.47208	-2.54314	1.45413	C	-6.51878	-1.08816	-0.01921
H	10.54083	-2.47125	1.68900	C	-7.35439	-1.40024	1.06631
H	8.91249	-2.81893	2.36234	H	-5.20679	-0.64446	3.61104
H	9.31574	-3.30684	0.67553	H	-4.60013	-0.35668	-0.65026
C	1.93407	1.45788	-0.72609	H	-6.87279	-1.19000	-1.04619
C	3.26148	1.19007	-0.40224	C	-3.33086	0.06627	1.73717
C	3.77391	-0.11268	-0.58712	C	-2.27928	-0.64328	0.96025
C	2.92437	-1.10222	-1.12712	H	-2.64436	-1.01050	-0.00318
C	1.59669	-0.78774	-1.41448	O	-1.13616	0.25636	0.58006
N	1.15300	0.46643	-1.20365	C	-0.12915	0.43990	1.50989
H	3.88409	1.97193	0.02945	C	0.02685	1.68429	2.11563
H	3.29745	-2.10810	-1.31361	C	0.78478	-0.60838	1.76481
Rh	-0.75495	0.83203	-1.46760	C	1.12113	1.92134	2.95639
C	1.21161	2.73643	-0.56967	H	-0.70814	2.46145	1.90231
C	1.80359	3.92206	-0.13141	C	1.87550	-0.36645	2.61080
C	1.01960	5.07031	-0.00525	C	2.04352	0.89827	3.19014
C	-0.33688	5.01017	-0.32826	H	1.25066	2.90237	3.41686
C	-0.87285	3.79933	-0.76570	H	2.60387	-1.15372	2.80465
N	-0.12225	2.69544	-0.87549	H	2.90659	1.07451	3.83573
H	1.46822	6.00246	0.34163	O	0.53886	-1.78752	1.14078
H	2.86525	3.94277	0.11189	C	1.41427	-2.88395	1.39373
H	-0.98338	5.88398	-0.24321	H	2.44601	-2.64696	1.08955
H	-1.92779	3.68514	-1.01301	H	1.39688	-3.15697	2.46063
C	-1.74527	-1.88938	-2.41296	H	1.03248	-3.71642	0.79150
C	-1.60068	-3.23992	-2.72843	H	-1.80352	-1.47341	1.51048
C	-0.33831	-3.82538	-2.61742	H	-7.52168	-1.46552	3.21201
C	0.74306	-3.04686	-2.19900	O	-8.64837	-1.86096	0.94569
C	0.53828	-1.70035	-1.89460	C	-9.15987	-2.05013	-0.36562
N	-0.70852	-1.14551	-2.00570	H	-10.18439	-2.42503	-0.24398
H	-0.19188	-4.88014	-2.85528	H	-9.18466	-1.10298	-0.93147
H	-2.70418	-1.37357	-2.48264	H	-8.56601	-2.79107	-0.92816
H	-2.46935	-3.81248	-3.05445	O	-2.96588	0.16922	3.12650
H	1.73819	-3.47987	-2.10309	H	-3.41026	1.46168	1.11677

<b>I-[Rh]-TS3'</b>							
O	4.93580	-0.97615	-1.33464	C	-4.03302	-2.27884	-3.04482
H	4.42513	-1.49736	-1.97661	H	-2.10873	-1.65271	-3.74682
H	2.39332	0.55495	0.94349	C	-4.15942	-3.01136	-0.73042
C	-2.82513	2.53777	2.72106	H	-2.32954	-2.92211	0.38039
C	-1.52612	2.02355	2.72337	C	-4.78948	-2.76693	-1.96246
C	-1.29132	0.63942	2.66396	H	-4.53381	-2.10184	-3.99841
C	-2.40337	-0.23033	2.65939	H	-4.72292	-3.37602	0.12815
C	-3.69691	0.26439	2.64809	O	-6.11282	-2.96724	-2.19740
C	-3.91589	1.65804	2.65029	C	-6.92703	-3.44435	-1.12736
H	-0.69433	2.72726	2.76345	H	-7.94233	-3.52280	-1.53439
H	-2.22649	-1.30619	2.62100	H	-6.58981	-4.43558	-0.78401
H	-4.55991	-0.40277	2.60438	H	-6.92190	-2.73808	-0.28143
C	0.05587	0.03466	2.52159	C	1.46104	-2.10958	-0.20846
C	1.24421	0.87795	2.29712	C	0.18148	-2.58004	-0.49802
H	2.16014	0.44386	2.70013	C	-0.60332	-1.91568	-1.46290
H	1.18568	1.96534	2.32645	C	-0.03704	-0.82643	-2.15586
H	-2.97323	3.61666	2.74868	C	1.23203	-0.37301	-1.80363
O	-5.21128	2.05742	2.56872	N	1.93949	-1.02556	-0.85620
C	-5.48515	3.45670	2.49999	H	-0.21965	-3.42963	0.05281
H	-6.57395	3.54512	2.40387	H	-0.63171	-0.26467	-2.87444
H	-5.15245	3.97081	3.41583	Rh	3.47559	-0.11704	-0.07387
H	-4.99766	3.90955	1.62170	C	2.36625	-2.59209	0.85304
O	0.20681	-1.19995	2.58486	C	2.18288	-3.77228	1.57604
O	0.32867	0.91391	0.35533	C	3.08341	-4.09750	2.59193
C	-0.19272	2.05689	-0.00136	C	4.14813	-3.23472	2.86434
C	0.56079	3.25861	-0.02242	C	4.28726	-2.07584	2.10251
C	-1.55905	2.11450	-0.44905	N	3.42429	-1.76663	1.12367
C	0.00786	4.45623	-0.47023	H	2.95162	-5.01597	3.16616
H	1.59659	3.21054	0.32019	H	1.34120	-4.42493	1.34513
C	-2.09856	3.31847	-0.91708	H	4.86857	-3.45034	3.65400
C	-1.32057	4.48437	-0.91961	H	5.09778	-1.36198	2.25907
H	0.60956	5.36782	-0.47639	C	3.54666	2.44825	-1.72163
H	-3.12995	3.35803	-1.26893	C	3.07899	3.32873	-2.69533
H	-1.76065	5.41794	-1.27718	C	1.95812	2.96969	-3.44722
O	-2.23200	0.94043	-0.41837	C	1.33845	1.74363	-3.20072
C	-3.58120	0.91096	-0.87746	C	1.85266	0.90083	-2.21247
H	-4.21131	1.60997	-0.30525	N	2.95697	1.26555	-1.48806
H	-3.63458	1.15454	-1.95074	H	1.56331	3.63868	-4.21339
H	-3.93194	-0.11444	-0.71368	H	4.40808	2.68293	-1.09455
C	-2.02300	-2.26597	-1.66358	H	3.58851	4.28044	-2.84903
C	-2.67529	-2.02807	-2.89228	H	0.45662	1.44247	-3.76560
C	-2.79221	-2.76292	-0.59549	O	4.97400	0.87399	0.88963
				H	5.53866	1.22809	0.18237

<b>I-[Rh]-TS3-Cl</b>				H	1.34683	4.54620	-0.73578
O	2.91611	2.45137	-1.09702	H	-0.31130	6.37087	-0.24652
H	3.53723	1.81068	-0.71174	H	-3.42159	3.36494	-0.31758
C	-4.22226	-1.51437	-0.57428	H	1.47118	1.24913	0.49689
C	-5.46952	-0.88634	-0.74751	C	4.40987	-3.33713	1.15603
C	-4.21755	-2.85249	-0.12142	C	3.58535	-2.69592	2.08082
C	-6.66880	-1.55208	-0.48912	C	3.62789	-1.30500	2.27406
H	-5.51563	0.14089	-1.11423	C	4.53732	-0.55675	1.49377
C	-5.40251	-3.52628	0.14588	C	5.37626	-1.18079	0.57900
H	-3.27077	-3.36809	0.05000	C	5.31712	-2.57580	0.40054
C	-6.64073	-2.88223	-0.03698	H	2.87929	-3.27996	2.67381
H	-7.61349	-1.03255	-0.64794	H	4.59231	0.52851	1.59099
H	-5.39347	-4.55564	0.50880	H	6.07542	-0.60301	-0.02826
O	-7.74765	-3.61671	0.24749	C	2.69099	-0.69783	3.26544
C	-9.02758	-3.00529	0.09182	C	2.63310	0.72158	3.39520
H	-9.19724	-2.70226	-0.95392	H	3.40261	1.38278	3.00259
H	-9.76137	-3.76884	0.37670	H	1.92307	1.13713	4.11209
H	-9.13059	-2.12955	0.75271	H	4.34063	-4.41697	1.02686
C	-0.58304	-0.79044	-1.31737	O	6.15172	-3.09651	-0.53729
C	-1.77929	-1.48904	-1.16361	C	6.07959	-4.49697	-0.80335
C	-2.95911	-0.79382	-0.82725	H	6.80650	-4.68836	-1.60171
C	-2.89009	0.60810	-0.67942	H	6.34896	-5.08292	0.08997
C	-1.67596	1.26530	-0.86014	H	5.07162	-4.78322	-1.14420
N	-0.56837	0.55433	-1.17541	O	1.90560	-1.43913	3.91927
H	-1.79154	-2.57118	-1.28701	O	1.47733	0.92943	1.56008
H	-3.77030	1.17415	-0.37865	C	0.16813	0.70242	1.94550
Rh	1.13600	1.47998	-1.25818	C	-0.59610	1.78755	2.43291
C	0.75307	-1.34939	-1.59003	C	-0.38215	-0.57754	1.87524
C	1.00666	-2.70085	-1.83473	C	-1.91935	1.56460	2.83811
C	2.31120	-3.11509	-2.11011	C	-1.70373	-0.79705	2.27841
C	3.33439	-2.16563	-2.13927	C	-2.46369	0.27579	2.75320
C	3.02631	-0.83428	-1.86662	H	-2.52857	2.38712	3.21279
N	1.77592	-0.43407	-1.59199	H	-2.13924	-1.79545	2.20805
H	2.52247	-4.16730	-2.30719	H	-3.49957	0.11726	3.06127
H	0.18467	-3.41632	-1.82013	H	0.23960	-1.38714	1.49019
H	4.36548	-2.44384	-2.35447	O	0.03776	2.98707	2.47234
H	3.78885	-0.05479	-1.86916	C	-0.65752	4.09687	3.03889
C	0.27917	4.34050	-0.64486	H	0.02280	4.95223	2.95231
C	-0.64975	5.34180	-0.37045	H	-1.58652	4.30896	2.48896
C	-1.99921	4.99803	-0.25500	H	-0.88824	3.90979	4.10009
C	-2.37762	3.66385	-0.40963	Cl	0.94412	1.89270	-3.68128
C	-1.40220	2.70340	-0.68907				
N	-0.08444	3.05986	-0.81022	<b>I-[Rh]-TS3-2Cl</b>			
H	-2.75088	5.75887	-0.03960	C	-4.29344	-1.49503	-0.60820

C	-5.53979	-0.86393	-0.77706	C	4.25601	-3.66047	1.02655
C	-4.29007	-2.84903	-0.20502	C	3.44542	-3.01544	1.96054
C	-6.74030	-1.54261	-0.56294	C	3.54214	-1.63393	2.19856
H	-5.58371	0.17573	-1.10703	C	4.49358	-0.89977	1.45589
C	-5.47637	-3.53521	0.01993	C	5.32102	-1.52945	0.53492
H	-3.34372	-3.36702	-0.03819	C	5.20553	-2.91369	0.30897
C	-6.71395	-2.88847	-0.15910	H	2.70696	-3.58787	2.52465
H	-7.68447	-1.02113	-0.71860	H	4.58698	0.17958	1.58211
H	-5.46959	-4.57692	0.34560	H	6.05101	-0.96167	-0.04486
O	-7.82166	-3.63644	0.08071	C	2.62294	-1.02161	3.20188
C	-9.10214	-3.02553	-0.07372	C	2.61794	0.39428	3.37381
H	-9.25550	-2.68448	-1.11016	H	3.40432	1.03978	2.98873
H	-9.83637	-3.80285	0.16964	H	1.92845	0.81459	4.10758
H	-9.22084	-2.17573	0.61761	H	4.14323	-4.73156	0.86039
C	-0.65040	-0.74401	-1.29506	O	6.02691	-3.43638	-0.63931
C	-1.84868	-1.44569	-1.18040	C	5.89390	-4.82064	-0.96138
C	-3.02888	-0.76435	-0.81751	H	6.62246	-5.01454	-1.75762
C	-2.96062	0.62975	-0.60847	H	6.12317	-5.45320	-0.08898
C	-1.74519	1.29381	-0.75033	H	4.87857	-5.04502	-1.32595
N	-0.63723	0.59141	-1.08338	O	1.81109	-1.75239	3.83606
H	-1.86241	-2.52031	-1.35736	O	1.42749	0.72947	1.57184
H	-3.84350	1.18434	-0.29496	C	0.11418	0.57140	1.97869
Rh	1.05306	1.52547	-1.16406	C	-0.57677	1.68911	2.49888
C	0.68623	-1.28930	-1.59018	C	-0.50441	-0.67563	1.90317
C	0.94802	-2.63057	-1.87459	C	-1.90396	1.53494	2.92216
C	2.25785	-3.02702	-2.15385	C	-1.82841	-0.82757	2.32974
C	3.27628	-2.07245	-2.14024	C	-2.52005	0.27931	2.83017
C	2.96041	-0.75113	-1.82723	H	-2.45987	2.38397	3.31972
N	1.70271	-0.36889	-1.56144	H	-2.31930	-1.79964	2.25508
H	2.47732	-4.07121	-2.38202	H	-3.55767	0.17402	3.15458
H	0.13117	-3.35197	-1.88409	H	0.06432	-1.51229	1.49534
H	4.31041	-2.34259	-2.35182	O	0.12934	2.84669	2.54683
H	3.71091	0.03949	-1.77722	C	-0.49505	3.99256	3.12476
C	0.20480	4.36755	-0.48316	H	0.23082	4.80866	3.03036
C	-0.72677	5.36256	-0.19416	H	-1.41790	4.25650	2.58742
C	-2.07474	5.01432	-0.07671	H	-0.72152	3.81557	4.18857
C	-2.45149	3.68106	-0.24535	Cl	0.79035	2.01414	-3.55720
C	-1.47471	2.72717	-0.54065	Cl	3.17918	2.58884	-0.90627
N	-0.15831	3.08824	-0.66031				
H	-2.82736	5.77092	0.14994				
H	1.27348	4.56855	-0.57917	<b>I-[Rh]-TS3a</b>			
H	-0.39063	6.39118	-0.06042	O	-3.30067	0.80012	1.89094
H	-3.49473	3.37950	-0.15494	H	-3.94288	0.29597	1.36433
H	1.44013	1.26608	0.62459	C	4.35337	-1.56306	0.11893
				C	5.46485	-0.86691	0.62864

C	4.59903	-2.64896	-0.75023	H	-1.55907	0.92352	-0.60785
C	6.77184	-1.23074	0.30048	C	-5.13601	-1.93725	-1.66456
H	5.31542	-0.03341	1.31778	C	-3.77796	-1.61951	-1.55848
C	5.89379	-3.01845	-1.09190	C	-3.34360	-0.35509	-1.12834
H	3.76255	-3.19761	-1.18735	C	-4.32695	0.61199	-0.82580
C	6.99342	-2.31334	-0.56745	C	-5.68128	0.31253	-0.93032
H	7.60546	-0.67343	0.72716	C	-6.09768	-0.96813	-1.34252
H	6.07905	-3.84961	-1.77478	H	-3.02538	-2.37216	-1.79989
O	8.22295	-2.74448	-0.95269	H	-4.02777	1.60960	-0.50155
C	9.36985	-2.05624	-0.45571	H	-6.44072	1.06213	-0.69880
H	9.42381	-2.11810	0.64314	C	-1.87559	-0.15398	-0.96940
H	10.23758	-2.56308	-0.89485	C	-1.68191	1.82323	-2.04507
H	9.36334	-0.99936	-0.76731	H	-2.74384	2.01335	-2.21763
C	0.61688	-1.67862	0.71566	O	-1.11643	2.96895	-1.52683
C	1.91915	-2.09662	0.44171	C	0.21936	3.29679	-1.55204
C	2.97436	-1.16029	0.46079	C	0.48686	4.63881	-1.26106
C	2.67925	0.18184	0.78677	C	1.29260	2.40841	-1.81541
C	1.36281	0.55263	1.04776	C	1.79601	5.12045	-1.21409
N	0.38417	-0.37668	0.99089	H	-0.36540	5.29276	-1.06874
H	2.11720	-3.14718	0.23263	C	2.60467	2.90429	-1.76573
H	3.46526	0.93570	0.79384	C	2.85762	4.24638	-1.46274
Rh	-1.44312	0.16818	1.34714	H	1.97996	6.17131	-0.98312
C	-0.59796	-2.51000	0.80874	H	3.43611	2.22686	-1.96066
C	-0.63228	-3.88844	0.58314	H	3.88951	4.60183	-1.42923
C	-1.83621	-4.57790	0.73595	O	0.99524	1.11368	-2.08690
C	-2.98155	-3.87894	1.12654	C	2.00717	0.26727	-2.62679
C	-2.88788	-2.50543	1.34171	H	2.38187	0.67512	-3.57953
N	-1.73455	-1.84100	1.18571	H	2.84442	0.13594	-1.92652
H	-1.87643	-5.65324	0.55469	H	1.51962	-0.69957	-2.79609
H	0.27676	-4.41183	0.28720	H	-1.13195	1.33543	-2.85245
H	-3.94099	-4.38011	1.25707	H	-5.42965	-2.93543	-1.99008
H	-3.74777	-1.90580	1.64332	O	-7.44679	-1.17111	-1.40369
C	-1.07224	3.17926	1.74492	C	-7.91373	-2.45368	-1.81054
C	-0.31060	4.31433	2.01134	H	-9.00907	-2.40042	-1.78102
C	1.08430	4.22016	1.97093	H	-7.58532	-2.69140	-2.83577
C	1.67379	3.00002	1.64621	H	-7.56559	-3.24140	-1.12210
C	0.85819	1.89685	1.37764	O	-1.05933	-0.95752	-1.50005
N	-0.50673	1.99971	1.44769				
H	1.70677	5.09074	2.18163				
H	-2.16281	3.18897	1.77406	<b>I-[Rh]-TS3b</b>			
H	-0.81102	5.25313	2.25041	H	2.25646	-1.77623	0.32587
H	2.75724	2.89535	1.60190	C	1.43937	-2.50988	0.13191
O	-1.18474	0.02310	3.38928	C	1.83305	-3.81825	-0.32056
H	-2.09221	0.29919	3.61649	C	0.40317	-2.50786	1.14539
				C	1.07286	-4.95211	-0.02718



H	2.71306	-3.89586	-0.96552	H	-6.81846	7.02908	-0.03958
C	-0.34134	-3.64473	1.44023	H	-5.11173	7.46771	-0.38681
C	-0.03423	-4.88251	0.83298	H	-5.94417	6.21846	-1.38287
H	1.36973	-5.91596	-0.45307	C	1.15465	1.74739	-1.15333
H	-1.16172	-3.58555	2.15799	C	-0.01061	2.50900	-1.10629
H	-0.62964	-5.76835	1.06379	C	-0.60740	2.79459	0.14124
O	0.22094	-1.28339	1.74605	C	0.02318	2.32369	1.31174
C	-0.84788	-1.14554	2.66496	C	1.19206	1.57184	1.21227
H	-1.81205	-1.40990	2.19952	N	1.70366	1.29757	-0.00453
H	-0.69305	-1.77412	3.55926	H	-0.47691	2.84689	-2.03065
H	-0.86898	-0.08924	2.96172	H	-0.38966	2.55504	2.29250
C	-4.06682	-4.37286	-0.98059	Rh	3.33476	0.22936	-0.11487
C	-2.88272	-3.65747	-1.17100	C	1.91279	1.33589	-2.35099
C	-2.76311	-2.31732	-0.75811	C	1.55869	1.66227	-3.66091
C	-3.87995	-1.70764	-0.14249	C	2.35766	1.21828	-4.71698
C	-5.06093	-2.40412	0.05581	C	3.49878	0.46186	-4.44215
C	-5.16350	-3.74775	-0.36264	C	3.80594	0.16648	-3.11499
H	-2.04330	-4.16714	-1.64478	N	3.03224	0.58390	-2.10337
H	-3.79383	-0.66803	0.17951	H	2.08900	1.46507	-5.74529
H	-5.92473	-1.93622	0.53209	H	0.66513	2.25649	-3.85042
C	-1.52390	-1.51732	-0.91540	H	4.14828	0.09880	-5.23909
C	-0.32917	-2.07579	-1.68075	H	4.68011	-0.42143	-2.82966
H	-0.48766	-1.76415	-2.73420	C	3.80516	-0.38936	2.84554
O	0.89099	-1.57720	-1.23042	C	3.51379	-0.31653	4.20634
H	-0.33626	-3.18179	-1.68088	C	2.42283	0.44991	4.62101
H	-4.12546	-5.41020	-1.30932	C	1.64826	1.10795	3.66455
O	-6.35374	-4.35397	-0.12894	C	1.97669	0.98309	2.31342
C	-6.51867	-5.71329	-0.53286	N	3.06433	0.24677	1.92671
H	-7.54228	-5.98735	-0.25073	H	2.17210	0.53362	5.67960
H	-6.39432	-5.81937	-1.62236	H	4.64926	-0.96802	2.46806
H	-5.80325	-6.36932	-0.01181	H	4.14034	-0.85209	4.92002
O	-1.46964	-0.36145	-0.47737	H	0.78707	1.70601	3.96086
C	-1.87194	3.55083	0.22531	O	4.95141	-0.94477	-0.34511
C	-2.21550	4.51595	-0.73867	H	5.52297	-0.82688	0.43202
C	-2.78082	3.32017	1.28200	O	4.42226	1.87563	0.03927
C	-3.40613	5.24019	-0.65720	H	4.21612	2.38817	-0.76352
H	-1.53054	4.73146	-1.56123				
C	-3.97397	4.02515	1.37026	<b>I-[2Rh]-IM1</b>			
H	-2.56292	2.55714	2.03181	O	0.00011	-0.94577	-1.66772
C	-4.29501	4.99715	0.40382	O	1.57102	-0.01033	-2.96768
H	-3.62805	5.99151	-1.41468	C	0.45961	-0.60434	-2.80258
H	-4.68026	3.83539	2.18052	C	-0.38307	-0.88743	-4.01518
O	-5.47614	5.64539	0.57507	H	-1.00642	-0.00040	-4.21525
C	-5.84614	6.64630	-0.37231	H	0.24862	-1.07067	-4.89402

H	-1.04785	-1.74061	-3.82987	C	0.62917	2.56375	0.90346
O	4.41439	0.36502	-2.92212	C	0.24743	3.90674	0.96233
H	5.25580	0.24515	-2.44989	C	-0.54638	4.43820	-0.05511
Rh	2.94299	0.13106	-1.38702	C	-0.93569	3.61293	-1.11161
C	5.86655	0.25430	2.24179	C	-0.51378	2.28486	-1.12222
C	5.30401	1.44366	1.76368	N	0.25152	1.76927	-0.14913
C	5.58865	-0.96270	1.61454	H	-0.85382	5.48423	-0.02073
C	4.44620	1.39028	0.66356	H	0.56284	4.52420	1.80280
H	5.52569	2.39658	2.24246	H	-1.55600	3.98380	-1.92773
C	4.72461	-0.97512	0.51473	H	-0.79083	1.60934	-1.93004
H	6.03046	-1.89049	1.97618	C	1.30386	-3.14415	0.48398
N	4.16558	0.18819	0.09267	C	1.75913	-4.25715	1.18471
H	6.52873	0.27879	3.10783	C	2.45310	-4.06642	2.38435
C	3.78623	2.50920	-0.01891	C	2.63633	-2.77078	2.86478
C	3.96437	3.85657	0.30987	C	2.14313	-1.69104	2.12578
C	3.33939	4.83457	-0.46197	N	1.51463	-1.89225	0.92450
C	2.56799	4.44455	-1.56183	H	2.83664	-4.91901	2.94660
C	2.41590	3.08804	-1.83314	H	0.76724	-3.23456	-0.46086
N	2.98455	2.14132	-1.06751	H	1.58038	-5.25448	0.78274
H	3.46275	5.89009	-0.21539	H	3.14848	-2.59099	3.80963
H	4.59211	4.12944	1.15778	H	3.10883	2.01825	4.88201
H	2.07562	5.17783	-2.20072	H	-2.15434	0.47665	0.82312
H	1.81985	2.73067	-2.67313	C	-7.50131	1.26513	-0.73645
C	3.04751	-2.82021	-2.13912	C	-6.13411	1.25418	-1.03575
C	3.52965	-4.12359	-2.03112	C	-5.16234	1.15724	-0.03086
C	4.43258	-4.43090	-1.01104	C	-5.59498	1.12537	1.30395
C	4.83960	-3.41994	-0.13951	C	-6.95120	1.13934	1.62356
C	4.33026	-2.12917	-0.30229	C	-7.91502	1.19035	0.60270
N	3.42329	-1.84823	-1.29302	H	-5.82804	1.30695	-2.08430
H	4.81981	-5.44412	-0.89505	H	-4.84883	1.06841	2.09711
H	2.34567	-2.53647	-2.92333	H	-7.28606	1.09523	2.66208
H	3.19005	-4.87989	-2.73915	C	-3.68135	1.07647	-0.39143
H	5.55336	-3.62335	0.65801	C	-3.34680	-0.16221	-1.23817
O	-1.07922	-0.57851	1.07423	H	-2.33094	-0.07194	-1.64161
H	-1.49988	-1.26117	0.52158	O	-3.31423	-1.41116	-0.51909
C	1.41601	1.87972	1.93808	C	-4.39209	-1.75966	0.26705
C	1.97222	2.43358	3.09572	C	-4.18957	-1.93290	1.63596
C	2.65918	1.59915	3.98132	C	-5.66419	-2.00708	-0.30002
C	2.76528	0.22674	3.72640	C	-5.24867	-2.31661	2.46751
C	2.19616	-0.28863	2.55995	H	-3.19333	-1.72871	2.03233
N	1.57308	0.55397	1.69390	C	-6.72692	-2.36930	0.53888
H	1.87001	3.49902	3.29848	C	-6.51576	-2.52105	1.91665
H	3.28370	-0.43067	4.42326	H	-5.08276	-2.43926	3.53979
Rh	0.81425	-0.17885	0.09225	H	-7.71927	-2.54198	0.12192

H	-7.35562	-2.80552	2.55444	H	2.22218	5.45386	-1.46649
O	-5.76066	-1.86596	-1.64969	H	1.79957	3.10990	-2.27949
C	-7.03538	-2.06281	-2.25585	C	2.69895	-2.47394	-2.63322
H	-7.38378	-3.09850	-2.11232	C	3.07895	-3.81259	-2.73192
H	-7.78104	-1.36149	-1.84835	C	3.94182	-4.34280	-1.77166
H	-6.89269	-1.86728	-3.32549	C	4.42009	-3.51301	-0.75506
H	-4.05418	-0.22859	-2.07783	C	4.01422	-2.17770	-0.71461
H	-8.22858	1.33054	-1.54577	N	3.13516	-1.68377	-1.64308
O	-9.22403	1.17006	1.00154	H	4.24856	-5.38849	-1.81410
C	-10.22826	1.16795	-0.00709	H	2.03215	-2.01076	-3.35954
H	-11.18867	1.11607	0.52085	H	2.69384	-4.42113	-3.55000
H	-10.19286	2.08955	-0.61152	H	5.11075	-3.89617	-0.00498
H	-10.12572	0.29222	-0.66967	O	-1.12009	-0.82636	1.96846
H	-3.47959	1.91468	-1.09206	H	-1.50048	-1.68960	1.73289
O	-2.87405	1.21278	0.75471	C	1.44733	1.61220	2.16448
				C	2.06358	1.93888	3.37771
				C	2.68257	0.92511	4.11414
				C	2.66387	-0.39833	3.65585
				C	2.03764	-0.68198	2.44022
				N	1.48199	0.32978	1.72707
				H	2.06017	2.96578	3.74108
				H	3.13106	-1.19163	4.23794
				Rh	0.63916	-0.09326	0.05505
				C	0.68490	2.49702	1.26964
				C	0.38176	3.83387	1.54533
				C	-0.42155	4.54555	0.65236
				C	-0.91993	3.89810	-0.48053
				C	-0.59179	2.55951	-0.69521
				N	0.22101	1.89063	0.13479
				H	-0.66024	5.59229	0.84592
				H	0.76215	4.30509	2.45079
				H	-1.56179	4.41484	-1.19411
				H	-0.96025	2.00550	-1.55510
				C	0.91763	-3.11250	-0.03404
				C	1.28183	-4.35310	0.48509
				C	1.97876	-4.40120	1.69619
				C	2.26381	-3.20919	2.36350
				C	1.86011	-1.99522	1.80195
				N	1.21444	-1.96335	0.59331
				H	2.28997	-5.35589	2.12200
				H	0.38163	-3.00995	-0.97826
				H	1.02811	-5.26107	-0.06180
				H	2.78825	-3.21924	3.31837
				H	3.17700	1.16395	5.05608
<b>I-[2Rh]-TS1</b>							
O	-0.17825	-0.53111	-1.79995				
O	1.42573	0.52204	-2.96524				
C	0.28502	-0.03566	-2.86980				
C	-0.58001	-0.08485	-4.10192				
H	-1.16334	0.84844	-4.15566				
H	0.03610	-0.15812	-5.00704				
H	-1.28282	-0.92450	-4.03698				
O	4.23677	0.65804	-2.82343				
H	5.09213	0.52790	-2.37976				
Rh	2.78378	0.30776	-1.41481				
C	5.75948	-0.30463	2.11344				
C	5.28231	0.97949	1.82541				
C	5.38235	-1.39791	1.32853				
C	4.40559	1.14586	0.75043				
H	5.58690	1.83202	2.43059				
C	4.50390	-1.18905	0.26018				
H	5.76283	-2.39471	1.54669				
N	4.03332	0.05983	0.02840				
H	6.43563	-0.45226	2.95580				
C	3.81401	2.39610	0.24641				
C	4.08908	3.66716	0.75715				
C	3.50855	4.78357	0.15430				
C	2.68302	4.60632	-0.95960				
C	2.43887	3.31403	-1.42033				
N	2.96795	2.23914	-0.81820				
H	3.70729	5.78203	0.54553				
H	4.75285	3.77939	1.61359				

H	-1.64583	-0.22188	1.28101	H	1.42352	-1.32288	-5.13431
C	-6.68559	0.89768	-1.61111	H	1.22018	0.44404	-5.26233
C	-5.39476	0.35515	-1.65746	H	2.86710	-0.24145	-5.21880
C	-4.43928	0.64106	-0.67406	O	4.86993	1.31675	-1.14416
C	-4.80063	1.52542	0.35261	H	5.37883	1.10778	-0.34232
C	-6.07705	2.08252	0.41668	Rh	2.91728	0.58714	-0.71914
C	-7.03569	1.76220	-0.56048	C	3.37834	0.55580	3.91705
H	-5.13976	-0.31231	-2.48601	C	2.89322	1.70121	3.27513
H	-4.04197	1.75376	1.10315	C	3.75214	-0.56802	3.17560
H	-6.36098	2.76429	1.22211	C	2.77131	1.69505	1.88413
C	-3.01896	0.05367	-0.71563	H	2.60972	2.58263	3.84916
C	-3.03880	-1.49210	-0.71260	C	3.61569	-0.53635	1.78393
H	-2.03185	-1.84215	-0.96954	H	4.14160	-1.45721	3.66990
O	-3.29270	-2.08819	0.57733	N	3.11173	0.57617	1.18994
C	-4.45352	-1.80533	1.24587	H	3.46908	0.54231	5.00362
C	-4.36037	-1.28677	2.53953	C	2.32350	2.78947	1.01427
C	-5.72723	-2.11319	0.70615	C	1.97568	4.06791	1.46233
C	-5.50931	-1.04957	3.30367	C	1.62182	5.04359	0.53246
H	-3.35955	-1.05401	2.90902	C	1.64584	4.72692	-0.83044
C	-6.87616	-1.85644	1.46814	C	1.99265	3.43641	-1.21795
C	-6.76619	-1.32742	2.76206	N	2.29821	2.48240	-0.32135
H	-5.41820	-0.63754	4.31129	H	1.34054	6.04340	0.86621
H	-7.86242	-2.07716	1.05922	H	1.98884	4.29014	2.52881
H	-7.67366	-1.13924	3.34051	H	1.38934	5.46453	-1.59088
O	-5.74216	-2.65714	-0.53936	H	2.02184	3.13564	-2.26548
C	-6.99815	-2.87656	-1.16269	C	4.06876	-2.13300	-1.45794
H	-7.59603	-3.61945	-0.60819	C	4.69522	-3.34628	-1.17918
H	-7.56665	-1.93584	-1.24747	C	4.95352	-3.68573	0.15062
H	-6.77666	-3.26252	-2.16503	C	4.59581	-2.79169	1.16072
H	-3.75911	-1.88081	-1.44829	C	3.98352	-1.58247	0.82059
H	-7.40273	0.64589	-2.39332	N	3.70871	-1.27711	-0.48864
O	-8.26509	2.33753	-0.41523	H	5.43155	-4.63363	0.40171
C	-9.27132	2.01350	-1.35959	H	3.84751	-1.82705	-2.48052
H	-10.17195	2.55718	-1.04823	H	4.96469	-4.01067	-2.00051
H	-8.98859	2.33095	-2.37817	H	4.79616	-3.02325	2.20621
H	-9.48299	0.93013	-1.36714	C	-0.43543	1.42924	1.30916
H	-2.65190	0.26612	-1.75556	C	-0.69018	1.85217	2.61678
O	-2.19806	0.59913	0.23075	C	-0.41933	0.98157	3.67520
				C	0.08624	-0.30011	3.42450
				C	0.34217	-0.68034	2.10628
<b>I-[2Rh]-IM2</b>				N	0.10219	0.19978	1.09535
O	0.92222	-0.83907	-2.69322	H	-1.10393	2.84288	2.80058
O	2.68966	0.54246	-2.79524	H	0.28241	-0.99277	4.24212
C	1.82374	-0.21595	-3.33566	Rh	0.46100	-0.34561	-0.70645
C	1.84601	-0.35577	-4.83300				

C	-0.73611	2.13992	0.06456	O	-6.02813	-1.61547	-1.44304
C	-1.41787	3.35697	0.00120	C	-7.20037	-0.81847	-1.29756
C	-1.72031	3.90763	-1.24503	H	-8.04170	-1.41710	-0.91225
C	-1.32525	3.22789	-2.39896	H	-7.01630	0.03721	-0.62802
C	-0.63358	2.02378	-2.27465	H	-7.44150	-0.45269	-2.30303
N	-0.33981	1.48801	-1.07850	H	-4.17099	-1.29413	-2.87130
H	-2.26165	4.85230	-1.31096	H	-5.38780	2.68569	-0.75185
H	-1.72351	3.85325	0.92145	O	-5.24087	2.49539	1.97957
H	-1.54242	3.61849	-3.39334	C	-6.10989	3.52535	1.52267
H	-0.30504	1.46540	-3.15107	H	-6.51677	4.00172	2.42347
C	1.33225	-3.22289	-0.29986	H	-5.56304	4.27533	0.92702
C	1.56102	-4.36774	0.45761	H	-6.93727	3.11368	0.92087
C	1.43869	-4.29594	1.84994	H	-2.05098	-0.11471	-2.54218
C	1.05799	-3.09093	2.43733	O	-1.31980	-1.46855	-1.13614
C	0.82536	-1.97728	1.62372				
N	1.00135	-2.05053	0.26691				
H	1.62696	-5.17356	2.47009	<b>I-[2Rh]-TS2</b>			
H	1.42334	-3.22047	-1.38645	O	-1.23968	-0.18774	-2.89310
H	1.84220	-5.29472	-0.04235	O	-3.33887	-0.72943	-2.28631
H	0.92857	-3.00779	3.51615	C	-2.42982	-0.55167	-3.15618
H	-0.61022	1.29742	4.70122	C	-2.77142	-0.82857	-4.59541
C	-4.73850	1.90947	-0.34652	H	-2.59620	-1.89964	-4.78995
C	-4.01876	1.08332	-1.21887	H	-3.82894	-0.61063	-4.79276
C	-3.16342	0.08007	-0.74610	H	-2.12450	-0.24603	-5.26366
C	-3.04046	-0.07800	0.64254	O	-5.20386	-0.24312	-0.17570
C	-3.74292	0.73334	1.52921	H	-5.38584	0.10524	0.71358
C	-4.59618	1.73581	1.03947	C	3.53318	3.31544	-0.67506
H	-4.12484	1.23778	-2.29665	C	3.17524	2.31198	-1.57361
H	-2.37995	-0.85365	1.02943	C	3.02216	0.97598	-1.16423
H	-3.64083	0.60773	2.60885	C	3.23792	0.66924	0.19671
C	-2.37987	-0.79792	-1.72250	C	3.62465	1.65157	1.09802
C	-3.27463	-1.79925	-2.48043	C	3.75649	2.98596	0.67382
H	-2.70058	-2.21016	-3.32241	H	3.00974	2.55677	-2.62405
O	-3.64110	-2.96669	-1.72112	H	3.09131	-0.34477	0.56790
C	-4.23002	-2.81281	-0.48745	H	3.78992	1.41300	2.14964
C	-3.60834	-3.40442	0.61368	C	2.66753	-0.04698	-2.18800
C	-5.46306	-2.13759	-0.31905	H	0.98454	-0.18357	-1.59052
C	-4.17314	-3.31107	1.89131	C	2.80308	-1.53022	-1.82990
H	-2.65901	-3.91774	0.44939	H	2.19591	-2.11667	-2.52900
C	-6.01977	-2.03540	0.96277	O	4.16791	-1.96322	-2.05379
C	-5.37322	-2.61694	2.06234	C	5.09283	-1.52395	-1.12546
H	-3.66817	-3.76798	2.74499	C	6.05605	-0.59201	-1.50895
H	-6.95969	-1.50282	1.10893	C	5.06828	-2.01663	0.20011
H	-5.82186	-2.52451	3.05394	C	6.99687	-0.12110	-0.58481
				H	6.03683	-0.22807	-2.53800

C	6.00497	-1.53622	1.12555	H	-0.84653	-2.76964	-2.70878
C	6.96041	-0.59002	0.73058	H	-0.40773	-5.20525	-2.36705
H	7.74155	0.61610	-0.89131	H	0.74848	-4.29475	1.69844
H	5.99113	-1.89242	2.15569	H	1.45391	-0.53488	4.46610
H	7.68002	-0.22337	1.46594	Rh	-3.07605	-0.15482	-0.29024
O	4.09024	-2.91922	0.48984	C	-2.26260	1.20329	4.09396
C	3.97612	-3.36970	1.83820	C	-2.31001	-0.16269	3.78635
H	4.89020	-3.89644	2.15595	C	-2.47288	2.16046	3.09810
H	3.77776	-2.52766	2.51994	C	-2.55481	-0.55184	2.46902
H	3.13041	-4.06610	1.85232	H	-2.15642	-0.91336	4.56071
H	2.49839	-1.75835	-0.80126	C	-2.71664	1.73453	1.78795
O	2.56535	0.26853	-3.39390	H	-2.44889	3.22412	3.33231
H	3.62698	4.34369	-1.02353	N	-2.72952	0.40253	1.51127
O	4.08002	3.89026	1.63661	H	-2.06347	1.52065	5.11802
C	4.16897	5.26588	1.26972	C	-2.67446	-1.91251	1.93842
H	4.41686	5.80722	2.19076	C	-2.59401	-3.07731	2.71018
H	4.96253	5.42696	0.52254	C	-2.77745	-4.31541	2.09960
H	3.20765	5.63133	0.87392	C	-3.05841	-4.36328	0.72789
C	0.42653	0.83780	1.53092	C	-3.11945	-3.17562	0.00851
C	0.88430	0.77719	2.84860	N	-2.91292	-1.97791	0.58815
C	1.09948	-0.47426	3.43670	H	-2.71083	-5.23283	2.68610
C	0.86973	-1.64784	2.71134	H	-2.38959	-3.00342	3.77812
C	0.40273	-1.55227	1.39710	H	-3.21689	-5.31088	0.21269
N	0.17244	-0.32161	0.86179	H	-3.32810	-3.15797	-1.06164
H	1.07726	1.69405	3.40387	C	-3.51384	2.51803	-1.67787
H	1.04929	-2.62389	3.16018	C	-3.66305	3.90249	-1.70961
Rh	-0.48618	-0.21929	-0.93236	C	-3.46166	4.63445	-0.53578
C	0.21276	2.02554	0.70362	C	-3.12918	3.95617	0.63644
C	0.49957	3.33686	1.10219	C	-3.00510	2.56339	0.61307
C	0.32930	4.37943	0.19554	N	-3.18457	1.86012	-0.55349
C	-0.09972	4.08697	-1.10576	H	-3.56151	5.72076	-0.53184
C	-0.37455	2.76847	-1.44734	H	-3.66112	1.90584	-2.56818
N	-0.24986	1.76052	-0.56358	H	-3.92695	4.39145	-2.64782
H	0.54491	5.40666	0.49258	H	-2.97302	4.49761	1.56916
H	0.86656	3.52667	2.11043				
H	-0.22892	4.87128	-1.85165				
H	-0.71496	2.48719	-2.44425	<b>I-[2Rh]-IM3</b>			
C	-0.49879	-3.15052	-1.74841	O	-1.26981	-0.16902	-2.89601
C	-0.24675	-4.50444	-1.54752	O	-3.35858	-0.74098	-2.28313
C	0.20110	-4.93551	-0.29452	C	-2.45758	-0.54154	-3.15643
C	0.39673	-3.99264	0.71285	C	-2.80618	-0.80156	-4.59722
C	0.14916	-2.64125	0.45083	H	-2.62051	-1.86771	-4.80838
N	-0.31775	-2.23614	-0.77852	H	-3.86741	-0.59259	-4.78407
H	0.39578	-5.99178	-0.10398	H	-2.17051	-0.20232	-5.26150
				O	-5.21293	-0.31087	-0.16299

H	-5.39546	0.03482	0.72720	H	1.08421	1.68952	3.39312
C	3.45579	3.37864	-0.73496	H	1.10532	-2.62649	3.12125
C	3.15862	2.34801	-1.62300	Rh	-0.49624	-0.21425	-0.94139
C	3.05770	1.01177	-1.19501	C	0.18149	2.02863	0.70726
C	3.26323	0.73417	0.17418	C	0.43797	3.34277	1.11827
C	3.59221	1.74577	1.06557	C	0.23849	4.39017	0.22393
C	3.67249	3.07836	0.62258	C	-0.19051	4.10095	-1.07872
H	2.99843	2.57016	-2.67929	C	-0.43712	2.78064	-1.43224
H	3.15412	-0.27930	0.55906	N	-0.28261	1.76584	-0.56007
H	3.75027	1.53102	2.12336	H	0.42921	5.41928	0.53111
C	2.77012	-0.03773	-2.20645	H	0.80284	3.53080	2.12753
H	0.94381	-0.16625	-1.63706	H	-0.34278	4.88981	-1.81538
C	2.86462	-1.51264	-1.80522	H	-0.77783	2.50186	-2.42974
H	2.25585	-2.10395	-2.49873	C	-0.47377	-3.13868	-1.77943
O	4.22287	-1.97815	-1.99644	C	-0.19457	-4.48916	-1.59390
C	5.14544	-1.50941	-1.07927	C	0.27686	-4.92309	-0.35016
C	6.11000	-0.58973	-1.48762	C	0.46683	-3.98612	0.66337
C	5.11432	-1.96131	0.26033	C	0.19037	-2.63691	0.41717
C	7.04881	-0.09302	-0.57486	N	-0.29803	-2.22944	-0.80333
H	6.09560	-0.25794	-2.52757	H	0.49421	-5.97713	-0.17214
C	6.04911	-1.45514	1.17397	H	-0.83994	-2.75571	-2.73215
C	7.00743	-0.52291	0.75356	H	-0.35235	-5.18554	-2.41784
H	7.79598	0.63321	-0.90083	H	0.83723	-4.29074	1.64128
H	6.03166	-1.78029	2.21422	H	1.49795	-0.54163	4.43689
H	7.72582	-0.13622	1.47980	Rh	-3.08467	-0.19086	-0.28272
O	4.13240	-2.85156	0.57295	C	-2.24844	1.11800	4.11279
C	4.02698	-3.27939	1.92955	C	-2.27796	-0.24407	3.78596
H	4.94226	-3.80341	2.24846	C	-2.48111	2.08560	3.13208
H	3.83611	-2.42592	2.59893	C	-2.52810	-0.61855	2.46550
H	3.17902	-3.97250	1.96128	H	-2.10760	-1.00327	4.54844
H	2.53866	-1.70642	-0.77600	C	-2.72905	1.67464	1.81798
O	2.68660	0.24429	-3.41655	H	-2.47189	3.14606	3.38133
H	3.50863	4.40514	-1.09668	N	-2.72502	0.34634	1.52198
O	3.94066	4.00912	1.57492	H	-2.04594	1.42389	5.13968
C	3.98414	5.38236	1.18869	C	-2.63315	-1.97306	1.91771
H	4.19475	5.94528	2.10595	C	-2.52821	-3.14680	2.67318
H	4.78478	5.56169	0.45353	C	-2.69911	-4.37927	2.04824
H	3.01706	5.70490	0.77073	C	-2.99320	-4.41306	0.67857
C	0.42614	0.83831	1.52070	C	-3.07911	-3.21729	-0.02418
C	0.89746	0.77411	2.83320	N	-2.88414	-2.02377	0.56870
C	1.13407	-0.47855	3.41094	H	-2.61277	-5.30333	2.62161
C	0.91209	-1.64984	2.67969	H	-2.31405	-3.08365	3.73990
C	0.43574	-1.55189	1.36900	H	-3.14270	-5.35607	0.15236
N	0.18528	-0.32027	0.84332	H	-3.29874	-3.18912	-1.09190

C	-3.57275	2.49473	-1.62793	C	1.30716	-0.47444	2.16039
C	-3.74665	3.87654	-1.63749	N	1.19879	-1.32913	1.07995
C	-3.54610	4.59482	-0.45489	H	3.16750	-2.41567	4.25493
C	-3.18903	3.90540	0.70334	H	1.68828	-3.16946	0.26039
C	-3.04136	2.51532	0.65828	H	2.97730	-3.94565	2.24832
N	-3.22102	1.82572	-0.51665	H	2.07237	-0.16857	4.15239
H	-3.66547	5.67896	-0.43370	H	-0.20516	3.86862	3.21790
H	-3.71881	1.89324	-2.52576	Rh	-2.18194	-1.60914	0.20783
H	-4.02897	4.37445	-2.56558	C	-3.71946	2.31701	2.19530
H	-3.03258	4.43565	1.64245	C	-3.00625	1.38333	2.96112
<b>I-[2Rh]-TS3</b>				C	-3.98104	2.07393	0.84461
O	0.22356	-2.19158	-1.75264	C	-2.54698	0.21720	2.35089
O	-1.43500	-3.32348	-0.74038	H	-2.80732	1.56617	4.01660
C	-0.45862	-3.24175	-1.55340	C	-3.50698	0.89271	0.26268
C	-0.05850	-4.47997	-2.31091	H	-4.54345	2.79127	0.24754
H	-0.85676	-5.23203	-2.29353	N	-2.79133	0.01998	1.02325
H	0.19906	-4.21772	-3.34640	H	-4.07451	3.23787	2.65917
H	0.84431	-4.90061	-1.83849	C	-1.82700	-0.89823	2.96636
O	-3.89472	-2.73233	0.60020	C	-1.50824	-0.98511	4.32707
H	-4.60261	-2.06988	0.67878	C	-0.87804	-2.12811	4.81068
C	-0.47636	2.12916	0.30668	C	-0.59423	-3.17675	3.92346
C	-0.61733	3.18176	1.21082	C	-0.92536	-3.03476	2.58217
C	-0.10033	3.04901	2.50649	N	-1.51091	-1.92034	2.10400
C	0.54966	1.87101	2.89058	H	-0.61822	-2.20788	5.86728
C	0.66602	0.82547	1.96908	H	-1.76001	-0.15889	4.99167
N	0.14453	0.97569	0.71736	H	-0.10652	-4.09124	4.26169
H	-1.12851	4.09553	0.91059	H	-0.72065	-3.81754	1.85124
H	0.95628	1.76240	3.89591	C	-3.29183	-1.33590	-2.61116
Rh	0.16534	-0.52195	-0.46855	C	-4.06531	-0.72854	-3.59661
C	-0.91438	2.06382	-1.07956	C	-4.67894	0.49806	-3.31873
C	-1.53229	3.11256	-1.77902	C	-4.50094	1.07540	-2.06299
C	-1.84204	2.95659	-3.12339	C	-3.71836	0.41861	-1.10649
C	-1.51027	1.74487	-3.75904	N	-3.11338	-0.78213	-1.40034
C	-0.92875	0.72838	-3.01895	H	-5.28727	1.00022	-4.07238
N	-0.64637	0.85811	-1.70209	H	-2.79926	-2.29462	-2.77797
H	-2.32028	3.76478	-3.67865	H	-4.17753	-1.21549	-4.56571
H	-1.75243	4.04380	-1.25664	H	-4.97336	2.02536	-1.81458
H	-1.72054	1.58315	-4.81670	H	1.83376	-0.29417	-1.39113
H	-0.68234	-0.23749	-3.46178	O	2.64322	-0.42349	-2.09010
C	1.79429	-2.53721	1.14273	C	3.43341	-1.53841	-1.80052
C	2.51036	-2.96042	2.25693	C	3.39983	-2.63359	-2.65983
C	2.61651	-2.10901	3.36477	C	4.24315	-1.53329	-0.64555
C	2.00532	-0.85819	3.31111	C	4.17486	-3.76210	-2.37393
				H	2.75409	-2.59012	-3.53802



C	5.02701	-2.66382	-0.37139	C	-3.91782	-1.93249	0.78883
C	4.98334	-3.76672	-1.23203	C	-4.19627	-0.28171	3.03550
H	4.14702	-4.62763	-3.03814	H	-2.10108	-0.71298	3.40820
H	5.66057	-2.69028	0.51496	C	-5.14580	-1.32968	1.06544
H	5.59462	-4.64148	-0.99976	C	-5.28623	-0.49302	2.18868
O	4.18523	-0.42446	0.12504	H	-4.29542	0.36420	3.91195
C	5.04108	-0.33220	1.26613	H	-5.99960	-1.49395	0.40632
H	4.84909	-1.15467	1.96971	H	-6.25072	-0.02123	2.39076
H	6.09784	-0.33839	0.95666	O	-3.68288	-2.74119	-0.29309
H	4.79629	0.62443	1.74258	C	-4.76090	-2.99899	-1.18079
C	1.55493	5.03931	-0.34818	H	-5.15094	-2.06704	-1.62302
C	1.63997	4.18362	-1.44642	H	-4.35566	-3.63780	-1.97592
C	2.39538	2.99581	-1.40389	C	0.50618	0.51193	2.45823
C	3.05931	2.67843	-0.19495	C	0.44261	1.50992	3.43140
C	2.97351	3.51227	0.90889	C	-0.56053	2.48294	3.33600
C	2.21645	4.69962	0.84368	C	-1.49963	2.43347	2.30396
H	1.11991	4.43816	-2.37100	C	-1.40424	1.41255	1.35154
H	3.62146	1.74883	-0.10927	N	-0.38650	0.51984	1.43374
H	3.46734	3.25504	1.84773	H	1.16092	1.52784	4.25007
C	2.46278	2.14773	-2.61146	H	-2.29824	3.17169	2.24141
C	3.45257	1.07205	-2.67328	Rh	-0.30127	-0.88212	0.12748
H	3.66870	0.71236	-3.68005	C	1.42113	-0.63618	2.40617
H	4.29670	1.08514	-1.98370	C	2.39529	-0.91900	3.36788
O	1.72747	2.37092	-3.61267	C	3.14999	-2.08572	3.25095
H	0.96125	5.95045	-0.41925	C	2.89719	-2.95714	2.18659
O	2.16969	5.44208	1.98163	C	1.92307	-2.61643	1.25221
C	1.32288	6.58940	2.00387	N	1.22115	-1.47420	1.34116
H	1.39539	6.99731	3.01929	H	3.91885	-2.31788	3.98918
H	1.66042	7.34653	1.27796	H	2.54905	-0.23195	4.19952
H	0.27776	6.31290	1.79017	H	3.45324	-3.88704	2.06726
<b>I-[2Rh]-IM4</b>				H	1.69026	-3.25549	0.40001
O	-0.22113	-2.37087	-1.33639	C	-2.70431	-0.21859	-1.63519
O	0.53671	-0.96175	-2.91160	C	-3.88483	0.46233	-1.93029
C	0.05175	-2.07854	-2.54362	C	-4.28165	1.51954	-1.10979
C	-0.21693	-3.12329	-3.59117	C	-3.48151	1.86987	-0.02177
H	-1.27270	-3.42850	-3.54056	C	-2.30989	1.14963	0.22546
H	0.01978	-2.74591	-4.59287	N	-1.93233	0.11027	-0.58898
H	0.39682	-4.01108	-3.37356	H	-5.20075	2.07021	-1.31482
O	2.44457	1.20475	-3.08548	H	-2.36514	-1.05146	-2.24883
H	3.28954	0.72603	-3.03772	H	-4.47367	0.16112	-2.79661
O	-1.61189	-2.26753	1.32533	H	-3.76229	2.69160	0.63548
C	-2.77551	-1.71844	1.62941	H	-0.61612	3.27676	4.08171
C	-2.96269	-0.88736	2.75739	Rh	1.30699	0.38767	-1.50294
				C	3.00875	3.16859	1.82669



H	1.62063	-4.95527	1.54380	C	1.88328	0.33170	-2.70388
H	-0.16282	-3.89717	0.12976	C	2.82765	0.23005	-3.73039
C	-4.28308	-0.15997	-1.09073	C	3.57194	-0.94598	-3.85900
C	-5.36074	0.71298	-1.22735	C	3.34316	-2.01892	-2.98950
C	-5.50887	1.75461	-0.30900	C	2.40050	-1.88385	-1.96910
C	-4.58706	1.87939	0.73109	N	1.74466	-0.69613	-1.82283
C	-3.53678	0.96323	0.83064	H	2.96530	1.05282	-4.43168
N	-3.38599	-0.03517	-0.09916	H	3.88876	-2.95420	-3.11028
H	-6.33477	2.46195	-0.39615	Rh	0.34564	-0.61424	-0.52650
H	-4.12488	-0.98515	-1.78527	C	0.94227	1.42443	-2.45462
H	-6.06229	0.57319	-2.04997	C	0.87569	2.59833	-3.21059
H	-4.68577	2.67387	1.46979	C	-0.08936	3.55855	-2.90732
O	1.01594	0.81814	-2.88961	C	-0.96515	3.31921	-1.84497
H	2.24762	0.77150	-2.60881	C	-0.85020	2.13545	-1.11899
H	0.78364	1.76099	-2.92179	N	0.07485	1.20304	-1.40844
O	3.36446	0.61678	-2.33846	H	-0.15869	4.47558	-3.49479
C	3.79869	1.50137	-1.44199	H	1.57282	2.75164	-4.03413
C	3.15676	2.72491	-1.16832	H	-1.74253	4.03242	-1.57067
C	4.98198	1.19753	-0.70276	H	-1.51646	1.90901	-0.28617
C	3.65956	3.61513	-0.20896	C	0.70909	-3.26663	0.93423
H	2.24704	2.97080	-1.72038	C	1.20444	-4.56307	1.05365
C	5.47845	2.08506	0.25495	C	2.11787	-5.03661	0.10546
C	4.81649	3.30053	0.50505	C	2.52491	-4.18339	-0.91749
H	3.13081	4.55251	-0.01884	C	2.00717	-2.88464	-0.97713
H	6.38201	1.83726	0.81368	N	1.08981	-2.44566	-0.05923
H	5.21324	3.98607	1.25717	H	2.50891	-6.05372	0.16515
O	5.55993	-0.00472	-1.01919	H	0.01209	-2.85828	1.66269
C	6.66349	-0.43644	-0.23719	H	0.86374	-5.18552	1.88167
H	6.39792	-0.49957	0.83174	H	3.24436	-4.51573	-1.66587
H	6.92782	-1.43543	-0.60681	H	4.31008	-1.03931	-4.65662
H	7.52913	0.23713	-0.35605	Rh	1.94618	0.60135	1.27360
				C	3.96001	3.79844	-1.44551
				C	4.51218	2.51636	-1.35489
<b>II-[2Rh]-IM1</b>				C	2.82107	4.12744	-0.70111
O	3.14200	1.17962	2.83417	C	3.89198	1.56507	-0.53944
H	2.58494	1.67795	3.45539	H	5.42523	2.26803	-1.89583
H	-1.08902	-0.61813	0.76828	C	2.22194	3.14890	0.09495
H	-1.38336	-1.18308	3.08218	H	2.41027	5.13611	-0.73651
O	-0.16211	-1.98399	3.85396	N	2.74295	1.88973	0.10923
O	0.86287	-0.71963	2.38877	H	4.43557	4.55249	-2.07414
C	0.86958	-1.38091	3.49931	C	4.35215	0.20847	-0.22627
C	2.13686	-1.46380	4.31733	C	5.53364	-0.36008	-0.71101
H	2.63030	-2.42561	4.09566	C	5.90988	-1.63303	-0.28280
H	2.81538	-0.63475	4.07033	C	5.09718	-2.30487	0.63490
H	1.88216	-1.47734	5.38562				

C	3.92420	-1.69434	1.07409	C	-6.92322	-1.37094	-1.36090
N	3.54418	-0.48336	0.64183	H	-7.76927	-0.25774	0.29206
H	6.83368	-2.08603	-0.64656	H	-5.88980	-2.59889	-2.80469
H	6.16053	0.19995	-1.40470	H	-7.70013	-1.07954	-2.07076
H	5.36182	-3.29252	1.01361	O	-3.87267	-3.46332	-1.19880
H	3.25327	-2.17195	1.78665	C	-3.66738	-3.81064	-2.55346
C	-0.42645	2.13020	2.38083	H	-4.49873	-4.42263	-2.94400
C	-1.15624	3.29416	2.61569	H	-3.54741	-2.91127	-3.18159
C	-0.75437	4.49246	2.01647	H	-2.73838	-4.39260	-2.57975
C	0.35877	4.48635	1.17830	H	-2.36938	-2.39478	-0.07488
C	1.05186	3.29037	0.96420				
N	0.65647	2.12866	1.58221				
H	-1.30297	5.41835	2.19726	<b>II-[2Rh]-TS1</b>			
H	-0.71997	1.16126	2.79433	O	3.18995	0.65485	2.98958
H	-2.03042	3.25043	3.26468	H	2.82961	1.42333	3.46287
H	0.69432	5.40191	0.69092	H	-0.97209	-0.41766	0.63102
O	-1.00811	-1.63692	-1.72370	H	-1.31047	-1.08188	3.35507
H	-1.17205	-1.09223	-2.51122	O	-0.51173	-1.64363	4.08037
C	-2.14736	-0.73865	1.31539	O	0.77360	-0.95759	2.43996
O	-1.98339	-0.49540	2.65210	C	0.65146	-1.40617	3.62091
C	-4.59774	2.16618	0.94037	C	1.84650	-1.70675	4.47990
C	-3.69482	1.24839	1.49292	H	2.25226	-2.69135	4.19245
C	-3.06183	0.28988	0.69888	H	2.61450	-0.94049	4.28582
C	-3.36286	0.24722	-0.67751	H	1.55523	-1.75561	5.53615
C	-4.25471	1.14858	-1.23919	C	1.61828	1.09281	-2.65994
C	-4.88557	2.11616	-0.43236	C	2.53592	1.25409	-3.70191
H	-3.50395	1.24702	2.56622	C	3.34485	0.16954	-4.06347
H	-2.87280	-0.50854	-1.29474	C	3.21137	-1.06033	-3.41083
H	-4.51096	1.10892	-2.29865	C	2.28007	-1.17776	-2.37218
H	-5.09037	2.88948	1.59065	N	1.55760	-0.09460	-2.00698
O	-5.75248	2.94238	-1.06518	H	2.61348	2.20196	-4.23393
C	-6.50551	3.85848	-0.29093	H	3.81752	-1.91431	-3.71278
H	-7.16506	4.38243	-0.99321	Rh	0.20594	-0.31422	-0.60451
H	-7.11585	3.33602	0.46542	C	0.62570	2.05801	-2.17435
H	-5.85407	4.59342	0.21440	C	0.45294	3.33910	-2.71152
C	-2.56454	-2.18260	0.98365	C	-0.56301	4.16145	-2.23016
H	-1.98390	-2.87221	1.60978	C	-1.39192	3.67426	-1.21366
O	-3.92381	-2.41356	1.34421	C	-1.16982	2.39931	-0.70620
C	-4.89895	-2.10223	0.43316	N	-0.18336	1.59865	-1.15812
C	-5.94957	-1.28204	0.84686	H	-0.71270	5.15824	-2.64839
C	-4.88951	-2.61544	-0.88704	H	1.10882	3.67810	-3.51360
C	-6.96213	-0.91226	-0.04283	H	-2.20971	4.26894	-0.80674
H	-5.92942	-0.91749	1.87472	H	-1.79261	1.98520	0.08439
C	-5.89507	-2.22400	-1.78065	C	0.70807	-3.21651	0.20607
				C	1.21796	-4.49963	0.00946

C	2.13023	-4.71615	-1.02581	C	-3.81718	1.34574	1.53669
C	2.50900	-3.63426	-1.81960	C	-3.20154	0.32647	0.79728
C	1.95444	-2.37289	-1.58219	C	-3.52288	0.18591	-0.56956
N	1.04851	-2.17715	-0.56915	C	-4.42612	1.04515	-1.17301
H	2.54309	-5.70918	-1.21097	C	-5.04868	2.06335	-0.42223
H	0.01226	-2.99167	1.00855	H	-3.58781	1.43141	2.59992
H	0.89247	-5.31009	0.66273	H	-3.00471	-0.57593	-1.15637
H	3.22270	-3.76661	-2.63258	H	-4.68952	0.94300	-2.22648
H	4.06702	0.27831	-4.87399	H	-5.21645	2.98461	1.54489
Rh	1.98817	0.32550	1.34331	O	-5.92729	2.83996	-1.09271
C	4.53771	3.16296	-1.30893	C	-6.64603	3.83475	-0.38268
C	4.89075	1.81273	-1.18658	H	-7.31343	4.30724	-1.11312
C	3.42918	3.66291	-0.61940	H	-7.24587	3.39109	0.42977
C	4.10528	0.97121	-0.39849	H	-5.96853	4.59718	0.03994
H	5.77812	1.42640	-1.68737	C	-2.40304	-2.09308	1.10340
C	2.65960	2.79345	0.16020	H	-1.72543	-2.67129	1.74321
H	3.17067	4.72005	-0.67910	O	-3.71617	-2.55343	1.43372
N	2.98741	1.47218	0.20538	C	-4.69522	-2.36763	0.49005
H	5.14534	3.83081	-1.92090	C	-5.84680	-1.66891	0.85258
C	4.34560	-0.43424	-0.06635	C	-4.56161	-2.88104	-0.82266
C	5.45139	-1.18155	-0.49057	C	-6.85401	-1.42359	-0.08482
C	5.61573	-2.48540	-0.03036	H	-5.91237	-1.29542	1.87562
C	4.67572	-3.01231	0.86532	C	-5.56037	-2.60489	-1.76593
C	3.59080	-2.23004	1.24192	C	-6.69852	-1.87742	-1.39655
N	3.40724	-0.98598	0.76706	H	-7.74620	-0.86592	0.20591
H	6.47619	-3.07727	-0.34685	H	-5.46131	-2.97141	-2.78808
H	6.18429	-0.73178	-1.16061	H	-7.46965	-1.67772	-2.14354
H	4.77971	-4.01947	1.26973	O	-3.44194	-3.60909	-1.07264
H	2.82689	-2.58268	1.93188	C	-3.10673	-3.90408	-2.41756
C	-0.17258	2.19633	2.37121	H	-3.86288	-4.55639	-2.88648
C	-0.73824	3.45430	2.57262	H	-2.98197	-2.97850	-3.00181
C	-0.15189	4.57515	1.97458	H	-2.14530	-4.43026	-2.37828
C	0.96861	4.39842	1.16506	H	-2.16759	-2.25275	0.04439
C	1.49400	3.11377	0.98681				
N	0.92477	2.02898	1.61191	<b>II-[2Rh]-IM2</b>			
H	-0.56784	5.57220	2.12880	O	3.02146	0.83355	3.07206
H	-0.61194	1.28756	2.78938	H	2.70771	1.67159	3.45055
H	-1.62879	3.54213	3.19554	H	-0.72081	-0.34732	0.58595
H	1.44057	5.24953	0.67425	H	-1.34223	-1.06233	3.86436
O	-1.13945	-1.19771	-1.92114	O	-0.56403	-1.41611	4.43990
H	-1.38370	-0.51820	-2.57112	O	0.56600	-0.70984	2.68348
C	-2.28125	-0.61882	1.48350	C	0.56836	-1.17079	3.84234
O	-1.99310	-0.32067	2.70542	C	1.80686	-1.49357	4.61715
C	-4.73425	2.21609	0.94047	H	2.16727	-2.49111	4.31633

H	2.56706	-0.73779	4.35650	C	5.47151	-2.48461	0.20750
H	1.58823	-1.52217	5.69143	C	4.49926	-2.98353	1.08459
C	1.66525	1.06874	-2.77539	C	3.41561	-2.18052	1.41686
C	2.63856	1.24237	-3.76329	N	3.26030	-0.94038	0.92112
C	3.49990	0.17383	-4.05459	H	6.33335	-3.09220	-0.07321
C	3.37346	-1.04848	-3.38245	H	6.08003	-0.76573	-0.95388
C	2.38137	-1.17759	-2.40226	H	4.57616	-3.98582	1.50666
N	1.59388	-0.11564	-2.11886	H	2.62925	-2.52039	2.08721
H	2.72919	2.18451	-4.30436	C	-0.36720	2.30350	2.27082
H	4.03362	-1.88150	-3.62611	C	-0.95654	3.56142	2.37619
Rh	0.25093	-0.29999	-0.66313	C	-0.36672	4.65282	1.72788
C	0.62888	2.01388	-2.33460	C	0.78263	4.44593	0.96773
C	0.39864	3.25999	-2.93106	C	1.33112	3.16127	0.88574
C	-0.66600	4.05065	-2.50430	N	0.75797	2.10912	1.55967
C	-1.49165	3.57092	-1.47988	H	-0.80292	5.65004	1.80579
C	-1.20797	2.33979	-0.90153	H	-0.79347	1.41680	2.74383
N	-0.16961	1.57271	-1.29714	H	-1.86728	3.67466	2.96439
H	-0.85999	5.01591	-2.97511	H	1.25628	5.27245	0.43816
H	1.04348	3.59121	-3.74556	O	-1.27657	-1.15309	-1.76401
H	-2.35200	4.13872	-1.12565	H	-1.64319	-0.44537	-2.31871
H	-1.81125	1.92904	-0.09411	C	-2.75865	-0.59477	1.89708
C	0.68205	-3.19573	0.12751	O	-2.38452	-0.28220	3.04198
C	1.20773	-4.47694	-0.02553	C	-4.70864	2.49349	0.97047
C	2.19163	-4.69635	-0.99529	C	-4.01032	1.53459	1.69832
C	2.60984	-3.62244	-1.77900	C	-3.50848	0.37218	1.08319
C	2.03848	-2.35817	-1.59384	C	-3.72630	0.18653	-0.30077
N	1.07828	-2.15589	-0.62567	C	-4.41876	1.13668	-1.03669
H	2.62149	-5.68853	-1.14259	C	-4.91737	2.29554	-0.41108
H	-0.08471	-2.97051	0.86479	H	-3.85065	1.66234	2.77076
H	0.83833	-5.28607	0.60583	H	-3.28296	-0.66808	-0.81326
H	3.36582	-3.76218	-2.55191	H	-4.58782	1.00984	-2.10671
H	4.26674	0.29221	-4.82166	H	-5.10135	3.37590	1.47586
Rh	1.83960	0.41065	1.42038	O	-5.56501	3.16844	-1.20928
C	4.45319	3.11420	-1.30100	C	-6.15984	4.32363	-0.63628
C	4.80394	1.77276	-1.10458	H	-6.65196	4.85097	-1.46178
C	3.31805	3.63947	-0.67766	H	-6.90949	4.05040	0.12448
C	3.99262	0.96484	-0.30765	H	-5.40035	4.98293	-0.18154
H	5.70897	1.36677	-1.55532	C	-2.55648	-2.00520	1.37255
C	2.52301	2.80398	0.11324	H	-1.87044	-2.53430	2.04606
H	3.05819	4.69138	-0.79491	O	-3.81631	-2.68774	1.44473
N	2.85272	1.48694	0.23182	C	-4.56161	-2.71398	0.29225
H	5.08078	3.75565	-1.92091	C	-5.85162	-2.18525	0.31390
C	4.22060	-0.42463	0.09027	C	-4.04055	-3.27717	-0.89798
C	5.33027	-1.19155	-0.28701	C	-6.63273	-2.16915	-0.84637

H	-6.21402	-1.76654	1.25423	H	6.82990	-3.67710	-0.52046
C	-4.81184	-3.21620	-2.06682	H	7.04023	0.55362	-1.36021
C	-6.10071	-2.66763	-2.03665	H	8.14480	-1.55392	-0.66591
H	-7.64068	-1.75114	-0.82090	O	4.39086	0.74673	-1.98729
H	-4.41830	-3.61558	-3.00149	C	5.07771	1.99134	-2.06235
H	-6.68991	-2.64293	-2.95589	H	5.52271	2.25879	-1.09065
O	-2.80862	-3.83998	-0.81050	H	5.86508	1.96168	-2.83324
C	-2.14685	-4.18298	-2.02006	H	4.32144	2.73711	-2.33690
H	-2.71483	-4.94199	-2.58398	H	1.14177	-1.19165	-0.79948
H	-1.97237	-3.27830	-2.62288	O	2.63048	-2.24930	1.13256
H	-1.18024	-4.60676	-1.72213	H	6.65310	-0.40168	3.12115
H	-2.15254	-1.99489	0.35013	O	6.73893	2.30938	2.81128
<b>II-[2Rh]-TS2</b>				C	7.86160	1.78268	3.52209
O	-2.48790	-0.92627	-3.35717	H	8.42978	1.08040	2.89199
H	-1.66884	-1.03841	-3.86946	H	8.48868	2.64686	3.77090
H	1.93567	-2.67288	-2.03621	H	7.54067	1.27875	4.44725
O	1.25772	-3.39529	-2.30678	H	0.84278	0.09606	0.48641
O	-0.30996	-1.94341	-1.68648	C	-2.97017	1.48679	2.10056
C	-0.00301	-3.04417	-2.16335	C	-4.18916	1.65042	2.77021
C	-1.00599	-4.07416	-2.56870	C	-4.82578	0.51869	3.28830
H	-1.30053	-4.63292	-1.66511	C	-4.24204	-0.74877	3.16505
H	-1.89388	-3.57329	-2.97352	C	-3.03052	-0.86292	2.47797
H	-0.58019	-4.77686	-3.29485	N	-2.46453	0.24289	1.94191
C	5.82866	0.06047	2.57928	H	-4.62781	2.64053	2.88966
C	4.80335	-0.73102	2.07322	H	-4.72465	-1.62708	3.59239
C	3.74330	-0.17181	1.33504	Rh	-0.69708	0.08239	1.08188
C	3.71388	1.22651	1.14105	C	-2.10356	2.53402	1.53927
C	4.71563	2.03108	1.66266	C	-2.39712	3.89860	1.59003
C	5.78970	1.45326	2.37039	C	-1.49597	4.81910	1.05302
H	4.82884	-1.81250	2.21686	C	-0.31371	4.34951	0.47700
H	2.89560	1.69010	0.58931	C	-0.07213	2.97743	0.44699
H	4.69912	3.11362	1.52723	N	-0.93916	2.08353	0.95631
C	2.75166	-1.08418	0.73898	H	-1.71723	5.88683	1.08415
C	1.99986	-0.62802	-0.47255	H	-3.32779	4.23208	2.04841
H	2.16506	0.36823	-0.86966	H	0.41966	5.02955	0.04293
O	3.00530	-1.51290	-1.74568	H	0.83171	2.56448	0.00011
C	4.33242	-1.55826	-1.51771	C	-0.35443	-2.98382	1.19472
C	4.97512	-2.73963	-1.12284	C	-0.72099	-4.27585	1.56424
C	5.09382	-0.35898	-1.61190	C	-1.88618	-4.46661	2.31220
C	6.34545	-2.74726	-0.82706	C	-2.65092	-3.35336	2.65225
H	4.37322	-3.64699	-1.03630	C	-2.24947	-2.08230	2.22698
C	6.45738	-0.36614	-1.30184	N	-1.09275	-1.90375	1.50721
C	7.07972	-1.56190	-0.90816	H	-2.19582	-5.46516	2.62444
				H	0.57481	-2.79861	0.65997

H	-0.08564	-5.11280	1.27241	H	-2.74127	-2.19005	0.95140
H	-3.57111	-3.46209	3.22565	Rh	1.07590	1.05114	1.00178
H	-5.77888	0.62561	3.80770	C	-0.90175	2.64232	-0.33690
Rh	-1.72888	-0.34220	-1.44208	C	-1.51483	3.69888	-1.01175
C	-4.34478	3.49870	-1.17927	C	-0.79305	4.87179	-1.24615
C	-4.84934	2.28303	-0.71189	C	0.52537	4.96580	-0.79754
C	-3.06098	3.56050	-1.73265	C	1.08695	3.87940	-0.12653
C	-4.04564	1.14115	-0.78046	N	0.39366	2.75541	0.09480
H	-5.85641	2.21715	-0.30171	H	-1.26074	5.70322	-1.77568
C	-2.28230	2.40316	-1.77915	H	-2.54483	3.60007	-1.35386
H	-2.66876	4.49784	-2.12459	H	1.12097	5.86434	-0.96074
N	-2.77824	1.23752	-1.26822	H	2.11159	3.88798	0.24845
H	-4.95729	4.39914	-1.12596	C	2.16215	-1.44725	2.37268
C	-4.40852	-0.22810	-0.41328	C	2.09299	-2.76060	2.83384
C	-5.66261	-0.61679	0.06350	C	0.90421	-3.47284	2.66209
C	-5.90457	-1.96525	0.32917	C	-0.18048	-2.85294	2.03907
C	-4.88650	-2.89455	0.10349	C	-0.05279	-1.53342	1.59964
C	-3.65166	-2.44675	-0.36290	N	1.12161	-0.85393	1.77367
N	-3.40908	-1.14936	-0.60583	H	0.81855	-4.50354	3.00963
H	-6.87773	-2.28442	0.70486	H	3.06294	-0.84284	2.48635
H	-6.43942	0.13094	0.21883	H	2.96204	-3.20803	3.31681
H	-5.03096	-3.95781	0.29588	H	-1.11883	-3.38661	1.89032
H	-2.82312	-3.13148	-0.54124	O	0.43691	1.71426	2.72818
C	0.72177	0.70482	-2.92114	H	1.29286	2.04228	3.07029
C	1.48043	1.69182	-3.54194	O	2.86483	1.79588	1.54420
C	1.00674	3.00866	-3.55319	H	3.49689	1.05778	1.55757
C	-0.22884	3.28511	-2.97268	C	-4.69310	-0.75603	-0.32134
C	-0.95029	2.25180	-2.36399	C	-5.74182	0.17330	-0.45454
N	-0.44692	0.97563	-2.30994	C	-5.00171	-2.12440	-0.49297
H	1.58474	3.80604	-4.02268	C	-7.04716	-0.22941	-0.73988
H	1.05034	-0.33276	-2.89714	H	-5.54996	1.23799	-0.30820
H	2.43226	1.42135	-3.99891	C	-6.29365	-2.53970	-0.78528
H	-0.63924	4.29452	-2.98721	H	-4.21403	-2.87678	-0.42235
O	0.28939	0.29467	2.93516	C	-7.33073	-1.59555	-0.90880
H	1.17154	0.60844	2.67531	H	-7.83208	0.52212	-0.82092
				H	-6.52444	-3.59661	-0.93019
				O	-8.56203	-2.09195	-1.19020
<b>b-TS1</b>				C	-9.64949	-1.17807	-1.32963
C	-1.55549	1.34861	-0.04785	H	-9.46952	-0.47250	-2.15643
C	-2.86240	0.97110	-0.35192	H	-10.52963	-1.79202	-1.55539
C	-3.31683	-0.32220	-0.00911	H	-9.81872	-0.61967	-0.39508
C	-2.42027	-1.19596	0.64403	H	1.95329	0.18153	-1.42603
C	-1.12285	-0.77250	0.92367	O	1.18274	0.72134	-1.89289
N	-0.73753	0.46938	0.56699	H	1.49810	1.63680	-1.84772
H	-3.51784	1.66853	-0.87178				



C	4.39170	1.15874	-1.49312	N	1.27018	2.85562	-0.16571
H	4.10017	1.01111	-2.54605	H	-0.29609	6.20291	0.95810
H	3.72950	1.91751	-1.04803	H	3.10549	3.78997	-0.22395
H	5.42472	1.54177	-1.46684	H	2.17766	6.02530	0.49894
C	4.24225	-0.16800	-0.71747	H	-1.72906	4.17479	0.67953
H	4.59394	0.04665	0.32500	C	-4.15052	-0.12118	-0.00254
O	2.94146	-0.63968	-0.72644	C	-4.80138	-1.13401	-0.73144
C	4.80346	-2.30182	-1.99544	C	-4.91999	0.62550	0.91722
C	5.24652	-1.19051	-1.26521	C	-6.16087	-1.40069	-0.56336
C	6.62875	-1.03287	-1.05919	H	-4.24662	-1.71736	-1.46889
C	7.54249	-1.95522	-1.57832	C	-6.27182	0.36632	1.10157
C	7.08779	-3.05790	-2.31512	H	-4.44806	1.40467	1.51868
C	5.71413	-3.22820	-2.51989	C	-6.90602	-0.64971	0.36161
H	3.72786	-2.42931	-2.13522	H	-6.62879	-2.18507	-1.15773
H	6.99232	-0.17852	-0.47948	H	-6.85932	0.93553	1.82424
H	8.61322	-1.81744	-1.40530	O	-8.22918	-0.83335	0.60504
H	7.80040	-3.78073	-2.72021	C	-8.91587	-1.86052	-0.10963
H	5.34916	-4.08843	-3.08780	H	-8.47739	-2.84923	0.10067
				H	-9.95189	-1.83382	0.24879
<b>b-IM1</b>				H	-8.89579	-1.66886	-1.19446
C	-0.47970	-0.59501	-0.78566	H	0.68619	-0.75058	1.55344
C	-1.83588	-0.87085	-0.62323	C	1.68680	-0.46481	1.94185
C	-2.71120	0.14980	-0.19069	O	2.14501	0.71723	1.34499
C	-2.17624	1.43170	0.06287	C	1.52208	-0.21612	3.44763
C	-0.81282	1.65969	-0.11913	H	2.49030	0.06810	3.89135
N	-0.02018	0.64997	-0.53524	H	0.80485	0.60364	3.61327
H	-2.20839	-1.87885	-0.79947	H	1.15357	-1.11678	3.96357
H	-2.82379	2.24740	0.38165	C	3.98925	-1.48994	1.55749
Rh	1.89289	0.97471	-0.66668	C	2.60451	-1.66129	1.70441
C	0.59393	-1.53199	-1.17734	C	2.07644	-2.96011	1.64111
C	0.38956	-2.86803	-1.52940	C	2.90960	-4.06367	1.42891
C	1.48557	-3.65541	-1.88623	C	4.28992	-3.88189	1.27785
C	2.76341	-3.09199	-1.88364	C	4.82658	-2.59027	1.34484
C	2.90853	-1.75631	-1.51334	H	4.40646	-0.48137	1.58711
N	1.85612	-1.00132	-1.16934	H	0.99634	-3.10381	1.74022
H	1.33987	-4.70074	-2.16278	H	2.47996	-5.06675	1.36727
H	-0.61777	-3.28363	-1.52485	H	4.94195	-4.74084	1.10157
H	3.64430	-3.67378	-2.15513	H	5.90231	-2.43888	1.22297
H	3.87876	-1.26009	-1.47945	O	1.74640	1.43413	-2.64476
C	2.04389	3.93804	-0.01656	H	2.41518	0.86496	-3.06219
C	1.51721	5.16494	0.38646	O	3.89395	1.31243	-0.75830
C	0.14719	5.25770	0.64067	H	4.10604	1.31574	0.19200
C	-0.65761	4.12641	0.48667				
C	-0.07431	2.92402	0.08135	<b>b-TS2</b>			

O	-3.72148	1.67293	-0.95649	H	-3.78433	-3.18905	-2.38455
H	-3.80332	2.61736	-1.17319	H	0.42387	-3.16935	-1.38164
C	4.17978	-0.25598	0.03808	O	-1.39548	1.88076	-2.50526
C	4.74773	-1.31592	-0.69367	H	-2.31460	2.02296	-2.80797
C	5.01270	0.43905	0.94346	C	-2.55795	-0.60547	2.06110
C	6.08734	-1.67600	-0.54373	O	-1.19267	-0.57471	2.16976
H	4.14357	-1.86252	-1.42022	H	-2.96451	0.13301	1.30704
C	6.34534	0.08675	1.10983	C	-3.25282	-0.21716	3.39244
H	4.60648	1.25182	1.54844	H	-4.35436	-0.21415	3.32693
C	6.89675	-0.97370	0.36553	H	-2.91774	0.78976	3.69346
H	6.49093	-2.49416	-1.13968	H	-2.94809	-0.92771	4.18048
H	6.98168	0.61676	1.82083	C	-4.94048	-3.34842	0.74852
O	8.20750	-1.24552	0.58906	C	-4.44847	-2.10366	1.15422
C	8.81368	-2.31590	-0.13514	C	-3.11855	-1.95872	1.59007
H	8.78722	-2.12412	-1.21979	C	-2.29298	-3.09089	1.59368
H	9.85520	-2.35616	0.20555	C	-2.77928	-4.34134	1.19154
H	8.31558	-3.27371	0.08476	C	-4.10682	-4.47585	0.76967
C	0.97713	1.75602	-0.03849	H	-5.10248	-1.22623	1.12348
C	2.32178	1.43168	0.13142	H	-1.25528	-2.95413	1.90728
C	2.76205	0.11659	-0.13542	H	-2.11812	-5.21247	1.19956
C	1.81242	-0.83422	-0.57034	H	-5.97527	-3.44112	0.40753
C	0.48005	-0.45924	-0.72814	H	-4.48842	-5.44836	0.44850
N	0.11465	0.81332	-0.46674				
H	3.02621	2.19616	0.45543				
H	2.10957	-1.86415	-0.76130	<b>acetophenone</b>			
Rh	-1.77019	1.28534	-0.68529	C	0.42653	1.19944	-0.00002
C	0.32400	3.05386	0.22567	C	-0.21002	-0.05586	0.00001
C	0.99473	4.19255	0.67449	C	0.57448	-1.22488	-0.00000
C	0.27078	5.36140	0.91876	C	1.96617	-1.14292	-0.00003
C	-1.10982	5.36601	0.71294	C	2.59213	0.11135	-0.00006
C	-1.72603	4.19947	0.26232	C	1.82161	1.27987	-0.00005
N	-1.03080	3.07847	0.02369	H	-0.16200	2.11822	-0.00001
H	0.78397	6.25837	1.26885	H	0.07060	-2.19316	0.00001
H	2.07245	4.16078	0.83216	H	2.56760	-2.05467	-0.00004
H	-1.71166	6.25671	0.89500	H	3.68261	0.17717	-0.00008
H	-2.80144	4.14477	0.08776	H	2.30908	2.25713	-0.00006
C	-2.93379	-1.32880	-1.71392	C	-1.69838	-0.19621	0.00004
C	-2.88013	-2.68118	-2.04987	C	-2.54954	1.04729	0.00005
C	-1.66503	-3.35600	-1.92736	H	-2.33151	1.66347	-0.88661
C	-0.53463	-2.66209	-1.48818	H	-3.60873	0.76132	0.00006
C	-0.64409	-1.30661	-1.17667	H	-2.33149	1.66348	0.88670
N	-1.84809	-0.66549	-1.29839	O	-2.21676	-1.31269	0.00005
H	-1.59270	-4.41718	-2.16969				
H	-3.85142	-0.74299	-1.78044	<b>e-TS1</b>			
				C	0.08611	1.17236	-0.02027

C	1.47850	1.12262	-0.00163	H	8.41574	1.49694	0.40210
C	2.13688	-0.12610	-0.03273	H	9.64613	0.24054	0.03522
C	1.34958	-1.29590	-0.10780	H	8.49256	0.75964	-1.23990
C	-0.03979	-1.19413	-0.11999	H	-2.92207	0.00234	2.62117
N	-0.61923	0.02364	-0.05868	H	-1.88056	1.07159	2.86816
H	2.05212	2.04556	0.06471	O	-3.54286	-0.76729	2.42222
H	1.81868	-2.27652	-0.17000	H	-4.15925	-0.39891	1.73985
Rh	-2.57475	0.11185	-0.02535				
C	-0.76692	2.37641	0.00416				
C	-0.27007	3.68111	0.00829	<b>I-[Ir]-IM1</b>			
C	-1.16343	4.75414	0.01279	O	-2.89521	1.62710	-0.54438
C	-2.53477	4.49752	0.00886	H	-2.82305	1.52969	-1.50960
C	-2.97106	3.17288	0.00767	H	-1.43048	1.83126	-0.06195
N	-2.11540	2.14284	0.01053	C	3.82073	-0.02103	-1.10772
H	-0.78801	5.77851	0.01615	C	2.53699	0.41998	-1.44970
H	0.80568	3.85411	0.00608	C	1.66228	0.95128	-0.49285
H	-3.26779	5.30470	0.00823	C	2.08554	0.97566	0.84543
H	-4.03310	2.92599	0.01015	C	3.35362	0.52509	1.20822
C	-3.30900	-2.82509	-0.21049	C	4.23799	0.04038	0.22945
C	-3.03147	-4.18825	-0.30088	H	2.22554	0.35798	-2.49560
C	-1.69897	-4.60442	-0.33186	H	1.41206	1.36452	1.60946
C	-0.68121	-3.65007	-0.27391	H	3.68394	0.55383	2.24846
C	-1.01816	-2.29785	-0.18775	C	0.29883	1.47721	-0.91304
N	-2.33048	-1.91297	-0.15620	C	0.38420	2.60700	-1.95572
H	-1.44938	-5.66432	-0.40124	H	-0.61979	2.78722	-2.36455
H	-4.32738	-2.43532	-0.17726	O	0.76382	3.87842	-1.39954
H	-3.85371	-4.90300	-0.34471	C	1.91172	3.94733	-0.63951
H	0.36640	-3.94929	-0.29750	C	1.80489	4.36752	0.68629
O	-2.55790	0.22515	-1.98210	C	3.18521	3.66542	-1.18926
H	-3.51821	0.21544	-2.15943	C	2.94193	4.47307	1.49646
O	-4.59809	0.04864	0.03551	H	0.80674	4.57590	1.07522
H	-4.93583	0.95458	0.12674	C	4.31876	3.74786	-0.36932
C	3.60947	-0.20518	0.02200	C	4.19345	4.14838	0.96844
C	4.41399	0.85353	-0.43981	H	2.84324	4.79178	2.53620
C	4.25833	-1.34128	0.55578	H	5.30327	3.50943	-0.77220
C	5.80666	0.79610	-0.37956	H	5.08851	4.20818	1.59159
H	3.95063	1.73823	-0.88061	O	3.21203	3.32075	-2.50525
C	5.64305	-1.40893	0.63060	C	4.46990	2.99085	-3.08795
H	3.67184	-2.17407	0.94813	H	5.15260	3.85584	-3.06699
C	6.43126	-0.33990	0.16344	H	4.93687	2.13842	-2.56922
H	6.39376	1.63184	-0.75946	H	4.25633	2.71577	-4.12790
H	6.14010	-2.28083	1.05957	H	1.05674	2.32637	-2.78061
O	7.77498	-0.49123	0.27727	H	4.47455	-0.42468	-1.88035
C	8.61970	0.57252	-0.16159	O	5.47226	-0.35898	0.66653
				C	6.44480	-0.70631	-0.31466

H	7.36580	-0.93201	0.23677	C	4.66939	-3.70496	0.39534
H	6.13987	-1.59302	-0.89170	H	4.55567	-3.40489	2.54790
H	6.62392	0.13611	-1.00356	H	4.45644	-3.92606	-1.73982
H	-0.22405	0.65370	-1.43950	O	5.97025	-4.08874	0.30814
O	-0.44879	1.89498	0.20752	C	6.76463	-4.04761	1.49321
C	-1.44585	-1.70911	-0.83610	H	6.39814	-4.76971	2.24043
C	-0.20403	-2.34068	-0.80876	H	7.78025	-4.32281	1.18441
C	0.61364	-2.25396	0.33898	H	6.76993	-3.03552	1.92806
C	0.11417	-1.53532	1.44749	Ir	-3.62162	-0.17362	0.18322
C	-1.12793	-0.91711	1.38215				
N	-1.87316	-1.01381	0.25139				
H	0.12479	-2.89532	-1.68589	<b>I-[Ir]-TS1</b>			
H	0.71254	-1.41510	2.34762	O	2.78167	-1.17186	-2.43346
C	-2.40725	-1.66221	-1.94913	H	2.56794	-0.24160	-2.26173
C	-2.19660	-2.23581	-3.20595	H	1.99941	-1.67393	-1.93144
C	-3.16900	-2.10041	-4.19679	C	-3.23820	-0.84729	0.94029
C	-4.34017	-1.38992	-3.91391	C	-2.23321	-0.64938	-0.01390
C	-4.50570	-0.84086	-2.64628	C	-1.21841	-1.59269	-0.22409
N	-3.57118	-0.97449	-1.68730	C	-1.22411	-2.75040	0.56826
H	-3.01143	-2.54339	-5.18140	C	-2.22022	-2.97522	1.51540
H	-1.27230	-2.77907	-3.40240	C	-3.23503	-2.02330	1.70761
H	-5.12235	-1.25962	-4.66241	H	-2.24746	0.27046	-0.60516
H	-5.39575	-0.28020	-2.35667	H	-0.42657	-3.48003	0.42446
C	-3.63592	1.25139	2.91173	H	-2.22478	-3.87922	2.12807
C	-3.08531	1.63277	4.13139	C	-0.13134	-1.36496	-1.27547
C	-1.83177	1.13021	4.49421	C	-0.72123	-1.29008	-2.70176
C	-1.16572	0.27082	3.62123	H	0.06110	-0.91907	-3.37865
C	-1.76123	-0.07283	2.40447	O	-1.07009	-2.57337	-3.26222
N	-3.00018	0.41677	2.07001	C	-1.91246	-3.39583	-2.55143
H	-1.37366	1.40908	5.44440	C	-1.44469	-4.65587	-2.17686
H	-4.61014	1.61409	2.58184	C	-3.24560	-3.02371	-2.25256
H	-3.63708	2.31274	4.78116	C	-2.26796	-5.54786	-1.47896
H	-0.18262	-0.12763	3.87160	H	-0.40754	-4.90020	-2.41288
O	-5.53493	0.52877	0.00824	C	-4.06050	-3.90904	-1.53416
H	-5.81262	0.89725	0.86168	C	-3.57024	-5.16527	-1.14951
O	-4.41870	-1.88687	0.94719	H	-1.88468	-6.52629	-1.18175
H	-5.37164	-1.69220	0.88939	H	-5.08242	-3.62723	-1.27963
C	1.97576	-2.82429	0.36577	H	-4.22099	-5.84236	-0.59162
C	2.70403	-2.92416	1.56735	O	-3.64540	-1.79837	-2.69242
C	2.63186	-3.21608	-0.82214	C	-4.95349	-1.35484	-2.34476
C	4.02978	-3.35538	1.59502	H	-5.72346	-2.00404	-2.79278
H	2.23677	-2.66283	2.51746	H	-5.08511	-1.32559	-1.25116
C	3.95108	-3.65012	-0.81263	H	-5.04567	-0.34082	-2.75255
H	2.12089	-3.14315	-1.78294	H	-1.58360	-0.60611	-2.74350
				H	-4.00669	-0.08621	1.07878

O	-4.16823	-2.31575	2.66832	C	-2.48406	6.06976	-0.34564
C	-5.22004	-1.38122	2.87946	H	-0.39763	5.59372	-0.37643
H	-5.85323	-1.80804	3.66741	C	-3.79312	5.61230	-0.10316
H	-4.82904	-0.40547	3.21349	H	-5.00182	3.89812	0.47930
H	-5.81937	-1.23962	1.96443	H	-2.33717	7.10897	-0.64572
H	0.21283	-0.31178	-1.11607	O	-4.78944	6.51943	-0.28037
O	0.90501	-2.27852	-1.18889	C	-6.13410	6.10322	-0.04680
C	1.76241	2.18226	-0.33046	H	-6.27359	5.78218	0.99806
C	0.73004	3.11312	-0.42196	H	-6.75922	6.98156	-0.24798
C	-0.44471	2.94188	0.34198	H	-6.41900	5.28446	-0.72698
C	-0.50892	1.84512	1.22704	Ir	3.01247	-0.26750	0.51023
C	0.53480	0.92618	1.27480				
N	1.61666	1.09475	0.47021				
H	0.82323	3.95341	-1.10879	<b>I-[Ir]-IM2</b>			
H	-1.37475	1.70635	1.87219	C	1.87618	1.64671	-1.81243
C	3.05478	2.19999	-1.03444	C	0.47888	1.77110	-1.79708
C	3.47108	3.21717	-1.89849	C	-0.26395	1.55456	-0.63170
C	4.72292	3.13307	-2.50690	C	0.43137	1.20529	0.53823
C	5.54008	2.03066	-2.24036	C	1.81633	1.09438	0.55133
C	5.07672	1.04443	-1.37535	C	2.54940	1.30793	-0.62910
N	3.87096	1.12280	-0.78635	H	-0.03852	2.02996	-2.72529
H	5.05643	3.92216	-3.18253	H	-0.13293	1.00976	1.45027
H	2.81665	4.06727	-2.08886	H	2.35171	0.82019	1.46200
H	6.52530	1.92684	-2.69569	C	-1.78135	1.71051	-0.61935
H	5.66979	0.16075	-1.13825	C	-2.23026	3.16834	-0.44293
C	1.85835	-2.23366	2.55785	H	-3.32780	3.19162	-0.49436
C	0.94632	-2.63000	3.53197	O	-1.94010	3.75733	0.83835
C	-0.15432	-1.81206	3.80341	C	-0.64792	3.96372	1.25767
C	-0.32067	-0.63001	3.08338	C	-0.35891	3.62481	2.58292
C	0.61258	-0.28634	2.10347	C	0.36391	4.55091	0.45644
N	1.70223	-1.09179	1.86577	C	0.92138	3.80667	3.11576
H	-0.88340	-2.09452	4.56397	H	-1.16135	3.17844	3.17388
H	2.74453	-2.81898	2.30770	C	1.65249	4.70560	0.98649
H	1.10714	-3.56547	4.06837	C	1.93157	4.33397	2.30829
H	-1.17358	0.02141	3.26936	H	1.12654	3.52072	4.14949
O	4.32908	-1.81091	0.58409	H	2.44311	5.13115	0.36822
H	5.12189	-1.58711	0.07087	H	2.94253	4.46806	2.69910
O	3.85091	0.73635	1.98534	O	0.01832	4.92884	-0.80640
H	3.50571	0.34168	2.80646	C	1.04448	5.39544	-1.67714
C	-1.58631	3.86796	0.20525	H	1.48464	6.33458	-1.30435
C	-2.90204	3.43003	0.44825	H	1.83532	4.63775	-1.79877
C	-1.40366	5.20939	-0.19726	H	0.55771	5.57701	-2.64311
C	-3.99818	4.28115	0.29631	H	-1.81720	3.78344	-1.25283
H	-3.08780	2.39323	0.73628	H	2.42194	1.80372	-2.74308
				O	3.90303	1.14284	-0.53144

C	4.67403	1.18156	-1.72661	H	3.61043	-2.84663	-2.01567
H	5.70545	0.95434	-1.42973	C	6.21865	-2.08780	0.03700
H	4.32485	0.42515	-2.44848	H	6.02170	-1.41384	2.09744
H	4.63801	2.17948	-2.19452	H	6.08356	-2.78102	-2.00132
H	-2.13502	1.48512	-1.64641	O	7.57441	-2.06039	-0.06378
O	-2.40202	0.89971	0.33853	C	8.32925	-1.63539	1.06974
C	-0.11711	-1.56895	-1.22215	H	8.16453	-2.30442	1.92971
C	1.25163	-1.80899	-1.21485	H	9.38163	-1.68235	0.76473
C	1.91587	-2.07029	0.00366	H	8.07218	-0.60137	1.35101
C	1.14502	-2.13632	1.18284	Ir	-2.68716	-1.09632	-0.07954
C	-0.22363	-1.87557	1.13589				
N	-0.80957	-1.58449	-0.05337	<b>I-[Ir]-TS2</b>			
H	1.81286	-1.73294	-2.14459	O	3.52411	2.36344	0.01456
H	1.61620	-2.36050	2.13875	H	4.21469	1.75266	-0.28855
C	-0.95578	-1.20939	-2.37672	C	4.08191	-3.38375	0.41486
C	-0.49417	-1.12028	-3.69210	C	2.81075	-2.86583	0.69885
C	-1.37608	-0.74662	-4.70615	C	2.63710	-1.57853	1.21254
C	-2.70912	-0.46939	-4.38630	C	3.78601	-0.80541	1.45827
C	-3.11769	-0.56912	-3.05990	C	5.05930	-1.29408	1.17277
N	-2.26714	-0.92533	-2.07993	C	5.21345	-2.58773	0.64072
H	-1.02499	-0.67269	-5.73652	H	1.91816	-3.45910	0.48865
H	0.55005	-1.33899	-3.91313	H	3.68224	0.21260	1.84433
H	-3.42891	-0.17524	-5.15067	H	5.95040	-0.68402	1.33766
H	-4.13806	-0.35357	-2.73858	C	1.21203	-1.05068	1.45687
C	-3.39181	-1.31287	2.87766	C	0.97364	-1.02298	2.99047
C	-3.11053	-1.54101	4.22146	H	1.86640	-0.65505	3.51544
C	-1.81301	-1.91508	4.58546	O	-0.04790	-0.09813	3.41334
C	-0.83539	-2.04549	3.59845	C	-1.33580	-0.10289	2.94577
C	-1.16847	-1.80254	2.26291	C	-1.92843	1.15411	2.77500
N	-2.45254	-1.44331	1.92527	C	-2.12230	-1.26558	2.74130
H	-1.56146	-2.10102	5.63082	C	-3.26836	1.28163	2.39140
H	-4.37896	-1.01600	2.51898	H	-1.30397	2.03352	2.94588
H	-3.89953	-1.42347	4.96496	C	-3.44724	-1.13071	2.30614
H	0.18399	-2.33055	3.85869	C	-4.02475	0.13550	2.14117
O	-4.69256	-0.56025	-0.11348	H	-3.70372	2.27528	2.26789
H	-4.61291	0.37651	0.13932	H	-4.04373	-2.02412	2.11795
O	-3.21851	-3.05121	-0.33217	H	-5.06355	0.21209	1.81336
H	-3.49462	-3.13374	-1.26018	O	-1.54441	-2.47058	3.01293
C	3.38882	-2.15923	0.03579	C	-2.07448	-3.62246	2.36260
C	4.10930	-1.77929	1.18312	H	-3.05524	-3.90628	2.77789
C	4.12859	-2.52453	-1.11059	H	-2.16604	-3.44912	1.27846
C	5.50447	-1.73751	1.19454	H	-1.35696	-4.43194	2.54676
H	3.57630	-1.46495	2.08225	H	0.74444	-2.04292	3.33315
C	5.51724	-2.49578	-1.11285	H	4.17586	-4.38811	0.00077

O	6.49787	-2.97718	0.36333	C	-0.77253	3.01204	0.03106
C	6.69078	-4.25218	-0.23827	N	0.58225	3.20212	0.17858
H	7.77171	-4.35273	-0.39809	H	-1.88400	5.89882	1.45146
H	6.34170	-5.06492	0.42030	H	2.13306	4.39978	0.83688
H	6.16913	-4.31862	-1.20790	H	0.60952	6.20622	1.70013
O	0.26421	-1.69695	0.76257	H	-2.74250	3.82225	0.36034
H	1.26596	0.07315	1.21236	O	1.75128	2.59054	-2.37496
C	-3.99252	-0.65519	-1.31355	H	1.49875	3.51364	-2.19423
C	-5.14563	0.14483	-1.40170	Ir	1.69789	1.67210	-0.62314
C	-4.16897	-2.05088	-1.19075				
C	-6.42755	-0.40836	-1.37115				
H	-5.05046	1.22717	-1.51034	<b>I-[Ir]-IM3</b>			
C	-5.43768	-2.61618	-1.15328	O	2.87191	0.98832	-1.17460
H	-3.30042	-2.70371	-1.08515	H	3.43960	0.31397	-0.76956
C	-6.58008	-1.79907	-1.24234	C	-5.06285	-1.02693	-0.29036
H	-7.29479	0.24680	-1.45028	C	-6.10471	-0.29082	-0.88324
H	-5.56884	-3.69400	-1.04060	C	-5.41464	-2.05478	0.61276
O	-7.78057	-2.43617	-1.19399	C	-7.44592	-0.56190	-0.60319
C	-8.96854	-1.64939	-1.26189	H	-5.87221	0.50041	-1.59914
H	-9.02496	-1.09725	-2.21386	C	-6.74438	-2.33191	0.90577
H	-9.80267	-2.35874	-1.19935	H	-4.63359	-2.62874	1.11559
H	-9.02307	-0.94089	-0.41950	C	-7.77333	-1.58852	0.29830
C	-0.23658	-0.23717	-1.53858	H	-8.22317	0.02331	-1.09425
C	-1.51090	-0.77842	-1.70110	H	-7.01107	-3.11829	1.61437
C	-2.64223	-0.05871	-1.27232	O	-9.04448	-1.92920	0.64220
C	-2.45076	1.23358	-0.73697	C	-10.12286	-1.19757	0.06233
C	-1.16380	1.73983	-0.59286	H	-10.13109	-1.30581	-1.03435
N	-0.09884	0.99394	-0.99081	H	-11.03929	-1.63125	0.48058
H	-1.62071	-1.76858	-2.14112	H	-10.06565	-0.12957	0.32798
H	-3.30072	1.81561	-0.38829	C	-1.32332	-1.42600	-0.71039
C	1.05128	-0.84938	-1.90797	C	-2.66418	-1.73803	-0.50545
C	1.17972	-2.07849	-2.56333	C	-3.64531	-0.72624	-0.57638
C	2.44727	-2.55553	-2.88773	C	-3.22685	0.58918	-0.86802
C	3.57269	-1.79225	-2.55784	C	-1.87595	0.86670	-1.06182
C	3.38890	-0.57567	-1.91166	N	-0.96115	-0.14117	-0.98096
N	2.16532	-0.11270	-1.59777	H	-2.95060	-2.76751	-0.29281
H	2.55725	-3.51588	-3.39392	H	-3.94992	1.40375	-0.89283
H	0.28760	-2.65362	-2.80963	C	-0.17007	-2.33449	-0.65821
H	4.58247	-2.13156	-2.78930	C	-0.25267	-3.70950	-0.42096
H	4.22952	0.06089	-1.63577	C	0.91361	-4.47343	-0.38413
C	1.04754	4.32521	0.75734	C	2.14570	-3.84639	-0.59372
C	0.19231	5.31416	1.23220	C	2.17190	-2.47492	-0.82735
C	-1.18826	5.13889	1.09249	N	1.05083	-1.73222	-0.85287
C	-1.67189	3.98027	0.48581	H	0.85956	-5.54666	-0.19498
				H	-1.22731	-4.17155	-0.26523

H	3.08193	-4.40514	-0.57402	C	8.84183	-2.06387	-0.65390
H	3.10405	-1.93606	-0.99833	H	9.80691	-1.82516	-1.11616
C	0.79023	3.33846	-1.44157	H	9.00424	-2.66978	0.25135
C	0.13198	4.55382	-1.60138	H	8.21593	-2.62037	-1.36903
C	-1.26644	4.57236	-1.60763	O	2.50259	-1.51410	2.33014
C	-1.96325	3.37657	-1.43912	O	1.02696	0.02840	-3.24021
C	-1.25609	2.18117	-1.28161	H	1.09056	0.92393	-3.61049
N	0.12026	2.17994	-1.30079	Ir	0.91534	0.31201	-1.11399
H	-1.81023	5.50961	-1.73470				
H	1.87773	3.25240	-1.42303				
H	0.71430	5.46813	-1.71949	<b>I-[Ir]-TS3</b>			
H	-3.05297	3.36290	-1.42811	O	2.91303	2.83491	-0.72793
H	0.91742	0.50613	0.46864	H	3.63725	2.29629	-1.08376
C	6.29545	-1.95485	0.57959	C	-4.34451	-1.04506	-0.73123
C	5.04813	-1.82549	1.18234	C	-5.57003	-0.35413	-0.73572
C	4.50123	-0.56320	1.47938	C	-4.38205	-2.44777	-0.56689
C	5.25295	0.59002	1.15864	C	-6.78883	-1.02028	-0.59022
C	6.49841	0.47669	0.55818	H	-5.58462	0.72815	-0.87943
C	7.02934	-0.79507	0.26162	C	-5.58643	-3.12387	-0.41559
H	4.46979	-2.71752	1.42939	H	-3.45094	-3.01707	-0.53095
H	4.86482	1.58710	1.37121	C	-6.80245	-2.41565	-0.42737
H	7.08483	1.36110	0.30367	H	-7.71627	-0.44835	-0.61198
C	3.15378	-0.50041	2.08371	H	-5.60906	-4.20621	-0.27556
C	2.57467	0.87734	2.36029	O	-7.93179	-3.15759	-0.27372
H	2.57938	1.43504	1.40914	C	-9.18890	-2.48387	-0.26355
O	1.25278	0.72048	2.84354	H	-9.36710	-1.96189	-1.21758
C	0.34265	1.69407	2.53349	H	-9.94700	-3.26434	-0.12565
C	0.67385	3.02029	2.25284	H	-9.24569	-1.76328	0.56837
C	-1.01362	1.28112	2.50468	C	-0.69507	-0.33575	-1.43555
C	-0.33518	3.95034	1.95592	C	-1.92712	-0.98478	-1.40317
H	1.71919	3.33172	2.26552	C	-3.05615	-0.33649	-0.86258
C	-2.01271	2.21815	2.22711	C	-2.90553	0.98696	-0.39797
C	-1.67066	3.55135	1.94968	C	-1.66168	1.60791	-0.45468
H	-0.06384	4.98371	1.73134	N	-0.58888	0.93343	-0.95889
H	-3.05804	1.91011	2.19874	H	-2.01253	-1.99671	-1.79685
H	-2.46119	4.26835	1.71957	H	-3.74773	1.51361	0.04811
O	-1.23153	-0.04572	2.73416	C	0.59212	-0.87785	-1.89006
C	-2.58145	-0.48562	2.86294	C	0.76571	-2.16033	-2.41847
H	-3.06498	-0.01147	3.73310	C	2.04136	-2.58771	-2.78582
H	-3.16417	-0.26839	1.95670	C	3.12298	-1.71778	-2.62482
H	-2.53172	-1.57096	3.01254	C	2.89461	-0.45225	-2.09292
H	3.20392	1.41810	3.08900	N	1.66766	-0.03626	-1.73183
H	6.68966	-2.94647	0.35906	H	2.18807	-3.58880	-3.19432
O	8.24694	-0.80645	-0.32629	H	-0.09517	-2.81811	-2.53372
				H	4.13764	-2.01169	-2.89150



H	3.70451	0.26209	-1.94653	O	5.69639	-3.08952	-0.98011
C	0.44918	4.47757	0.37133	C	5.60081	-4.43915	-1.43186
C	-0.40633	5.38247	0.99030	H	6.23433	-4.50285	-2.32477
C	-1.75974	5.05399	1.12594	H	5.97102	-5.14091	-0.66742
C	-2.21305	3.82712	0.64410	H	4.56153	-4.69332	-1.69608
C	-1.31185	2.94716	0.03794	O	1.71097	-2.06416	3.89507
N	0.01491	3.29053	-0.09469	Ir	1.14268	1.80766	-0.93396
H	-2.45466	5.74462	1.60604				
H	1.51411	4.67183	0.23584				
H	-0.01080	6.32981	1.35795	<b>I-[Ir]-IM4</b>			
H	-3.25986	3.54158	0.74438	C	-0.18935	-1.09631	-0.82771
O	0.93894	2.46244	-2.93587	C	-1.57781	-1.06307	-0.90305
H	0.68172	3.39596	-2.84276	C	-2.25486	0.17408	-0.84423
H	1.38070	1.14150	0.71512	C	-1.48761	1.35538	-0.76482
C	4.16172	-3.59509	0.85321	C	-0.09876	1.28024	-0.68113
C	3.40961	-3.09308	1.91729	N	0.50718	0.06311	-0.69370
C	3.40803	-1.72818	2.24665	H	-2.13564	-1.99305	-1.00248
C	4.21446	-0.86328	1.47538	H	-1.97805	2.32634	-0.71127
C	4.97797	-1.34605	0.42017	C	0.67903	-2.28201	-0.81483
C	4.94790	-2.71443	0.09190	C	0.22092	-3.59369	-0.96338
H	2.78782	-3.77048	2.50539	C	1.12833	-4.64948	-0.89120
H	4.23133	0.20819	1.67884	C	2.48243	-4.37256	-0.67767
H	5.59040	-0.67465	-0.18435	C	2.88523	-3.04697	-0.54482
C	2.49821	-1.25015	3.33342	N	2.01252	-2.02650	-0.60999
C	2.47746	0.13878	3.65722	H	0.78152	-5.67837	-0.99887
H	3.29580	0.80699	3.39756	H	-0.84094	-3.77949	-1.12222
O	1.43568	0.78136	1.87825	H	3.22431	-5.16901	-0.61254
C	0.11791	0.49691	2.18107	H	3.92846	-2.77489	-0.37928
C	-0.68745	1.42641	2.84263	C	3.09688	2.94388	-0.04015
C	-0.41621	-0.75641	1.79530	C	2.79885	4.30349	-0.04044
C	-2.01431	1.11416	3.15808	C	1.48031	4.70714	-0.27297
H	-0.25278	2.39376	3.10269	C	0.49858	3.74116	-0.49567
C	-1.73950	-1.07529	2.12872	C	0.84821	2.38874	-0.48285
C	-2.53001	-0.13756	2.80442	N	2.15168	2.01182	-0.25395
H	-2.64026	1.84493	3.67389	H	1.21690	5.76592	-0.28204
H	-2.16465	-2.03736	1.84262	H	4.10189	2.55846	0.13891
H	-3.56431	-0.39259	3.04585	H	3.59380	5.02824	0.13753
O	0.41574	-1.55888	1.09042	H	-0.53610	4.03033	-0.67843
C	0.03320	-2.91374	0.88409	O	4.41202	0.09024	0.12692
H	-0.12930	-3.41595	1.85110	H	4.75948	-0.81200	0.20523
H	-0.87955	-2.98362	0.27117	O	2.88141	0.12537	-2.30808
H	0.86830	-3.38633	0.35508	H	2.96017	1.07526	-2.50089
H	1.79084	0.46220	4.44148	O	2.07019	-0.24380	1.72978
H	4.12664	-4.65962	0.62148	C	0.86165	-0.69354	2.08927
				C	0.56861	-2.06360	2.21128



H	-3.84083	2.04322	-1.81114	N	1.92583	-3.01423	-0.44995
C	-6.50993	0.13034	-0.90639	H	-0.10513	-6.30894	-0.47916
H	-6.37229	-1.83295	0.02527	H	-1.23315	-4.12661	-0.94989
H	-6.31525	2.07289	-1.82424	H	2.36991	-6.31875	0.01508
O	-7.86332	0.24182	-0.96043	H	3.60805	-4.12158	-0.01148
C	-8.65240	-0.83982	-0.46707	C	4.23755	1.47717	-0.96444
H	-8.46373	-1.01116	0.60500	C	4.30545	2.83150	-1.28809
H	-9.69729	-0.54021	-0.61246	C	3.12359	3.51665	-1.57592
H	-8.45202	-1.76535	-1.03054	C	1.90989	2.82651	-1.53726
Ir	2.50659	-0.01465	-0.46928	C	1.90422	1.46371	-1.22965
				N	3.07334	0.81036	-0.93979
<b>1a-TS</b>				H	3.14103	4.57906	-1.82277
O	3.42299	-1.63858	-2.56660	H	5.12274	0.88806	-0.71876
H	3.93401	-0.85372	-2.82631	H	5.27324	3.33365	-1.30100
H	2.51592	-0.88674	0.93481	H	0.97330	3.33370	-1.76630
C	-3.08580	0.48744	-1.37302	O	0.88896	1.30748	1.63413
C	-3.44565	1.78233	-1.81238	C	1.45198	2.47211	1.66942
C	-4.13185	-0.38907	-1.02761	C	2.81940	2.68355	1.99741
C	-4.77437	2.17695	-1.89695	C	0.69450	3.65776	1.34198
H	-2.67779	2.49842	-2.10720	C	3.39637	3.96036	2.00149
C	-5.47254	-0.00938	-1.10953	H	3.42025	1.79942	2.23146
H	-3.91230	-1.39261	-0.66165	C	1.27451	4.92511	1.33846
C	-5.80376	1.28454	-1.54347	C	2.63573	5.08536	1.66987
H	-5.04001	3.17833	-2.24050	H	4.45449	4.07108	2.25652
H	-6.24523	-0.72222	-0.82317	H	0.67789	5.80080	1.07485
O	-7.07329	1.75419	-1.65072	H	3.08072	6.08312	1.66471
C	-8.14897	0.88755	-1.29164	O	-0.62085	3.40373	1.02290
H	-9.06668	1.46654	-1.45026	C	-1.40291	4.47458	0.52000
H	-8.16388	-0.01010	-1.93040	H	-1.52509	5.27560	1.26955
H	-8.07899	0.58853	-0.23340	H	-0.95626	4.90286	-0.39419
C	0.02301	-1.63759	-0.94155	H	-2.38719	4.05106	0.28105
C	-1.31624	-1.28166	-1.07814	O	4.73293	-1.70611	-0.11003
C	-1.66921	0.07422	-1.26960	H	4.98607	-1.95059	-1.02078
C	-0.62858	1.02373	-1.34572	C	1.07354	-1.00583	3.05022
C	0.69706	0.61956	-1.20125	H	1.87475	-1.74435	2.97544
N	0.97909	-0.68409	-0.99535	H	1.30396	-0.02856	3.46846
H	-2.07869	-2.05673	-1.03238	C	-2.58273	-0.72815	2.52072
H	-0.84709	2.08160	-1.47158	C	-1.28060	-0.37891	2.78650
Rh	2.81394	-1.18153	-0.59693	C	-0.21919	-1.34483	2.70370
C	0.57953	-2.98368	-0.70756	C	-0.54394	-2.68164	2.28330
C	-0.16648	-4.16491	-0.73088	C	-1.84136	-3.03562	2.01884
C	0.46712	-5.38000	-0.46848	C	-2.87776	-2.06858	2.15083
C	1.83782	-5.39032	-0.19520	H	-1.02572	0.64939	3.04002
C	2.53510	-4.18394	-0.20246	H	0.25836	-3.41753	2.20336

H	-2.11378	-4.04708	1.71669	H	-2.02424	5.30683	-2.05006
H	-3.37528	0.01557	2.58700	H	-3.14960	3.06641	-1.80425
O	-4.10393	-2.50824	1.90769	C	-3.38930	-2.56890	-0.92967
C	-5.24383	-1.66326	2.15950	C	-3.35095	-3.96343	-0.92123
H	-6.11376	-2.25699	1.86038	C	-2.11446	-4.60476	-0.84596
H	-5.29353	-1.42359	3.23113	C	-0.94872	-3.83536	-0.80219
H	-5.18822	-0.74535	1.56090	C	-1.04456	-2.44369	-0.83634
<b>1b-TS</b>				N	-2.27275	-1.82796	-0.88338
O	-2.48740	-0.10156	-3.15171	H	-2.05147	-5.69386	-0.83112
H	-2.55015	-1.06866	-3.24490	H	-4.32622	-2.01317	-0.97961
H	-1.61524	0.87214	0.63041	H	-4.28406	-4.52565	-0.96387
C	3.86130	-1.11947	-0.64080	H	0.03194	-4.30967	-0.76906
C	4.38449	-2.40304	-0.91185	O	-1.84363	0.68334	2.70356
C	4.74861	-0.13790	-0.16123	C	-2.50413	-0.45277	2.42831
C	5.73073	-2.68681	-0.71945	C	-3.89080	-0.45441	2.20328
H	3.73287	-3.18680	-1.30323	C	-1.81332	-1.70002	2.40101
C	6.10257	-0.40972	0.04313	C	-4.60356	-1.65101	2.06508
H	4.37613	0.85836	0.08665	H	-4.40252	0.51059	2.19395
C	6.60296	-1.69205	-0.23890	C	-2.52828	-2.89744	2.29320
H	6.13369	-3.67640	-0.94278	C	-3.92089	-2.86864	2.12851
H	6.75300	0.37484	0.42904	H	-5.68497	-1.62991	1.91385
O	7.90153	-2.05872	-0.07756	H	-2.00737	-3.85480	2.31500
C	8.82909	-1.08247	0.39428	H	-4.46467	-3.81118	2.03607
H	9.80071	-1.58899	0.43963	O	-0.45958	-1.62594	2.52012
H	8.89009	-0.22758	-0.29835	C	0.28435	-2.83765	2.60260
H	8.55183	-0.72566	1.39928	H	0.01243	-3.40372	3.50874
C	0.63509	0.76463	-1.24151	H	0.12543	-3.46926	1.71532
C	2.00015	0.49068	-1.12739	H	1.33864	-2.54017	2.65573
C	2.42883	-0.81891	-0.84017	O	-4.10898	0.72562	-1.03229
C	1.45470	-1.83893	-0.71887	H	-4.32594	0.95293	-1.95367
C	0.10926	-1.52952	-0.89003	C	-1.08281	1.54387	1.44095
N	-0.25457	-0.25025	-1.14444	C	0.33687	1.38747	1.54309
H	2.72394	1.29613	-1.24287	C	1.19925	2.47572	1.70024
H	1.74835	-2.85674	-0.46590	C	0.69237	3.78049	1.71557
Rh	-2.14912	0.19429	-1.18431	C	-0.70266	3.97216	1.61072
C	-0.00659	2.07204	-1.46613	C	-1.56401	2.89850	1.47253
C	0.68146	3.28354	-1.57356	H	0.75103	0.37933	1.52573
C	-0.03721	4.46214	-1.78197	H	2.27127	2.28596	1.77314
C	-1.42894	4.40786	-1.88822	H	-1.09045	4.99378	1.61092
C	-2.06460	3.17395	-1.75936	H	-2.63673	3.07372	1.36155
N	-1.37794	2.04297	-1.55314	O	1.46020	4.92096	1.81725
H	0.48959	5.41465	-1.85769	C	2.87043	4.75813	1.80566
H	1.76750	3.30133	-1.48963	H	3.29777	5.76846	1.84339
				H	3.21972	4.18306	2.68036

H	3.20743	4.25206	0.88386	C	0.82105	-2.63348	3.40966
				C	-1.21466	-3.46078	2.36749
				C	1.34061	-2.35624	2.14635
<b>[2Rh]-1a-TS</b>				H	1.40985	-2.42188	4.30195
O	0.82169	0.22107	-2.66034	C	-0.66862	-3.17385	1.11225
O	2.01830	-1.68443	-2.59155	H	-2.21195	-3.89411	2.44335
C	1.59996	-0.63479	-3.17840	N	0.57257	-2.60916	1.04145
C	2.10335	-0.37316	-4.57424	H	-0.88863	-3.38423	4.50109
H	2.28360	-1.31585	-5.10742	C	2.66093	-1.83827	1.80815
H	1.39429	0.25440	-5.12943	C	3.68861	-1.60443	2.73356
H	3.06069	0.16878	-4.49897	C	4.93724	-1.18993	2.28450
O	2.23246	-4.06417	-1.06210	C	5.14796	-1.03698	0.90259
H	1.85579	-4.65413	-0.38725	C	4.09668	-1.27394	0.02989
C	-1.36977	-0.02560	1.65572	N	2.87446	-1.65057	0.45825
C	-1.68015	0.02208	3.01456	H	5.74350	-1.00018	2.99474
C	-0.71674	0.48448	3.92442	H	3.49631	-1.75370	3.79633
C	0.54468	0.89367	3.47353	H	6.11266	-0.71805	0.50679
C	0.83255	0.84455	2.10647	H	4.20759	-1.15892	-1.04900
N	-0.12941	0.39553	1.23856	C	-0.88810	-3.27282	-2.52011
H	-2.65992	-0.30518	3.36265	C	-2.05911	-3.97194	-2.79183
H	1.29665	1.24990	4.17780	C	-2.84832	-4.41970	-1.72272
Rh	0.31989	0.23625	-0.60772	C	-2.43724	-4.14909	-0.42103
C	-2.21146	-0.45945	0.55382	C	-1.24373	-3.44751	-0.20101
C	-3.52151	-0.95009	0.68178	N	-0.48259	-3.00927	-1.26454
C	-4.24763	-1.28457	-0.45236	H	-3.77385	-4.96817	-1.90464
C	-3.65930	-1.08694	-1.71832	H	-0.23939	-2.90636	-3.31711
C	-2.35923	-0.61941	-1.79277	H	-2.34495	-4.15738	-3.82775
N	-1.62155	-0.32879	-0.69474	H	-3.02442	-4.49023	0.43154
H	-5.26071	-1.67892	-0.36450	H	-0.47312	1.99653	-1.05899
H	-3.95512	-1.06259	1.67569	O	-0.58789	2.93254	-1.54010
H	-4.20045	-1.31489	-2.63716	C	0.57740	3.67999	-1.39553
H	-1.85255	-0.48205	-2.74933	C	1.33842	3.99235	-2.51777
C	3.06974	1.54213	-0.67801	C	0.95103	4.13466	-0.11155
C	4.17971	2.14620	-0.10566	C	2.49487	4.77017	-2.37903
C	4.22780	2.31115	1.28910	H	1.01521	3.61599	-3.48982
C	3.15500	1.86408	2.05251	C	2.10270	4.92054	0.02029
C	2.04549	1.27597	1.42621	C	2.86633	5.22989	-1.11259
N	2.01709	1.10960	0.05103	H	3.09738	5.01325	-3.25610
H	5.09063	2.77663	1.76780	H	2.41237	5.28086	1.00104
H	2.99529	1.38966	-1.75525	H	3.76638	5.83695	-0.99362
H	4.99472	2.48388	-0.74652	O	0.13921	3.76703	0.90830
H	3.16041	1.97278	3.13738	C	0.40444	4.28276	2.21186
H	-0.95073	0.52128	4.98920	H	1.39305	3.95888	2.57085
Rh	1.30472	-2.23134	-0.69129	H	0.34902	5.38292	2.21064
C	-0.46837	-3.17723	3.51620				



C	5.80093	4.49292	0.71073	Rh	0.38227	-0.36512	2.12265
H	6.41705	5.04390	1.43297	C	0.88781	-2.13407	-0.09381
H	6.41143	4.24815	-0.17542	C	0.70627	-3.10309	-1.08259
H	4.95008	5.12423	0.40040	C	-0.49285	-3.81831	-1.12912
Rh	-2.84960	0.09688	-0.61269	C	-1.47843	-3.55841	-0.17657
C	-2.61310	1.11257	3.92849	C	-1.24401	-2.56881	0.77736
C	-2.76933	-0.21862	3.52278	N	-0.10484	-1.86784	0.81136
C	-2.57777	2.14250	2.98467	H	-0.64751	-4.57677	-1.89803
C	-2.86906	-0.50135	2.15965	H	1.50045	-3.29809	-1.80283
H	-2.80450	-1.02284	4.25654	H	-2.42586	-4.09821	-0.16740
C	-2.68131	1.81909	1.62811	H	-1.98235	-2.32922	1.54122
H	-2.46392	3.18066	3.29479	C	1.02273	1.84386	4.10765
N	-2.80129	0.51750	1.26280	C	1.83973	2.81503	4.68505
H	-2.52073	1.34686	4.98948	C	3.13624	2.98399	4.19439
C	-3.04911	-1.81053	1.52130	C	3.57850	2.18208	3.14053
C	-3.23511	-3.01108	2.21298	C	2.71591	1.22587	2.60007
C	-3.45307	-4.18518	1.49419	N	1.44951	1.07220	3.09905
C	-3.49498	-4.13204	0.09681	H	3.80041	3.73489	4.62521
C	-3.29139	-2.91094	-0.53939	H	0.00059	1.66539	4.44504
N	-3.05607	-1.78258	0.15056	H	1.45617	3.42350	5.50457
H	-3.59652	-5.13068	2.01912	H	4.58414	2.29697	2.73674
H	-3.21326	-3.01742	3.30238	O	-1.31211	-0.09613	3.19465
H	-3.67149	-5.02576	-0.50171	H	-1.99152	-0.69857	2.85144
H	-3.30676	-2.81392	-1.62530	O	0.91524	-1.76139	3.48300
C	-2.84705	2.88447	-1.85181	H	0.14467	-1.67233	4.07390
C	-2.82488	4.27731	-1.80283	C	5.63867	-0.63611	-1.12123
C	-2.71053	4.91020	-0.56271	C	6.49841	0.47522	-1.20393
C	-2.64668	4.13224	0.59396	C	6.01654	-1.81191	-1.80738
C	-2.69079	2.74031	0.48596	C	7.68588	0.43133	-1.93566
N	-2.76608	2.13327	-0.74265	H	6.23106	1.41052	-0.70836
H	-2.67425	5.99829	-0.49355	C	7.19903	-1.87353	-2.53280
H	-2.92941	2.34633	-2.79639	H	5.38816	-2.70278	-1.75187
H	-2.88627	4.84683	-2.73035	C	8.04566	-0.75106	-2.60440
H	-2.56986	4.59613	1.57665	H	8.31669	1.31853	-1.98464
				H	7.49387	-2.78880	-3.04929
				O	9.17986	-0.90018	-3.33569
<b>1c-IM1</b>				C	10.07609	0.20623	-3.43309
C	2.12532	-1.35192	0.09119	H	10.44896	0.50197	-2.43937
C	3.29189	-1.41005	-0.66930	H	10.91295	-0.13952	-4.05175
C	4.38567	-0.57937	-0.34172	H	9.58978	1.06762	-3.91834
C	4.24790	0.30925	0.74687	O	-0.20320	1.06541	0.75980
C	3.05739	0.33845	1.47088	H	-0.81353	1.61933	1.27751
N	2.05361	-0.50223	1.13804	C	-4.74299	-2.84164	-1.83794
H	3.34567	-2.08185	-1.52485	C	-4.02947	-1.66042	-1.61357
H	5.06992	0.96284	1.03546				

C	-3.91421	-1.10651	-0.33169	C	4.14321	-0.39982	-0.45728
C	-4.54350	-1.76832	0.73845	C	3.90240	-0.18784	0.91829
C	-5.26363	-2.94496	0.53331	C	2.68678	-0.57679	1.47614
C	-5.36507	-3.49088	-0.75818	N	1.75219	-1.15834	0.69297
H	-3.53313	-1.17106	-2.45412	H	3.27931	-1.19266	-2.29216
H	-4.45361	-1.36376	1.75032	H	4.66802	0.26115	1.54925
H	-5.74414	-3.46458	1.36448	Rh	0.02474	-1.59154	1.50392
C	-3.12447	0.16736	-0.11405	C	0.79819	-2.10203	-1.24320
C	-3.96644	1.41278	-0.44391	C	0.79627	-2.57429	-2.55677
H	-4.19118	1.41572	-1.52134	C	-0.29138	-3.32216	-3.01398
O	-3.16651	2.57510	-0.11380	C	-1.35043	-3.58362	-2.14525
C	-2.65711	3.30854	-1.16129	C	-1.30737	-3.05734	-0.85348
C	-1.27656	3.48148	-1.26574	N	-0.27223	-2.32852	-0.41854
C	-3.51911	3.94597	-2.08759	H	-0.30081	-3.70533	-4.03550
C	-0.73233	4.27290	-2.28561	H	1.64933	-2.37578	-3.20518
H	-0.64023	2.96672	-0.54357	H	-2.21148	-4.17694	-2.45227
C	-2.96909	4.72229	-3.11702	H	-2.11994	-3.22399	-0.14635
C	-1.57995	4.88442	-3.21177	C	0.49940	-0.80565	4.39604
H	0.35028	4.39761	-2.35668	C	1.25186	-0.29585	5.45424
H	-3.62196	5.21371	-3.83893	C	2.54893	0.15327	5.20214
H	-1.16907	5.49682	-4.01762	C	3.05991	0.07799	3.90420
O	-4.85343	3.75832	-1.89492	C	2.26132	-0.44129	2.88402
C	-5.76118	4.32154	-2.83742	N	0.99086	-0.87163	3.15318
H	-5.69331	5.42149	-2.84637	H	3.16357	0.55824	6.00757
H	-5.57274	3.93120	-3.85061	H	-0.52203	-1.16654	4.52569
H	-6.76175	4.01758	-2.50671	H	0.81750	-0.25572	6.45347
H	-4.80456	-3.24889	-2.84713	H	4.07115	0.41977	3.68499
O	-6.07569	-4.65024	-0.86822	O	-1.68932	-1.97037	2.47167
C	-6.18404	-5.25402	-2.15438	H	-2.34037	-2.28250	1.82225
H	-6.78141	-6.16288	-2.01153	O	0.62865	-3.38316	1.99843
H	-6.69552	-4.58637	-2.86695	H	-0.14281	-3.64448	2.54039
H	-5.19195	-5.52499	-2.55149	C	5.41918	0.01516	-1.07294
O	-1.94862	0.16646	-0.90240	C	6.16254	1.09065	-0.55112
H	-2.85617	0.23214	0.95675	C	5.93502	-0.65346	-2.20566
C	-5.28093	1.52358	0.33293	C	7.36835	1.49523	-1.12493
H	-5.61737	2.56656	0.26703	H	5.78536	1.64990	0.30725
H	-5.11103	1.28778	1.40050	C	7.13833	-0.26822	-2.78170
O	-6.31557	0.72282	-0.22111	H	5.40140	-1.50681	-2.62842
H	-6.05748	-0.20834	-0.10111	C	7.86671	0.81164	-2.24714
H	-1.20795	0.50945	-0.28960	H	7.90502	2.34252	-0.69889
				H	7.54111	-0.79682	-3.64754
				O	9.02985	1.12033	-2.87496
<b>1c-TS1</b>				C	9.81225	2.20053	-2.36644
C	1.93968	-1.40291	-0.62026	H	10.12863	2.00570	-1.32920
C	3.13668	-1.02391	-1.22571				



H	10.69465	2.26224	-3.01455	H	-5.69279	0.21692	-0.45182
H	9.25356	3.14903	-2.41200	H	-0.69496	1.14785	1.01434
O	-0.02753	1.40939	1.78939				
H	-0.51321	1.15480	2.58971	<b>1c-IM2</b>			
C	-4.04489	-1.70954	-2.48516	C	0.42687	1.13836	-1.60078
C	-3.43325	-0.68476	-1.75988	C	1.66998	1.71176	-1.33528
C	-3.55167	-0.59435	-0.36499	C	2.81212	0.88852	-1.23119
C	-4.31837	-1.57080	0.29620	C	2.65820	-0.50392	-1.41128
C	-4.92503	-2.61338	-0.40903	C	1.39356	-1.02880	-1.66891
C	-4.78395	-2.69183	-1.80418	N	0.33547	-0.19802	-1.77217
H	-2.82907	0.05718	-2.28713	H	1.74582	2.78395	-1.15904
H	-4.43623	-1.51964	1.38222	H	3.51605	-1.17034	-1.33477
H	-5.50245	-3.38339	0.10665	Rh	-1.44379	-0.98393	-1.72653
C	-2.85842	0.54690	0.37021	C	-0.88033	1.81790	-1.70654
C	-3.69476	1.83601	0.18132	C	-1.05213	3.20371	-1.74999
H	-3.67966	2.11652	-0.88309	C	-2.33389	3.72767	-1.92694
O	-3.06702	2.88868	0.95943	C	-3.41735	2.85625	-2.05996
C	-2.46712	3.91720	0.27324	C	-3.18807	1.48312	-1.99476
C	-1.12302	4.20042	0.52202	N	-1.95921	0.98128	-1.81420
C	-3.20428	4.73811	-0.61730	H	-2.48267	4.80790	-1.96350
C	-0.49197	5.28150	-0.10729	H	-0.18774	3.86171	-1.66241
H	-0.58413	3.53326	1.19886	H	-4.43368	3.22640	-2.19554
C	-2.56358	5.80803	-1.25738	H	-3.99461	0.75411	-2.08099
C	-1.21222	6.07816	-0.99987	C	-0.78408	-3.95796	-1.74781
H	0.56135	5.48797	0.09506	C	0.08020	-5.05103	-1.80922
H	-3.12032	6.44395	-1.94635	C	1.45588	-4.81981	-1.87599
H	-0.73143	6.91966	-1.50389	C	1.92990	-3.50669	-1.85622
O	-4.51953	4.42530	-0.77858	C	1.01746	-2.45352	-1.76848
C	-5.28362	5.16116	-1.72851	N	-0.32838	-2.69906	-1.73909
H	-5.35832	6.22331	-1.44381	H	2.15724	-5.65327	-1.93938
H	-4.84694	5.07914	-2.73711	H	-1.86815	-4.07275	-1.70018
H	-6.28247	4.70802	-1.72265	H	-0.32858	-6.06185	-1.81205
H	-3.92189	-1.75212	-3.56742	H	2.99822	-3.29732	-1.90204
O	-5.38034	-3.75903	-2.41506	O	-3.27425	-1.85031	-1.60857
C	-5.25719	-3.87718	-3.82968	H	-3.80477	-1.25202	-1.05671
H	-5.79846	-4.79100	-4.10436	O	-1.67671	-1.12593	-3.73902
H	-5.71089	-3.01367	-4.34316	H	-2.54441	-1.56882	-3.74977
H	-4.20136	-3.97161	-4.13247	C	4.13010	1.46543	-0.89951
O	-1.55478	0.72147	-0.06997	C	5.09767	0.70921	-0.21215
H	-2.91139	0.31415	1.45950	C	4.45489	2.79660	-1.24198
C	-5.15093	1.72831	0.64477	C	6.33920	1.24592	0.13135
H	-5.52941	2.74496	0.81206	H	4.87182	-0.31425	0.09290
H	-5.19981	1.18329	1.60717	C	5.68978	3.34172	-0.91460
O	-5.99845	1.13348	-0.33074	H	3.73911	3.40932	-1.79363

C	6.64297	2.57183	-0.22120	C	-2.64916	-1.29628	3.70550
H	7.05503	0.63181	0.67721	H	-2.11639	-1.64955	4.59971
H	5.94263	4.36678	-1.19163	H	-3.38647	-2.07090	3.42104
O	7.81953	3.18743	0.06455	O	-3.28369	-0.07784	4.06532
C	8.81843	2.45020	0.76858	H	-3.77895	0.23120	3.28624
H	9.13415	1.56393	0.19500				
H	9.66800	3.13354	0.88635				
H	8.45464	2.13901	1.76105	<b>1c-TS2</b>			
C	-3.37526	2.65479	1.20518	O	3.55865	2.25175	-0.90183
C	-2.57183	1.51622	1.26262	H	4.17014	1.50746	-0.77443
C	-3.10977	0.22674	1.11869	C	3.76109	-2.86904	0.64828
C	-4.49565	0.10609	0.92325	C	2.59684	-2.16879	0.97789
C	-5.31503	1.23517	0.84622	C	2.61798	-0.80387	1.29365
C	-4.75581	2.51569	0.97597	C	3.86072	-0.14383	1.26686
H	-1.49530	1.63169	1.40950	C	5.03425	-0.82004	0.92571
H	-4.94198	-0.88797	0.82559	C	4.98865	-2.18764	0.60858
H	-6.38897	1.14347	0.67211	H	1.63116	-2.67888	0.96158
C	-2.18607	-0.98173	1.17315	H	3.90624	0.92545	1.48857
C	-1.61115	-1.13443	2.59279	H	5.99371	-0.30010	0.88182
H	-0.99064	-0.25572	2.81502	C	1.29593	-0.08136	1.60123
O	-0.79243	-2.32898	2.63896	C	1.00461	-0.10111	3.12788
C	0.56699	-2.18442	2.50991	O	-0.03323	0.86152	3.44521
C	1.23549	-2.95364	1.55611	C	-1.27541	0.87136	2.87045
C	1.31179	-1.34591	3.37814	C	-1.78988	2.12309	2.51407
C	2.62736	-2.87591	1.41940	C	-2.10368	-0.27264	2.74029
H	0.63861	-3.60725	0.91731	C	-3.09828	2.26130	2.03157
C	2.69960	-1.24176	3.21141	H	-1.13281	2.98949	2.61723
C	3.35331	-2.00491	2.23418	C	-3.39141	-0.13519	2.21026
H	3.13472	-3.48600	0.67046	C	-3.89692	1.12865	1.87070
H	3.27858	-0.58272	3.85881	H	-3.47628	3.25096	1.76794
H	4.43687	-1.92031	2.12694	H	-4.01670	-1.01948	2.07942
O	0.60699	-0.69890	4.34893	H	-4.91144	1.21163	1.47509
C	1.30130	0.20778	5.20044	O	-1.59120	-1.46775	3.15708
H	2.07140	-0.31334	5.79217	C	-2.06452	-2.64570	2.50834
H	1.76829	1.01895	4.61869	H	-3.10313	-2.88071	2.79217
H	0.54281	0.62669	5.87283	H	-1.99148	-2.53623	1.41482
H	-2.92277	3.64023	1.31292	H	-1.40886	-3.46014	2.84205
O	-5.61638	3.56885	0.85002	H	0.67533	-1.11418	3.40435
C	-5.08142	4.88670	0.94123	H	3.70104	-3.92860	0.39835
H	-5.92939	5.56717	0.79544	O	6.17617	-2.76702	0.25210
H	-4.63228	5.06763	1.93151	C	6.17199	-4.15328	-0.07301
H	-4.32770	5.06582	0.15737	H	7.20944	-4.40873	-0.32236
O	-1.10924	-0.85321	0.29585	H	5.84033	-4.76321	0.78358
H	-2.79006	-1.88836	0.96129	H	5.52509	-4.35945	-0.94159
				O	0.25163	-0.58716	0.89498



O	-0.90380	-3.31616	0.49635	H	-0.11326	0.91400	-2.58220
C	-3.35172	-2.09412	0.00425	H	0.87220	1.58007	-1.25070
H	-3.35275	-2.99639	-0.63171	O	-1.11893	2.06162	-1.17856
H	-3.40008	-2.41888	1.05328	H	-1.98060	1.60512	-1.32715
O	-4.49245	-1.28323	-0.23127	O	-0.59022	0.85604	1.68583
H	-4.51196	-1.07365	-1.18027	H	-0.09637	0.32992	2.33385
				Na	-1.26421	2.77002	0.97433

**1c-A-TS3**

H	-0.41185	0.26380	0.60170
C	3.80872	0.59630	0.70386
C	2.48247	0.26436	0.41375
C	2.16795	-0.78272	-0.46895
C	3.22787	-1.51104	-1.04650
C	4.55145	-1.18126	-0.78302
C	4.85176	-0.12131	0.09472
H	1.67748	0.80318	0.91823
H	2.99495	-2.34050	-1.71757
H	5.37511	-1.73132	-1.24260
C	0.76374	-1.19495	-0.78015
C	-0.28465	-0.18297	-0.71852
O	-1.56046	-0.71482	-1.17552
C	-2.49962	-0.97917	-0.21118
C	-2.37432	-2.04900	0.67591
C	-3.62923	-0.13338	-0.13725
C	-3.37146	-2.29790	1.62842
H	-1.48717	-2.67995	0.59952
C	-4.62805	-0.38395	0.81054
C	-4.49354	-1.46809	1.68994
H	-3.26803	-3.13946	2.31669
H	-5.50322	0.26301	0.87521
H	-5.27767	-1.65501	2.42695
O	-3.64720	0.91148	-1.02289
C	-4.71050	1.86188	-0.92943
H	-5.67938	1.38267	-1.13847
H	-4.73300	2.33049	0.06750
H	-4.50033	2.62013	-1.69290
H	4.01815	1.40223	1.40717
O	6.17267	0.13082	0.30017
C	6.52961	1.19240	1.18315
H	7.62602	1.22020	1.19232
H	6.13957	2.15758	0.82157
H	6.15773	1.00245	2.20300
O	0.52876	-2.39889	-1.02435
C	-0.08904	1.10933	-1.49315

**1c-A-IM4**

H	-0.40011	0.06467	1.07108
C	3.81047	0.72527	0.52928
C	2.47538	0.37460	0.29474
C	2.12947	-0.77036	-0.44144
C	3.18124	-1.58002	-0.91729
C	4.51384	-1.24216	-0.70554
C	4.83947	-0.08137	0.01947
H	1.69424	1.00161	0.72666
H	2.93216	-2.49161	-1.46462
H	5.32344	-1.86669	-1.08948
C	0.71916	-1.23886	-0.70017
C	-0.30197	-0.29511	-0.90234
O	-1.58001	-0.84366	-1.28644
C	-2.51306	-0.95778	-0.28200
C	-2.40622	-1.93464	0.70988
C	-3.60955	-0.06574	-0.27149
C	-3.38368	-2.04327	1.70687
H	-1.53978	-2.59725	0.67617
C	-4.58789	-0.17469	0.72442
C	-4.47075	-1.16595	1.70916
H	-3.29212	-2.81241	2.47675
H	-5.43639	0.50958	0.74251
H	-5.24019	-1.24245	2.48062
O	-3.61501	0.88658	-1.25894
C	-4.68485	1.83536	-1.27946
H	-5.65029	1.32673	-1.42396
H	-4.70780	2.42582	-0.34969
H	-4.48088	2.49367	-2.13211
H	4.03357	1.61577	1.11737
O	6.16999	0.17377	0.18703
C	6.54338	1.34109	0.91312
H	7.64031	1.35669	0.91737
H	6.16496	2.25333	0.42320
H	6.17322	1.30091	1.95076
O	0.52750	-2.50339	-0.69979

C	-0.16995	1.08289	-1.45967	O	0.19743	-2.24980	-1.31564
H	-0.35417	1.07317	-2.55202	C	-0.32831	1.29654	-1.83821
H	0.83175	1.49365	-1.29083	H	-1.14555	1.89306	-2.24092
O	-1.11576	2.02939	-0.89008	H	0.67908	1.67982	-1.96714
H	-2.00783	1.70674	-1.15576	O	-0.35978	2.58115	0.01226
O	-0.53466	0.48321	1.97175	H	-1.10446	3.11347	-0.30740
H	0.29306	0.29395	2.44400	O	-0.27845	-1.10413	2.16382
Na	-1.20914	2.49376	1.30532	H	0.32282	-1.63505	1.61295
				Na	-0.71521	0.96206	1.37641

#### 1c-A-TS4

H	-1.09259	-1.64003	2.18575
C	3.42881	0.88453	0.27899
C	2.14382	0.61629	-0.20216
C	1.82961	-0.62117	-0.79708
C	2.85307	-1.59103	-0.88448
C	4.13601	-1.33237	-0.42622
C	4.43581	-0.08749	0.16289
H	1.38866	1.40110	-0.10381
H	2.61718	-2.56094	-1.32566
H	4.92838	-2.07894	-0.50855
C	0.46437	-1.03085	-1.25290
C	-0.54090	-0.03564	-1.60687
O	-1.84709	-0.54809	-1.79686
C	-2.56391	-0.75889	-0.62474
C	-2.59208	-2.01411	-0.01780
C	-3.30581	0.31643	-0.07377
C	-3.30455	-2.20897	1.17463
H	-2.02625	-2.82046	-0.48268
C	-3.99506	0.12283	1.13552
C	-3.98534	-1.13530	1.75452
H	-3.31730	-3.19366	1.64606
H	-4.55408	0.94383	1.58509
H	-4.52923	-1.26953	2.69189
O	-3.29351	1.47852	-0.77294
C	-3.94918	2.61553	-0.21349
H	-5.03080	2.43443	-0.10830
H	-3.51960	2.87768	0.76677
H	-3.78012	3.43531	-0.92155
H	3.63037	1.85038	0.74200
O	5.71312	0.08038	0.58935
C	6.07290	1.32597	1.18653
H	7.13567	1.23971	1.44274
H	5.92959	2.15866	0.47946
H	5.48633	1.51055	2.10070

#### 1c-A-IM5

C	3.15676	1.26880	0.35953
C	1.92204	0.65747	0.19148
C	1.83794	-0.70975	-0.15554
C	3.03235	-1.43005	-0.34725
C	4.27639	-0.83474	-0.16333
C	4.34311	0.52627	0.19583
H	1.01262	1.25076	0.29724
H	2.97281	-2.48249	-0.63152
H	5.18298	-1.42409	-0.29825
C	0.55490	-1.39823	-0.40699
C	-0.69107	-0.90195	0.25933
O	-1.79189	-1.16856	-0.52602
C	-3.00980	-0.63008	-0.13090
C	-4.00989	-1.46603	0.35238
C	-3.22355	0.75822	-0.28159
C	-5.25965	-0.93070	0.69363
H	-3.79676	-2.53178	0.45253
C	-4.47275	1.28770	0.06994
C	-5.48065	0.44112	0.55280
H	-6.04862	-1.58498	1.06912
H	-4.66599	2.35526	-0.03724
H	-6.44941	0.87022	0.81811
O	-2.17684	1.47461	-0.76513
C	-2.33016	2.88713	-0.89748
H	-3.13311	3.13218	-1.61086
H	-2.54412	3.35345	0.07755
H	-1.37137	3.25663	-1.28032
H	3.23197	2.32774	0.61266
O	5.49869	1.20052	0.39584
C	6.73736	0.50543	0.23902
H	7.52133	1.24276	0.44823
H	6.81315	-0.32917	0.95379
H	6.84921	0.12757	-0.78941

O	0.47716	-2.38455	-1.14451	C	-2.06865	-0.46308	-1.17925
C	-0.73809	-0.39034	1.50087	C	-1.74899	0.90962	-1.24820
H	0.18286	-0.24297	2.06394	C	-0.39108	1.28260	-1.33289
H	-1.68592	-0.13892	1.98265	C	0.59778	0.30083	-1.30224
<b>1c-A-TS5</b>				N	0.24295	-1.00105	-1.19199
C	4.27903	2.70106	1.69518	H	-3.10508	-0.78639	-1.09030
C	3.20457	1.88810	2.03755	H	-0.11126	2.33232	-1.40908
C	1.89514	2.19503	1.60891	Rh	1.63212	-2.29396	-0.78180
C	1.70798	3.38330	0.87879	C	-1.17338	-2.86772	-0.97943
C	2.77298	4.21088	0.52917	C	-2.36469	-3.57846	-1.13548
C	4.07576	3.85744	0.92029	C	-2.35675	-4.96726	-0.99364
H	3.38901	1.02517	2.67715	C	-1.15979	-5.61215	-0.67788
H	0.69818	3.65128	0.56443	C	-0.00140	-4.85019	-0.52999
H	2.58639	5.10868	-0.05953	N	-0.00242	-3.51901	-0.68960
C	0.67344	1.41130	1.96077	H	-3.27895	-5.53577	-1.12252
C	0.74484	-0.00698	2.30744	H	-3.28432	-3.04589	-1.37610
O	-0.40321	-0.42842	2.98538	H	-1.11170	-6.69375	-0.54813
C	-1.18054	-1.49672	2.57288	H	0.96210	-5.30077	-0.28689
C	-0.77520	-2.82280	2.72538	C	4.13386	-0.57501	-1.04915
C	-2.49080	-1.20103	2.12228	C	4.82064	0.60771	-1.31395
C	-1.65787	-3.87079	2.43245	C	4.09014	1.75734	-1.62480
H	0.22462	-3.03547	3.10367	C	2.69625	1.69517	-1.64309
C	-3.37611	-2.25390	1.85464	C	2.06014	0.48902	-1.34026
C	-2.95563	-3.58103	2.00964	N	2.79370	-0.63542	-1.06658
H	-1.32895	-4.90468	2.55079	H	4.59937	2.69595	-1.84784
H	-4.39107	-2.04325	1.51766	H	4.65067	-1.50842	-0.82015
H	-3.65580	-4.38955	1.79063	H	5.91048	0.61660	-1.28169
O	-2.80383	0.11459	2.00084	H	2.10229	2.57303	-1.89133
C	-4.14694	0.46092	1.67363	C	-2.81282	1.93010	-1.18049
H	-4.44075	0.05272	0.69461	C	-4.09857	1.68144	-1.69169
H	-4.84335	0.09941	2.44797	C	-2.58175	3.16793	-0.54228
H	-4.17263	1.55641	1.63321	C	-5.12493	2.62118	-1.58044
H	5.29149	2.46002	2.02394	H	-4.30711	0.73928	-2.20278
O	5.18775	4.56716	0.59844	C	-3.59570	4.10933	-0.41592
C	5.03700	5.73699	-0.20532	H	-1.60630	3.37891	-0.10082
H	6.04921	6.13282	-0.35122	C	-4.87728	3.84425	-0.93444
H	4.59262	5.48987	-1.18290	H	-6.10506	2.39552	-2.00006
H	4.41607	6.49063	0.30482	H	-3.42045	5.05830	0.09420
O	-0.42289	2.00803	2.00697	O	-5.80703	4.82137	-0.76563
C	1.75416	-0.90121	2.00861	C	-7.12678	4.59398	-1.25736
H	2.67854	-0.52398	1.57755	H	-7.69977	5.49513	-1.00764
H	1.84453	-1.82760	2.57755	H	-7.12364	4.45022	-2.34987
C	-1.04603	-1.40758	-1.13878	H	-7.58524	3.71823	-0.77034
				O	3.04291	-3.64301	-0.20233

H	3.68966	-3.13849	0.31900	C	-2.32625	-0.41078	-1.06189
H	1.41049	-1.76775	0.76286	C	-1.99950	0.95468	-1.21127
O	2.02002	-2.98225	-2.73554	C	-0.65040	1.31868	-1.38708
H	2.68869	-3.63957	-2.47158	C	0.33588	0.33208	-1.37844
				N	-0.02369	-0.95866	-1.19649
<b>1c-A-IM6</b>				H	-3.35796	-0.71554	-0.89326
C	5.03358	1.67957	1.89102	H	-0.37705	2.36390	-1.52156
C	3.73012	1.21623	2.05173	Rh	1.39968	-2.27410	-0.93200
C	2.62929	1.91566	1.50898	C	-1.42594	-2.79598	-0.73721
C	2.90159	3.14211	0.87515	C	-2.63738	-3.47114	-0.58430
C	4.19967	3.62940	0.71498	C	-2.62629	-4.83110	-0.26806
C	5.28165	2.87884	1.20040	C	-1.40375	-5.48808	-0.11420
H	3.57599	0.31310	2.64264	C	-0.22435	-4.76548	-0.28932
H	2.06064	3.71996	0.48916	N	-0.23558	-3.46151	-0.59601
H	4.35885	4.57546	0.19758	H	-3.56663	-5.36910	-0.13928
C	1.18879	1.50831	1.61006	H	-3.57670	-2.93293	-0.70456
C	0.81866	0.15024	1.75588	H	-1.35317	-6.54734	0.13913
O	-0.56658	0.03068	1.89158	H	0.76275	-5.22016	-0.19058
C	-1.33483	-1.04527	2.19205	C	3.88318	-0.54706	-1.41104
C	-0.92100	-2.33346	2.56023	C	4.54580	0.63884	-1.72050
C	-2.73291	-0.76692	2.13505	C	3.78778	1.78366	-1.97975
C	-1.86433	-3.33649	2.82494	C	2.39831	1.72012	-1.88449
H	0.13181	-2.57978	2.64514	C	1.78826	0.51139	-1.53681
C	-3.66193	-1.77861	2.38989	N	2.54585	-0.61620	-1.33862
C	-3.22822	-3.06872	2.73188	H	4.27483	2.72308	-2.24338
H	-1.51123	-4.33282	3.09819	H	4.42460	-1.47307	-1.21203
H	-4.72864	-1.56246	2.33180	H	5.63502	0.65343	-1.76166
H	-3.96479	-3.85063	2.92702	H	1.78710	2.60250	-2.06930
O	-3.06310	0.52083	1.84180	O	2.78760	-3.68488	-0.52166
C	-4.44539	0.85527	1.77225	H	3.57677	-3.47824	-1.04975
H	-4.95704	0.27653	0.98676	H	1.15040	-1.76765	0.84149
H	-4.94187	0.67944	2.74085	C	-3.04674	1.98946	-1.12098
H	-4.48593	1.92283	1.52595	C	-4.34638	1.76643	-1.60523
H	5.87844	1.12933	2.31022	C	-2.77512	3.21606	-0.47738
O	6.59009	3.24201	1.06632	C	-5.34947	2.72871	-1.47069
C	6.88324	4.43807	0.34902	H	-4.58346	0.82875	-2.11248
H	7.97668	4.52553	0.34113	C	-3.76589	4.17813	-0.32700
H	6.51131	4.38030	-0.68726	H	-1.78821	3.38937	-0.04376
H	6.44809	5.31980	0.84716	C	-5.06190	3.94310	-0.82476
O	0.31156	2.43874	1.57517	H	-6.34320	2.52608	-1.86959
C	1.65837	-1.03527	1.58330	H	-3.56330	5.11838	0.18917
H	2.64651	-0.77223	1.20093	O	-5.96689	4.93934	-0.63276
H	1.78724	-1.70178	2.44984	C	-7.30302	4.74011	-1.09095
C	-1.30411	-1.35523	-1.02921	H	-7.85113	5.65187	-0.82435

H	-7.33119	4.59955	-2.18351	H	6.87802	0.16872	0.70433
H	-7.76646	3.87239	-0.59430	C	5.88001	3.44573	-1.11365
O	1.43642	-2.85115	-2.84527	H	3.95540	3.22186	-0.20319
H	2.06201	-3.59641	-2.76474	C	7.16937	2.90890	-1.28796
<b>1c-A-TS6</b>				H	8.51389	1.29037	-0.73082
C	3.30383	-1.21555	1.91601	H	5.61627	4.36355	-1.64257
C	4.33578	-0.52658	1.28733	O	8.00318	3.59883	-2.11295
C	4.27194	0.87869	1.16711	C	9.31056	3.07673	-2.34116
C	3.18234	1.55166	1.75943	H	9.79557	3.77299	-3.03605
C	2.17944	0.82683	2.40097	H	9.88874	3.02958	-1.40412
N	2.25138	-0.53103	2.43832	H	9.26280	2.07424	-2.79668
H	5.14735	-1.08244	0.82008	C	3.30792	-2.41187	-1.49485
H	3.11009	2.63740	1.70737	C	2.11729	-1.96432	-0.93578
Rh	0.75135	-1.52394	3.13846	C	1.74903	-0.60041	-0.99622
C	3.13309	-2.67160	2.01015	C	2.64326	0.28071	-1.63709
C	4.08869	-3.61249	1.61394	C	3.84485	-0.14875	-2.19496
C	3.79046	-4.97209	1.69907	C	4.18833	-1.50788	-2.11868
C	2.53936	-5.36562	2.18953	H	1.51077	-2.69023	-0.39767
C	1.62993	-4.38691	2.57865	H	2.38233	1.33862	-1.67529
N	1.90790	-3.07402	2.48627	H	4.50926	0.57650	-2.66425
H	4.52583	-5.71582	1.38800	C	0.54788	0.01287	-0.37419
H	5.05477	-3.27630	1.23748	C	-0.48247	-0.81956	0.28414
H	2.26694	-6.41844	2.27360	O	-1.49918	0.07462	0.67984
H	0.64238	-4.62505	2.97883	C	-2.60060	-0.20039	1.42030
C	-1.01683	0.73389	4.15879	C	-3.10690	-1.46050	1.75198
C	-1.33764	2.06589	4.39673	C	-3.29585	0.96335	1.85552
C	-0.48783	3.06570	3.90800	C	-4.28640	-1.57657	2.50059
C	0.67397	2.69822	3.23035	H	-2.58353	-2.36176	1.44879
C	0.96630	1.34250	3.04719	C	-4.47866	0.83567	2.58829
N	0.09709	0.37348	3.49616	C	-4.97471	-0.43658	2.91195
H	-0.72646	4.12008	4.05586	H	-4.66075	-2.57161	2.74851
H	-1.65566	-0.08799	4.48708	H	-5.01267	1.72653	2.91831
H	-2.25520	2.30946	4.93321	H	-5.89918	-0.52221	3.48662
H	1.36112	3.45463	2.85046	O	-2.71600	2.15053	1.53251
O	-0.87362	-2.64184	3.76361	C	-3.38775	3.34598	1.91445
H	-0.42057	-2.81109	4.61608	H	-4.37172	3.41813	1.42392
O	1.30811	-1.99435	5.20616	H	-3.51911	3.39737	3.00693
H	0.85032	-1.28469	5.68795	H	-2.74818	4.17182	1.58270
H	0.08821	-1.21649	1.48986	H	3.59646	-3.46175	-1.42273
C	5.28540	1.60261	0.37405	O	5.34911	-2.03062	-2.59942
C	6.58030	1.08534	0.19158	C	6.29235	-1.13954	-3.19353
C	4.95931	2.80282	-0.29530	H	7.14866	-1.75919	-3.48618
C	7.51949	1.72272	-0.62284	H	5.86866	-0.65150	-4.08608
				H	6.61969	-0.37257	-2.47319





H	-0.00899	-2.94807	-2.43280	H	4.02552	-4.48487	0.92702
H	4.17362	-2.04399	-3.06672	O	5.55224	-3.23591	-0.97150
H	3.69333	0.30624	-2.28658	C	5.38413	-4.63155	-1.21451
C	0.48596	4.58130	-0.27531	H	5.96515	-4.85159	-2.11816
C	-0.36561	5.55715	0.23602	H	5.76981	-5.23049	-0.37406
C	-1.71913	5.25086	0.40789	H	4.32332	-4.87481	-1.38742
C	-2.17772	3.97746	0.07031	O	1.91082	-1.34268	3.90601
C	-1.27634	3.03258	-0.42715	C	1.97901	1.46151	4.39454
N	0.04822	3.35245	-0.59702	H	1.06044	0.92258	4.66646
H	-2.41224	5.99539	0.80270	H	2.62192	1.49306	5.29706
H	1.55056	4.75779	-0.43880	H	1.74010	2.50454	4.13877
H	0.03275	6.53996	0.49031				
H	-3.22664	3.71124	0.19830				
O	1.11401	2.48202	-3.34093	<b>1c-A-TS3a</b>			
H	1.06902	3.44611	-3.21803	C	4.14098	0.65424	-0.62431
H	1.48798	1.36272	0.34107	C	2.82110	0.49524	-1.06715
C	4.10562	-3.39967	0.99063	C	1.99552	-0.51500	-0.55631
C	3.42971	-2.71404	2.00084	C	2.53322	-1.39152	0.40654
C	3.48448	-1.31479	2.11371	C	3.83531	-1.23709	0.87121
C	4.27385	-0.60802	1.18020	C	4.64890	-0.20911	0.35824
C	4.96564	-1.27500	0.17794	H	2.44036	1.17055	-1.83745
C	4.87576	-2.67518	0.06529	H	1.91143	-2.19940	0.80020
H	2.82254	-3.26969	2.71737	H	4.24741	-1.90299	1.63236
H	4.33490	0.48030	1.21272	C	0.59136	-0.76830	-1.04937
H	5.56563	-0.72688	-0.55036	C	-0.38974	0.22190	-0.81556
C	2.66224	-0.65283	3.16587	H	-0.42307	-0.19298	0.89410
C	2.70137	0.78174	3.29311	O	-1.67264	-0.00629	-1.41993
O	1.51409	1.09840	1.49412	C	-2.64183	-0.55470	-0.60364
C	0.21208	0.86090	1.87637	C	-2.68653	-1.92826	-0.35949
C	-0.57146	1.87914	2.42554	C	-3.62060	0.29080	-0.03551
C	-0.33147	-0.43711	1.70758	C	-3.70695	-2.47568	0.42808
C	-1.88288	1.61994	2.83945	H	-1.90426	-2.54481	-0.80500
H	-0.13516	2.87584	2.51373	C	-4.64548	-0.25665	0.74522
C	-1.63822	-0.69929	2.13946	C	-4.68445	-1.63901	0.97233
C	-2.40524	0.33064	2.69956	H	-3.73662	-3.55218	0.60926
H	-2.49086	2.42161	3.26290	H	-5.40794	0.38701	1.18432
H	-2.07123	-1.69218	2.01769	H	-5.48826	-2.05468	1.58392
H	-3.42787	0.11574	3.01762	O	-3.47768	1.63230	-0.28713
O	0.47387	-1.33884	1.09928	C	-4.50087	2.52136	0.17385
C	0.06560	-2.70169	1.06661	H	-5.47170	2.24952	-0.26746
H	-0.07415	-3.08480	2.09003	H	-4.56922	2.50894	1.27263
H	-0.86645	-2.82665	0.49300	H	-4.20150	3.51907	-0.16794
H	0.87710	-3.24747	0.57252	H	4.75793	1.44560	-1.05024
H	3.49817	1.33326	2.79651	O	5.91149	-0.13123	0.86989
				C	6.77036	0.89960	0.39011

H	7.71528	0.78296	0.93498	H	-1.70762	3.56830	0.55852
H	6.95490	0.79386	-0.69156	O	1.34900	3.59920	2.34372
H	6.34836	1.89712	0.59547	H	0.66085	4.22978	2.62991
O	0.35171	-1.91210	-1.54072	C	4.67480	-1.66709	0.18798
C	-0.15955	1.67607	-0.55332	C	5.40647	-1.77931	-1.00876
H	-0.43798	2.29461	-1.42199	C	4.85614	-2.66797	1.16814
H	0.88329	1.87765	-0.28914	C	6.28549	-2.83944	-1.23333
O	-0.94632	2.18639	0.58534	H	5.27125	-1.04136	-1.80171
H	-1.89695	2.12091	0.31389	C	5.73377	-3.72411	0.96271
H	-0.76029	1.16109	1.55834	H	4.31800	-2.60887	2.11600
O	-0.55485	0.15319	1.89016	C	6.45564	-3.82129	-0.24254
H	0.34067	0.15665	2.28491	H	6.82237	-2.89769	-2.17965
				H	5.88139	-4.48879	1.72739
				O	7.28524	-4.88899	-0.36150
<b>1c-B-TS3</b>				C	8.04083	-5.03176	-1.56432
C	1.64341	0.27117	1.33003	H	8.71586	-4.17345	-1.71102
C	2.58462	-0.74811	1.21576	H	8.63160	-5.94721	-1.44003
C	3.71401	-0.56606	0.38789	H	7.37745	-5.13594	-2.43781
C	3.87246	0.66878	-0.27694	H	-0.90374	2.11414	-1.42854
C	2.90883	1.66429	-0.11906	O	-0.04031	2.01938	-2.00733
N	1.83829	1.42887	0.66421	H	0.15557	2.93214	-2.27123
H	2.42539	-1.69275	1.73090	C	-2.62744	-0.06586	-1.53828
H	4.74387	0.85080	-0.90447	H	-2.00314	0.28583	-2.37262
Rh	0.45237	2.80424	0.79396	C	-2.25502	0.75740	-0.26633
C	0.38152	0.24945	2.09943	H	-1.33478	0.24317	0.09075
C	-0.07699	-0.84351	2.83643	H	-3.03111	0.55649	0.50369
C	-1.30002	-0.74984	3.50534	O	-2.08350	2.09947	-0.51881
C	-2.02732	0.44022	3.44304	C	-7.58945	-1.03568	-1.40076
C	-1.52053	1.49961	2.69113	C	-6.46853	-0.37970	-1.90088
N	-0.36064	1.39794	2.03260	C	-5.18842	-0.56852	-1.34441
H	-1.67675	-1.60216	4.07279	C	-5.06355	-1.43806	-0.23584
H	0.51170	-1.75925	2.87614	C	-6.17539	-2.08752	0.28250
H	-2.98217	0.55263	3.95711	C	-7.44510	-1.89986	-0.29823
H	-2.04128	2.45224	2.57970	H	-6.57318	0.29720	-2.75092
C	1.64460	4.99052	-0.97290	H	-4.09153	-1.60689	0.22371
C	2.60873	5.53782	-1.81954	H	-6.08575	-2.75503	1.14161
C	3.74046	4.78153	-2.12706	C	-4.06255	0.19213	-1.93614
C	3.87771	3.50237	-1.58263	H	-8.56241	-0.87567	-1.86490
C	2.88131	3.00615	-0.74047	O	-8.46623	-2.58785	0.26471
N	1.77871	3.76522	-0.44887	C	-9.77588	-2.44571	-0.28792
H	4.51319	5.17966	-2.78655	H	-10.42616	-3.08954	0.31613
H	0.73441	5.52836	-0.70276	H	-10.12137	-1.40216	-0.21947
H	2.46326	6.53936	-2.22526	H	-9.79838	-2.77756	-1.33793
H	4.75144	2.89206	-1.80991	O	-4.26713	1.12276	-2.72343
O	-1.03014	4.16183	0.96472				

O	-2.40490	-1.46008	-1.28673	H	-1.54296	4.90919	-1.03293
C	-1.10792	-1.87516	-1.10469	H	-0.62122	5.95632	-3.14043
C	-0.04716	-1.49201	-1.92978	H	2.74997	3.26277	-2.82100
C	-0.88393	-2.79067	-0.04746	O	-2.40899	3.56181	1.07067
C	1.22751	-2.04495	-1.74291	H	-2.92658	3.02615	0.44229
H	-0.21681	-0.76174	-2.72175	O	0.23869	4.07033	2.03032
C	0.38494	-3.36008	0.11481	H	-0.25336	3.99802	2.86587
C	1.43532	-2.98964	-0.73718	C	4.62909	-0.48069	-0.12141
H	2.05186	-1.73526	-2.38874	C	5.13538	-0.62557	-1.42639
H	0.56510	-4.07774	0.91535	C	5.30802	-1.14502	0.92374
H	2.42253	-3.43299	-0.59206	C	6.26244	-1.40295	-1.69496
O	-1.95592	-3.04601	0.75394	H	4.62368	-0.15163	-2.26586
C	-1.80222	-4.00238	1.79908	C	6.43536	-1.91657	0.67405
H	-1.57093	-4.99879	1.38855	H	4.96212	-1.04385	1.95391
H	-1.01105	-3.70350	2.50440	C	6.92164	-2.05650	-0.63970
H	-2.76627	-4.03341	2.32097	H	6.61104	-1.50174	-2.72264
				H	6.96273	-2.41958	1.48651
				O	8.02341	-2.83455	-0.79289
<b>1c-B-IM4</b>				C	8.56016	-3.00149	-2.10478
C	1.42850	0.75291	1.46854	H	8.87565	-2.03469	-2.52875
C	2.59397	0.02016	1.25862	H	9.43299	-3.65549	-1.99077
C	3.40531	0.30218	0.13689	H	7.82652	-3.47824	-2.77446
C	3.00001	1.32926	-0.74315	C	-1.56528	-0.80950	-1.41815
C	1.82410	2.03397	-0.49012	H	-0.78506	-0.43509	-2.09959
N	1.08943	1.72967	0.60012	C	-1.50245	0.01669	-0.11736
H	2.85347	-0.78746	1.94032	H	-0.54242	-0.28083	0.34696
H	3.60518	1.58366	-1.61231	H	-2.30542	-0.31944	0.57107
Rh	-0.60777	2.64728	0.85348	O	-1.57263	1.37236	-0.41284
C	0.41814	0.55285	2.52839	C	-6.52977	-1.58864	-2.02047
C	0.51416	-0.40755	3.53582	C	-5.31566	-1.01961	-2.38878
C	-0.53371	-0.54593	4.44923	C	-4.12612	-1.28750	-1.68228
C	-1.65838	0.27245	4.33031	C	-4.18985	-2.16111	-0.57144
C	-1.69908	1.21576	3.30408	C	-5.39597	-2.73162	-0.18936
N	-0.68934	1.35590	2.43513	C	-6.57526	-2.45236	-0.90821
H	-0.47232	-1.29373	5.24122	H	-5.27162	-0.34298	-3.24414
H	1.39648	-1.04396	3.59730	H	-3.28932	-2.39839	-0.00761
H	-2.50049	0.18754	5.01774	H	-5.45256	-3.40323	0.66919
H	-2.55180	1.87884	3.14902	C	-2.89361	-0.60215	-2.12803
C	-0.59419	4.59455	-1.47197	H	-7.42985	-1.36024	-2.59071
C	-0.07432	5.15903	-2.63625	O	-7.70198	-3.05374	-0.46297
C	1.14176	4.68199	-3.13015	C	-8.93137	-2.80281	-1.14725
C	1.80161	3.65374	-2.45317	H	-9.69309	-3.38421	-0.61450
C	1.23330	3.12554	-1.29228	H	-9.18963	-1.73279	-1.11171
N	0.04438	3.61422	-0.82032	H	-8.87412	-3.13846	-2.19463
H	1.57621	5.10363	-4.03791				

O	-2.91873	0.23334	-3.03712	H	-1.46869	5.79048	1.38513
O	-1.34087	-2.19936	-1.13283	H	2.34393	4.29317	-0.00419
C	-0.07341	-2.51695	-0.68595	H	1.02270	6.10005	1.12684
C	1.03747	-2.43651	-1.52667	H	-2.52369	3.70208	0.50846
C	0.06709	-2.99040	0.63863	O	3.53765	2.19833	-1.40995
C	2.29701	-2.84749	-1.07297	H	3.71928	2.69080	-0.59185
H	0.90007	-2.06657	-2.54490	O	1.31192	2.39668	-2.99923
C	1.32816	-3.41159	1.08429	H	2.19186	2.80960	-3.10223
C	2.43492	-3.33688	0.22812	C	-4.15906	-0.64997	-1.14943
H	3.16143	-2.78896	-1.73625	C	-5.05368	-0.18293	-0.16779
H	1.45241	-3.78695	2.10019	C	-4.61489	-1.65916	-2.02708
H	3.41242	-3.66134	0.59097	C	-6.34676	-0.69343	-0.05032
O	-1.06177	-2.99521	1.39888	H	-4.73280	0.57546	0.54804
C	-1.02256	-3.66243	2.65898	C	-5.90104	-2.17212	-1.92712
H	-0.79506	-4.73238	2.52409	H	-3.96164	-2.03660	-2.81575
H	-0.27978	-3.21104	3.33295	C	-6.77928	-1.69654	-0.93429
H	-2.02406	-3.54639	3.09014	H	-7.00074	-0.31487	0.73479
				H	-6.25259	-2.94423	-2.61378
				O	-8.01304	-2.26036	-0.90433
<b>1c-B-TS4</b>				C	-8.94020	-1.81679	0.08642
C	-0.45033	-0.35684	-1.83869	H	-9.16207	-0.74406	-0.03155
C	-1.74632	-0.86818	-1.81965	H	-9.85388	-2.40116	-0.07540
C	-2.78797	-0.11390	-1.23641	H	-8.55495	-2.00685	1.10100
C	-2.47968	1.15813	-0.70738	C	-2.30858	-1.02152	2.10222
C	-1.16672	1.61957	-0.73916	C	-1.07058	-1.29657	1.52496
N	-0.20657	0.84992	-1.28954	C	-0.02342	-0.35752	1.53465
H	-1.93903	-1.86141	-2.22127	C	-0.25654	0.89578	2.14043
H	-3.25974	1.78202	-0.27573	C	-1.49156	1.18848	2.70809
Rh	1.63919	1.50774	-1.26290	C	-2.52615	0.23524	2.69340
C	0.76896	-1.00358	-2.36348	H	-0.89458	-2.26506	1.05422
C	0.80354	-2.26895	-2.94977	H	0.53197	1.65150	2.18404
C	2.02612	-2.78924	-3.37940	H	-1.67699	2.15794	3.17411
C	3.18690	-2.03068	-3.22197	C	1.26329	-0.75852	0.90090
C	3.09139	-0.76999	-2.63387	C	2.40667	0.16590	0.92890
N	1.91972	-0.27565	-2.21783	O	3.61211	-0.31688	0.40632
H	2.06756	-3.78071	-3.83296	C	4.16934	-1.53047	0.71805
H	-0.11613	-2.84287	-3.05936	C	5.14343	-1.98673	-0.17873
H	4.15998	-2.40186	-3.54388	C	3.88072	-2.30149	1.87218
H	3.95815	-0.12577	-2.48534	C	5.78825	-3.21246	0.01189
C	1.26630	4.20606	0.13616	H	5.37750	-1.36099	-1.04097
C	0.52082	5.20464	0.75954	C	4.51126	-3.54272	2.03925
C	-0.85726	5.02830	0.89968	C	5.45900	-4.00146	1.11656
C	-1.45083	3.86402	0.41037	H	6.53565	-3.54710	-0.71055
C	-0.65317	2.89590	-0.20346	H	4.26852	-4.14813	2.91335
N	0.69700	3.08424	-0.32563				



H	-4.24661	-1.56628	4.64485	H	2.66975	-5.81307	-1.01509
H	-5.74823	0.34208	5.13636	H	-1.20059	-4.09297	-1.94089
O	-3.10254	-2.04262	2.23768	H	0.25333	-6.14113	-1.66054
C	-2.58061	-2.87732	3.26671	H	3.53581	-3.49148	-0.70184
H	-2.03780	-2.28113	4.01791	O	-2.41240	-1.95664	-2.33802
H	-3.38103	-3.45418	3.75752	H	-3.16487	-1.43132	-1.96201
H	-1.88588	-3.56616	2.77080	C	4.77751	1.28124	-0.11451
H	2.96201	-0.81789	2.55724	C	5.66931	0.52440	0.66839
O	3.41704	-3.27406	1.44340	C	5.17469	2.58462	-0.48791
C	4.47043	-2.85311	2.31220	C	6.90546	1.03123	1.07051
H	5.24687	-3.62374	2.23491	H	5.38911	-0.47780	0.99802
H	4.88480	-1.88261	2.00071	C	6.40478	3.10042	-0.10142
H	4.11421	-2.78789	3.35264	H	4.52232	3.19816	-1.11205
O	-1.49728	0.73574	1.72620	C	7.28251	2.32839	0.68329
H	-2.45722	-1.69042	-0.22982	H	7.56066	0.41610	1.68665
				H	6.71315	4.10288	-0.40368
				O	8.46175	2.91243	1.01679
<b>1c-B-TS5</b>				C	9.39308	2.16554	1.79917
O	-0.22372	-1.03551	-3.65096	H	9.70341	1.24773	1.27439
H	-1.03495	-1.45412	-4.00291	H	10.26113	2.82101	1.93837
C	1.15648	1.03647	-1.18836	H	8.96592	1.90521	2.78091
C	2.38177	1.58313	-0.81186	O	-0.33491	-0.18320	1.18616
C	3.47075	0.73076	-0.52684	H	0.07999	-1.01641	1.46557
C	3.27675	-0.66363	-0.63826	H	-1.17596	-0.48609	0.76730
C	2.03081	-1.15954	-1.01757	C	-5.05321	3.33067	0.33304
N	1.02551	-0.30075	-1.28342	C	-4.96774	1.96717	0.03767
H	2.48420	2.66275	-0.71221	C	-3.92304	1.16361	0.52351
H	4.09667	-1.35295	-0.44241	C	-2.94271	1.77988	1.33023
Rh	-0.72418	-1.04997	-1.75605	C	-3.00008	3.13988	1.61678
C	-0.09400	1.75885	-1.49149	C	-4.05416	3.92779	1.11819
C	-0.22794	3.14613	-1.43360	H	-5.72336	1.50992	-0.60425
C	-1.45284	3.73209	-1.76608	H	-2.09556	1.20156	1.69804
C	-2.51121	2.91511	-2.16049	H	-2.22296	3.62050	2.21478
C	-2.32654	1.53163	-2.18239	C	-3.83072	-0.24958	0.04006
N	-1.15780	0.96844	-1.84774	C	-3.18144	-1.24653	0.76947
H	-1.57177	4.81571	-1.72002	H	-5.88232	3.91722	-0.06331
H	0.62044	3.76009	-1.13150	O	-4.01946	5.25311	1.43968
H	-3.48193	3.32951	-2.43176	C	-5.04880	6.09609	0.92983
H	-3.13496	0.84084	-2.42562	H	-4.82139	7.10526	1.29485
C	-0.14492	-4.02567	-1.67296	H	-5.05309	6.09629	-0.17259
C	0.67037	-5.14474	-1.51232	H	-6.03918	5.78601	1.30136
C	2.00668	-4.95772	-1.15372	O	-4.34403	-0.49951	-1.12432
C	2.49491	-3.66086	-0.97642	H	-3.17373	-2.26939	0.39509
C	1.63616	-2.57575	-1.16144	O	-3.10177	-1.10346	2.16994
N	0.32440	-2.78320	-1.49938				

C	-2.11977	-1.64491	2.95096	C	0.44754	-2.54852	-2.40686
C	-1.48577	-2.89281	2.71622	C	1.68478	-3.06644	-2.79373
C	-1.77132	-0.90429	4.08700	C	2.78933	-2.21459	-2.85532
C	-0.49495	-3.32927	3.60917	C	2.62299	-0.87362	-2.51443
C	-0.80022	-1.35860	4.98341	N	1.44345	-0.37758	-2.11162
H	-2.28061	0.04954	4.23979	H	1.78043	-4.12274	-3.05002
C	-0.15153	-2.57034	4.73522	H	-0.43344	-3.18823	-2.36430
H	0.00632	-4.28071	3.43155	H	3.77478	-2.57576	-3.15022
H	-0.54636	-0.75883	5.85997	H	3.44998	-0.16534	-2.56273
H	0.61919	-2.93990	5.41493	C	0.57002	4.34872	-0.44462
O	-1.88709	-3.61899	1.63104	C	-0.20492	5.37566	0.08824
C	-1.33554	-4.92076	1.45454	C	-1.57433	5.16323	0.27365
H	-1.81990	-5.33196	0.56125	C	-2.12313	3.92665	-0.06485
H	-0.24677	-4.87588	1.29528	C	-1.29486	2.92634	-0.58178
H	-1.55605	-5.56166	2.32405	N	0.04270	3.15954	-0.77796
<b>1c-C-TS3</b>				H	-2.20922	5.95040	0.68327
O	2.89310	2.39398	-1.49856	H	1.64183	4.45739	-0.61577
H	3.54613	1.67594	-1.46298	H	0.26531	6.32454	0.34822
C	-4.49039	-1.00669	-0.52779	H	-3.18491	3.73033	0.08173
C	-5.69146	-0.27401	-0.53437	O	0.96525	2.20555	-3.52991
C	-4.54999	-2.36470	-0.14269	H	1.84446	2.62689	-3.49185
C	-6.90926	-0.85888	-0.18282	H	1.36550	1.09844	0.13604
H	-5.68863	0.77349	-0.84207	C	4.50152	-3.28769	1.35679
C	-5.75315	-2.95870	0.21683	C	3.78867	-2.52637	2.28414
H	-3.63563	-2.95958	-0.09780	C	3.52389	-1.16009	2.08393
C	-6.94564	-2.21106	0.19751	C	3.99834	-0.56770	0.89211
H	-7.81882	-0.25949	-0.21314	C	4.72138	-1.30810	-0.03433
H	-5.79275	-4.00449	0.52696	C	4.96983	-2.67572	0.18198
O	-8.07592	-2.87281	0.55969	H	3.41101	-3.00106	3.19145
C	-9.31000	-2.15659	0.56182	H	3.76439	0.46699	0.64590
H	-9.55431	-1.78553	-0.44662	H	5.08410	-0.84962	-0.95504
H	-10.07345	-2.87498	0.88386	C	2.65656	-0.47078	3.08622
H	-9.27647	-1.31218	1.26896	C	2.52867	0.96466	3.15013
C	-0.89656	-0.54579	-1.61513	H	1.74106	1.28995	3.83688
C	-2.13271	-1.14443	-1.37983	H	4.68280	-4.34464	1.55159
C	-3.20233	-0.37632	-0.87567	O	5.64887	-3.32279	-0.80165
C	-2.98786	0.99865	-0.64466	C	5.87248	-4.72531	-0.66155
C	-1.73528	1.55516	-0.88892	H	6.41371	-5.03463	-1.56373
N	-0.73307	0.77713	-1.37078	H	6.48468	-4.94208	0.22839
H	-2.26501	-2.20691	-1.57816	H	4.91789	-5.27199	-0.59745
H	-3.77814	1.61402	-0.21811	O	1.95091	-1.17075	3.86063
Rh	1.04185	1.54553	-1.52160	C	3.50802	2.03018	2.78140
C	0.34383	-1.19791	-2.06563	H	4.02112	2.36355	3.70238
				H	4.29153	1.66275	2.10040



O	2.84664	3.17610	2.24810	H	3.65869	0.72847	-0.94824	
H	2.18344	2.80234	1.63345					
O	1.40732	1.05641	1.33346					
C	0.11556	0.81472	1.75323	<b>1c-C-TS4a</b>	H	-2.37539	0.08140	-0.89302
C	-0.66388	1.82820	2.31197	C	1.76403	-0.87691	-0.21530	
C	-0.39617	-0.49733	1.62471	C	0.49937	-0.28748	-0.30506	
C	-1.95948	1.54785	2.75894	C	0.31679	1.09151	-0.11242	
H	-0.23185	2.82758	2.39212	C	1.45234	1.88112	0.15526	
C	-1.68941	-0.77852	2.08454	C	2.71465	1.30948	0.26882	
C	-2.46253	0.24703	2.64339	C	2.87880	-0.07727	0.08693	
H	-2.57132	2.34117	3.19240	H	-0.35889	-0.90567	-0.57570	
H	-2.10269	-1.78303	1.99240	H	1.32850	2.95888	0.28267	
H	-3.47417	0.01936	2.98650	H	3.59391	1.91624	0.49516	
O	0.43020	-1.38813	1.02767	C	-1.02217	1.75929	-0.25254	
C	0.10164	-2.77197	1.08867	C	-2.22408	1.03448	0.11106	
H	0.00769	-3.09493	2.13784	H	1.87090	-1.94772	-0.38881	
H	-0.83252	-2.98721	0.54577	O	4.14874	-0.55283	0.21374	
H	0.93570	-3.29901	0.61100	C	4.36724	-1.95155	0.04467	
				H	5.44176	-2.10925	0.19854	
				H	3.79958	-2.53521	0.78761	
<b>1c-C-IM4</b>				H	4.08951	-2.27777	-0.97080	
H	4.19744	-2.11418	-0.17121	O	-1.04495	2.91075	-0.75322	
C	-2.07837	0.92438	0.21824	C	-2.24245	0.23063	1.39884	
C	-0.76308	1.36976	0.13383	H	-2.42900	0.87148	2.27951	
C	0.28928	0.50324	-0.21922	H	-1.28603	-0.28338	1.56494	
C	-0.01930	-0.84870	-0.48859	O	-3.24493	-0.81856	1.40722	
C	-1.32617	-1.30972	-0.40758	H	-4.11513	-0.38499	1.42173	
C	-2.36685	-0.42732	-0.05523	O	-2.57579	-0.88233	-1.68870	
H	-0.52920	2.41466	0.34588	H	-1.81311	-0.83063	-2.28696	
H	0.76791	-1.55082	-0.76764	Na	-3.08567	-2.38131	-0.22371	
H	-1.57133	-2.35263	-0.61569	H	-3.09588	1.70494	0.03200	
C	1.66728	1.04573	-0.28287					
C	2.82610	0.11556	-0.57547					
H	2.55945	-0.62559	-1.34446	<b>1c-C-IM5a</b>	H	-2.49589	-0.00191	-1.10194
H	-2.86972	1.62069	0.49478	C	1.71821	-0.85042	-0.14962	
O	-3.60875	-0.96166	-0.00452	C	0.43603	-0.29046	-0.20684	
C	-4.70776	-0.11512	0.33842	C	0.21906	1.08773	-0.06297	
H	-5.59702	-0.75592	0.31160	C	1.35078	1.90983	0.10811	
H	-4.58275	0.30204	1.35008	C	2.63279	1.37410	0.18333	
H	-4.81771	0.70211	-0.39168	C	2.82549	-0.01472	0.05977	
O	1.88759	2.23983	-0.05591	H	-0.41220	-0.94473	-0.40832	
C	3.29415	-0.62561	0.69017	H	1.20913	2.99036	0.18587	
H	2.47238	-1.24418	1.09370	H	3.50563	2.01331	0.33362	
H	3.56964	0.10920	1.46148	C	-1.14132	1.73834	-0.16790	
O	4.45249	-1.40655	0.44434					



H	6.64744	-3.59609	0.88919	H	-2.89537	-2.93746	0.04133
H	6.35764	-5.08847	-0.07679	C	-6.29848	-2.72814	-0.01874
O	-0.01274	-2.76190	-0.91402	H	-7.43148	-0.88298	0.20533
C	1.08685	0.47275	-2.15898	H	-4.91159	-4.36886	-0.21804
H	2.17109	0.41946	-2.26331	O	-7.33734	-3.58957	-0.18155
H	0.60759	1.31352	-2.66696	C	-8.66252	-3.06103	-0.18106
C	-1.61177	1.80878	0.00203	H	-9.32824	-3.91928	-0.33261
C	-2.78126	1.05585	-0.08789	H	-8.89652	-2.57821	0.78144
C	-2.81546	-0.24920	0.44756	H	-8.80040	-2.33766	-1.00088
C	-1.65779	-0.74964	1.07553	O	1.00005	3.32654	2.27589
C	-0.50823	0.03725	1.13114	H	1.82922	3.82803	2.18038
N	-0.52575	1.28845	0.61878	H	-0.76089	-0.56118	-1.89719
H	-3.64590	1.45503	-0.61728				
H	-1.65090	-1.75166	1.50145				
Rh	1.16156	2.24302	0.48360	<b>1c-C-IM7a</b>			
C	-1.35454	3.13786	-0.58438	C	4.60954	-1.36629	-1.00221
C	-2.32350	3.92598	-1.20993	C	3.26463	-1.06217	-1.19634
C	-1.95944	5.16410	-1.74216	C	2.27920	-2.07349	-1.23823
C	-0.63205	5.58687	-1.63977	C	2.72006	-3.39799	-1.05469
C	0.29272	4.75663	-1.00853	C	4.06261	-3.72322	-0.85762
N	-0.05584	3.56778	-0.49491	C	5.02257	-2.69758	-0.83174
H	-2.70740	5.79116	-2.22996	H	3.00078	-0.01020	-1.26471
H	-3.35245	3.57229	-1.27301	H	1.97012	-4.19015	-1.06156
H	-0.30701	6.54711	-2.04154	H	4.34946	-4.76630	-0.72245
H	1.34475	5.02782	-0.90695	C	0.79507	-1.86041	-1.39019
C	3.06221	0.29813	1.85402	C	0.22997	-0.64037	-1.81918
C	3.38200	-0.88028	2.52479	H	5.35759	-0.57242	-0.95386
C	2.37012	-1.80935	2.77711	O	6.35687	-2.89858	-0.64036
C	1.07319	-1.54161	2.33714	C	6.81762	-4.23519	-0.45762
C	0.81258	-0.34773	1.66090	H	7.90418	-4.16410	-0.32520
N	1.81374	0.56271	1.43887	H	6.36718	-4.69229	0.43846
H	2.58810	-2.73957	3.30385	H	6.59441	-4.85687	-1.33996
H	3.80796	1.06491	1.63899	O	0.04058	-2.85289	-1.10103
H	4.41036	-1.05706	2.84116	C	0.86043	0.61971	-2.15521
H	0.26645	-2.25279	2.51218	H	1.81555	0.58311	-2.69534
O	2.92239	3.23395	0.23521	H	0.17695	1.32912	-2.63935
H	3.57459	2.55804	-0.01325	C	-1.60827	1.81467	0.06924
H	1.34274	1.41030	-0.90821	C	-2.80280	1.10336	-0.02392
C	-4.01552	-1.09608	0.30011	C	-2.85267	-0.23692	0.42254
C	-5.30874	-0.54484	0.32034	C	-1.68679	-0.81597	0.95530
C	-3.88914	-2.48950	0.10828	C	-0.50661	-0.07273	0.99558
C	-6.44437	-1.34327	0.16953	N	-0.51555	1.21985	0.59887
H	-5.43910	0.52778	0.48000	H	-3.67646	1.56127	-0.48647
C	-5.01004	-3.29451	-0.05181	H	-1.69565	-1.84499	1.30968
				Rh	1.20873	2.11813	0.41877

C	-1.33063	3.17445	-0.43674	C	3.40985	0.54314	1.80371
C	-2.30274	4.04290	-0.93665	C	3.85209	1.47322	0.84134
C	-1.92082	5.30234	-1.40319	C	2.99581	2.54676	0.50902
C	-0.57368	5.66698	-1.36083	C	1.74577	2.65387	1.11349
C	0.35419	4.75878	-0.85298	N	1.36396	1.74032	2.04609
N	-0.01154	3.54849	-0.40755	H	4.01199	-0.33410	2.03831
H	-2.67160	5.99139	-1.79316	H	3.29209	3.27633	-0.24396
H	-3.34791	3.73511	-0.95349	Rh	-0.46431	1.75121	2.67454
H	-0.23508	6.64167	-1.71325	C	1.49646	-0.24302	3.31451
H	1.41959	4.98731	-0.79819	C	2.07533	-1.41767	3.80922
C	3.07228	0.06742	1.70469	C	1.33301	-2.24871	4.64703
C	3.38696	-1.18586	2.22674	C	0.02356	-1.88478	4.98574
C	2.37785	-2.14569	2.32681	C	-0.50239	-0.70567	4.46690
C	1.07858	-1.81518	1.93791	N	0.20592	0.09378	3.64985
C	0.82113	-0.53963	1.42971	H	1.77138	-3.17065	5.03244
N	1.83253	0.37691	1.30075	H	3.09659	-1.67622	3.52998
H	2.59541	-3.14230	2.71368	H	-0.59022	-2.50873	5.63642
H	3.82574	0.84787	1.58911	H	-1.52082	-0.37322	4.67668
H	4.41253	-1.40050	2.52728	C	-1.59803	4.11630	1.13142
H	0.27166	-2.54176	2.01925	C	-1.51208	5.23448	0.30908
O	2.98076	3.04334	0.11711	C	-0.28493	5.54080	-0.29024
H	3.65884	2.34762	0.09959	C	0.81482	4.71869	-0.04674
H	1.20729	1.24904	-1.18712	C	0.67438	3.60881	0.79299
C	-4.07965	-1.04299	0.27486	N	-0.53937	3.32055	1.37180
C	-5.35703	-0.47098	0.40605	H	-0.19164	6.40641	-0.94750
C	-3.99296	-2.42133	-0.02203	H	-2.52641	3.82159	1.62411
C	-6.51590	-1.23741	0.26651	H	-2.39694	5.84788	0.13625
H	-5.45455	0.58997	0.64668	H	1.78211	4.93251	-0.50170
C	-5.13779	-3.19315	-0.17350	O	-2.47652	1.58383	3.11312
H	-3.01284	-2.87897	-0.17614	H	-2.38009	2.17859	3.88517
C	-6.40988	-2.60807	-0.02486	O	-0.61848	3.07289	4.40627
H	-7.48973	-0.76436	0.39097	H	-0.92827	3.88768	3.97541
H	-5.07223	-4.25454	-0.41981	H	-0.63288	0.60788	1.41530
O	-7.47409	-3.43790	-0.18503	C	5.13175	1.25529	0.13793
C	-8.78571	-2.88921	-0.06517	C	6.16518	0.50284	0.72448
H	-9.47685	-3.72326	-0.23661	C	5.32577	1.71602	-1.18252
H	-8.95112	-2.47437	0.94218	C	7.33713	0.19570	0.03098
H	-8.95753	-2.10584	-0.82083	H	6.06363	0.14802	1.75177
O	1.22234	3.07535	2.19246	C	6.48352	1.41271	-1.88923
H	2.10407	3.48148	2.07434	H	4.54039	2.28574	-1.68269
H	-0.86479	-0.64154	-1.79631	C	7.49562	0.63840	-1.29244
				H	8.11304	-0.38834	0.52525
				H	6.61716	1.75001	-2.91878
<b>1c-C-TS7a</b>				O	8.58081	0.36325	-2.06589
C	2.15553	0.68704	2.38994				

C	9.59569	-0.48233	-1.52749	C	-0.00502	-4.29528	-1.98458
H	10.34569	-0.59411	-2.31988	C	1.12862	-4.10190	-2.77047
H	10.06397	-0.02750	-0.63971	C	1.26182	-2.90079	-3.47629
H	9.18600	-1.47136	-1.26434	C	0.26626	-1.93102	-3.37397
C	2.85096	-3.15683	0.30036	C	-0.84414	-2.16976	-2.55543
C	1.69148	-2.38879	0.33275	N	-0.96254	-3.36222	-1.88155
C	1.58626	-1.18663	-0.40325	H	2.13893	-2.71809	-4.09869
C	2.69345	-0.82630	-1.19779	H	-0.17090	-5.20713	-1.40858
C	3.85727	-1.59125	-1.25610	H	1.89202	-4.87878	-2.81635
C	3.94712	-2.76424	-0.49057	H	0.35503	-0.98555	-3.90726
H	0.87155	-2.74608	0.94852	O	-2.20634	-5.23163	0.12593
H	2.62981	0.09687	-1.77384	H	-3.04597	-5.63040	0.40875
H	4.68788	-1.25943	-1.87926	H	-1.37510	-2.52577	0.43969
C	0.41895	-0.25884	-0.41714	C	-2.87232	2.44733	-2.48187
C	-0.77697	-0.41520	0.38388	C	-3.97972	3.29560	-2.29598
H	2.92443	-4.07844	0.88100	C	-1.65147	3.04050	-2.87860
O	5.04185	-3.57515	-0.45722	C	-3.88657	4.67589	-2.48386
C	6.17068	-3.21175	-1.25080	H	-4.94633	2.87899	-2.00679
H	6.92934	-3.98225	-1.06691	C	-1.54693	4.40879	-3.08005
H	5.91360	-3.19665	-2.32249	H	-0.75642	2.42803	-2.98989
H	6.56409	-2.22715	-0.95293	C	-2.66059	5.24208	-2.86978
O	0.51250	0.78837	-1.12985	H	-4.76707	5.29763	-2.32417
C	-1.25020	-1.61085	1.12589	H	-0.59612	4.86113	-3.36573
H	-0.56781	-1.99306	1.89544	O	-2.45049	6.57397	-3.03423
H	-2.22384	-1.42253	1.59478	C	-3.52976	7.46899	-2.76693
C	-3.89850	-0.89614	-1.03118	H	-3.13297	8.47686	-2.93780
C	-3.93918	0.45539	-1.36678	H	-4.37513	7.28459	-3.44887
C	-2.94780	0.99613	-2.22164	H	-3.86849	7.37707	-1.72244
C	-1.96684	0.12770	-2.73675	O	-3.68341	-4.45187	-2.08682
C	-1.91948	-1.20017	-2.30699	H	-3.40947	-5.35115	-1.81995
N	-2.90312	-1.67660	-1.50498	H	-1.58739	0.17594	-0.05330
H	-4.69371	1.09867	-0.91714				
H	-1.20308	0.49869	-3.41555				
Rh	-2.63985	-3.44553	-0.71578	<b>1c-C-TS4b</b>			
C	-4.77914	-1.60849	-0.08362	C	-0.06588	-0.39821	-1.08072
C	-5.93676	-1.06342	0.47473	C	-1.45321	-0.52034	-1.11892
C	-6.68399	-1.82028	1.37914	C	-2.26281	0.54481	-0.66620
C	-6.25531	-3.10790	1.70760	C	-1.63023	1.70693	-0.17490
C	-5.09090	-3.59954	1.12023	C	-0.23832	1.77841	-0.15309
N	-4.37212	-2.87520	0.24956	N	0.48667	0.73048	-0.59077
H	-7.59122	-1.40559	1.82115	H	-1.90485	-1.43530	-1.49729
H	-6.24725	-0.05576	0.19980	H	-2.22046	2.56264	0.14863
H	-6.80761	-3.73213	2.41058	Rh	2.43369	0.93468	-0.72533
H	-4.70974	-4.59537	1.34997	C	0.93583	-1.36926	-1.56838
				C	0.63019	-2.62743	-2.09127

C	1.66491	-3.44498	-2.54987	H	-0.12323	-4.14009	0.68475
C	2.98322	-2.98867	-2.48249	H	1.29019	-0.52399	2.57403
C	3.22966	-1.72755	-1.94407	H	-1.05124	0.23754	2.85222
N	2.23566	-0.94830	-1.49920	C	2.12736	-2.94060	1.45860
H	1.43934	-4.43182	-2.95707	C	3.26842	-2.43418	2.31471
H	-0.40549	-2.96247	-2.13381	H	2.94723	-1.67060	3.03544
H	3.81667	-3.59763	-2.83348	H	-2.46466	-3.39878	0.98814
H	4.23127	-1.30350	-1.85994	O	-3.14669	-1.04547	2.19255
C	2.79587	3.74688	0.40089	C	-4.27476	-1.83863	1.81798
C	2.35482	4.93863	0.97488	H	-5.15805	-1.25850	2.10787
C	0.98773	5.11088	1.20026	H	-4.29030	-2.01718	0.73219
C	0.10067	4.09326	0.84236	H	-4.26858	-2.79987	2.35570
C	0.59928	2.92269	0.26696	O	2.34382	-3.85288	0.65112
N	1.94394	2.77189	0.05830	C	4.47218	-1.90723	1.49764
H	0.61040	6.02924	1.65273	H	4.68868	-2.67553	0.71855
H	3.85092	3.54599	0.20620	H	5.35041	-1.92498	2.18727
H	3.07846	5.71007	1.23950	O	4.25914	-0.65358	0.95627
H	-0.97021	4.20263	1.01311	O	2.89118	0.98343	2.30958
O	4.42195	1.13417	-0.96851	H	3.37913	1.81808	2.23246
H	4.65679	0.40690	-0.33248	H	3.59799	-3.31632	2.89189
O	2.14705	1.64579	-2.52613				
H	3.06907	1.67038	-2.84516				
C	-3.73388	0.44364	-0.71231	<b>1c-C-IM5b</b>			
C	-4.54274	1.18355	0.17008	C	0.19359	-0.47388	-1.03787
C	-4.37657	-0.42095	-1.62557	C	-1.19570	-0.49290	-1.14096
C	-5.93289	1.06889	0.16052	C	-1.94373	0.63514	-0.74085
H	-4.08487	1.83960	0.91226	C	-1.24815	1.76035	-0.24829
C	-5.75980	-0.54085	-1.65211	C	0.14288	1.73241	-0.16766
H	-3.78726	-0.99616	-2.34176	N	0.81048	0.62497	-0.55427
C	-6.55182	0.20030	-0.75502	H	-1.69759	-1.38283	-1.51554
H	-6.52114	1.64643	0.87313	H	-1.78823	2.66091	0.03978
H	-6.25274	-1.20264	-2.36642	Rh	2.75396	0.66655	-0.54851
O	-7.89353	0.01536	-0.84616	C	1.13942	-1.53653	-1.42758
C	-8.74349	0.74860	0.03528	C	0.76423	-2.77854	-1.94333
H	-8.62871	1.83378	-0.11689	C	1.75228	-3.70054	-2.29290
H	-9.76752	0.44834	-0.21718	C	3.09615	-3.36000	-2.12484
H	-8.53371	0.49704	1.08729	C	3.41223	-2.10717	-1.60240
H	3.48493	0.30350	1.78751	N	2.46342	-1.22375	-1.26050
C	-1.64794	-2.76955	1.34066	H	1.47171	-4.67602	-2.69309
C	-0.33058	-3.18498	1.17070	H	-0.29120	-3.02033	-2.06403
C	0.75194	-2.41339	1.63489	H	3.89731	-4.05064	-2.38921
C	0.47634	-1.17135	2.24578	H	4.44195	-1.77980	-1.44876
C	-0.83240	-0.72991	2.39700	C	3.29063	3.46450	0.49990
C	-1.90478	-1.53449	1.96780	C	2.92174	4.70897	1.00924
				C	1.56325	5.00470	1.14373







C	1.55853	1.95280	-1.64306	C	2.26735	4.01404	-0.66004
C	0.20570	1.58540	-1.80431	C	1.35310	3.04643	-0.23897
C	-0.81186	2.52009	-1.65751	N	0.02656	3.36334	-0.09995
C	-0.50244	3.85576	-1.33994	H	2.52429	6.07192	-1.26260
H	2.89351	3.59010	-1.24221	H	-1.47729	4.76685	-0.23411
H	-0.06412	0.55346	-2.03162	H	0.07247	6.60442	-0.99797
H	-1.85961	2.23311	-1.76319	H	3.32093	3.75757	-0.76816
C	2.68553	0.97089	-1.68453	O	-2.80795	2.83060	0.78652
C	2.39294	-0.45422	-1.67168	H	-3.55000	2.24259	0.49638
H	1.10347	5.28109	-0.97442	C	4.41147	-0.99899	0.15250
O	-1.56033	4.69180	-1.17480	C	5.40506	-0.50286	-0.71255
C	-1.30423	6.04761	-0.81069	C	4.71307	-2.15812	0.90233
H	-2.28780	6.52149	-0.70729	C	6.64741	-1.12550	-0.83799
H	-0.76462	6.10312	0.14843	H	5.20456	0.37679	-1.32696
H	-0.72558	6.56595	-1.59193	C	5.94743	-2.78467	0.79381
O	3.86486	1.39559	-1.61788	H	3.98057	-2.56492	1.60188
H	3.21542	-1.05155	-2.08667	C	6.92712	-2.27488	-0.07940
H	1.42195	-0.75541	-2.08229	H	7.38302	-0.71548	-1.52959

**1c-C-TS6b**

O	-0.76018	2.33456	2.41885	O	8.10262	-2.95192	-0.12403
H	-1.60093	2.81807	2.55612	C	9.13262	-2.46997	-0.98677
C	0.72830	-0.39690	0.78389	H	9.43908	-1.44990	-0.70484
C	1.95569	-1.05053	0.68132	H	9.97753	-3.15699	-0.85767
C	3.09878	-0.33257	0.26872	H	8.80507	-2.48163	-2.03863
C	2.95477	1.04033	-0.03296	O	-0.46942	1.13211	-2.29210
C	1.70291	1.64326	0.06867	H	-0.19925	2.05872	-2.40205
N	0.64381	0.91094	0.47090	H	-1.43448	1.21227	-2.07838
H	2.02050	-2.11484	0.90252	C	-5.02229	-3.02211	-0.59275
H	3.81867	1.63119	-0.33336	C	-5.06717	-1.62568	-0.65349
Rh	-1.10365	1.79427	0.57031	C	-4.00771	-0.87151	-1.17992
C	-0.56344	-0.97037	1.21239	C	-2.87103	-1.56732	-1.63991
C	-0.74545	-2.30273	1.58236	C	-2.79728	-2.95493	-1.56577
C	-2.00900	-2.73116	2.00007	C	-3.87379	-3.69345	-1.04099
C	-3.05757	-1.81407	2.04755	H	-5.94515	-1.10060	-0.27064
C	-2.82227	-0.49676	1.64994	H	-2.01488	-1.01232	-2.02722
N	-1.61412	-0.08942	1.24087	H	-1.90415	-3.48993	-1.89531
H	-2.16597	-3.77260	2.28510	C	-4.08119	0.63096	-1.15161
H	0.09321	-2.99735	1.54371	C	-3.40497	1.35654	-2.12461
H	-4.05755	-2.10649	2.36700	H	-5.86980	-3.57162	-0.18258
H	-3.61583	0.25109	1.61326	O	-3.71023	-5.04838	-1.00032
C	-0.40712	4.60185	-0.36971	C	-4.76806	-5.83572	-0.46190
C	0.46189	5.60711	-0.79169	H	-4.43111	-6.87786	-0.52364
C	1.81764	5.30727	-0.93643	H	-4.96296	-5.57390	0.59116
				H	-5.69385	-5.71416	-1.04797

O	-4.76101	1.15704	-0.18295
H	-3.49619	2.44693	-2.14292
H	-3.03873	0.86431	-3.02831