

## Supporting information for The mechanistic insights into the Palladium-catalyzed hydroaminocarbonylation of alkenes

### I. Computational Details

The calculations were conducted using Gaussian 09 program <sup>1</sup>. Geometries were optimized using the B3LYP functional <sup>2</sup>. Lanl2dz <sup>3</sup> basis set was used for Pd, a standard 6-31G(d) <sup>4</sup> basis set was used for other atoms. Frequency analyses were carried out to ensure these stationary points were at either a minimum or transition state. Solvation free energies are calculated with SMD<sup>5</sup> solvation model (solvent=methanol). The energetic results were further improved by single-point energy calculations at M06 <sup>6</sup> level of theory and the basis set SDD <sup>7</sup> for Pd and 6-311++G(d,p)<sup>8</sup> basis set for other atoms. The solvation model for the single point calculation was the same as described above. The energies presented in this paper are the M06-calculated single point energies added with B3LYP-optimized thermodynamic corrections.

### II. Free-energy profiles for other possible pathways

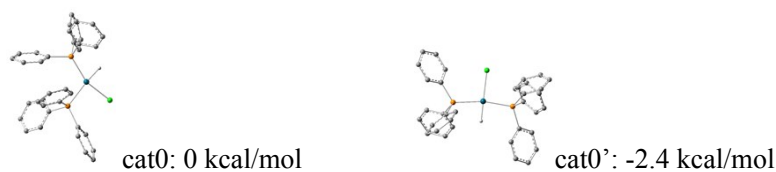


Figure S1. Free-energy for the cis-Pd(PPh<sub>3</sub>)<sub>2</sub>HCl and trans-Pd(PPh<sub>3</sub>)<sub>2</sub>HCl .

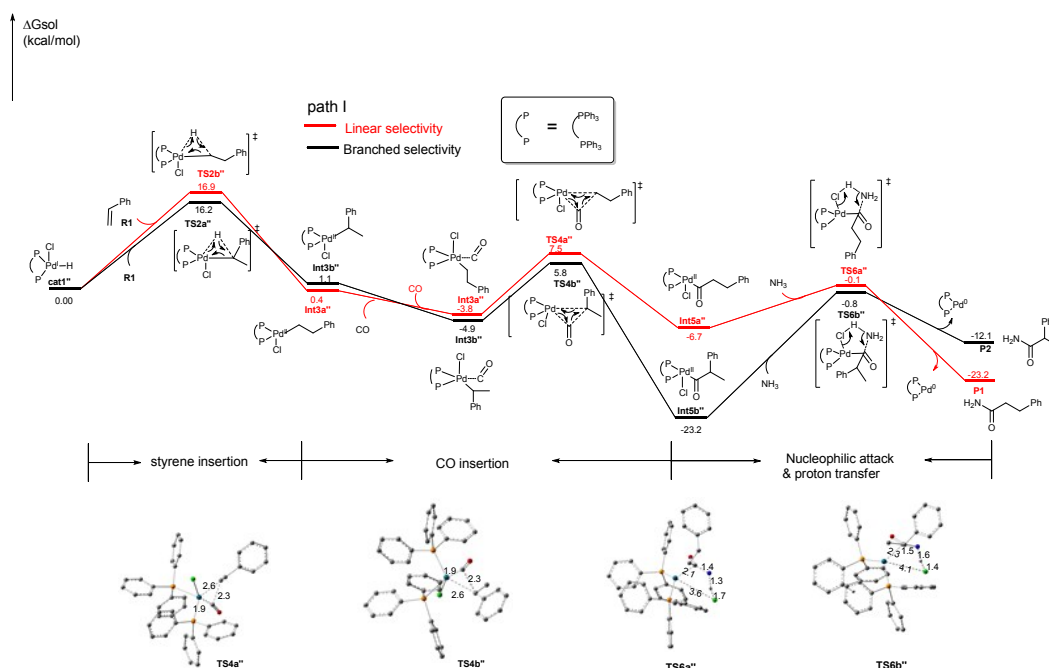


Figure S2. Free-energy profile for the path II' with Pd(II)/PPh<sub>3</sub> as the catalytic system. In the structure of the important intermediates and TSs, the hydrogen atom and the chloride anion were omitted for clarity.

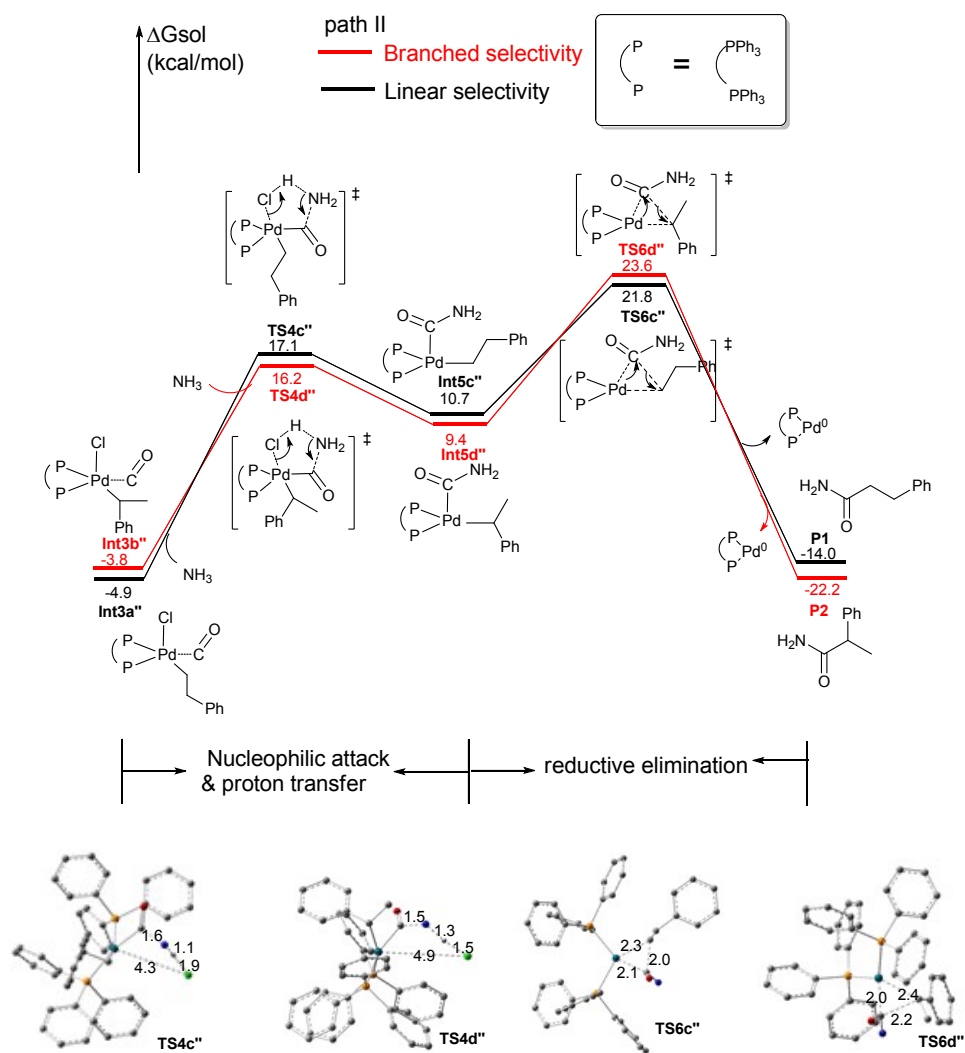


Figure S3. Free-energy profile for the path II' with Pd(II)/PPh<sub>3</sub> as the catalytic system. In the structure of the important intermediates and TSs, the hydrogen atom and the chloride anion were omitted for clarity.

### III. Cartesian coordinates and energies from the B3LYP method and electronic energies from M06

<b>cat1</b>				H	-3.13783	4.30783	3.23417
Number of imaginary frequencies=0				C	-3.50966	-0.24357	-1.37638
Charge = 0 Multiplicity = 1				C	-4.36225	-1.29177	-0.99867
C	-3.78052	3.25555	1.46488	C	-3.8565	0.5603	-2.47773
C	-3.50374	2.22731	0.56224	C	-5.5396	-1.53506	-1.7089
C	-2.36013	1.43242	0.72269	H	-4.1097	-1.92633	-0.15569
C	-1.49284	1.69645	1.79571	C	-5.04068	0.3167	-3.17585
C	-1.77605	2.72202	2.69678	H	-3.20557	1.38003	-2.7747
C	-2.92071	3.50526	2.53422	C	-5.88195	-0.73192	-2.79768
H	-4.66985	3.86395	1.32478	H	-6.18733	-2.35475	-1.40895
H	-4.17821	2.05277	-0.26802	H	-5.30004	0.94811	-4.02141

H	-6.79854	-0.92323	-3.34959	C	-0.32662	-3.30733	-3.79651
C	-1.66015	-1.39564	0.54602	C	-2.98488	-3.79427	-4.50637
C	-0.87837	-2.43484	0.01558	H	-3.35713	-3.98967	-2.39354
C	-2.22773	-1.55997	1.81974	C	-0.70052	-3.30461	-5.13759
C	-0.67141	-3.61137	0.73772	H	0.71092	-3.11041	-3.5342
H	-0.42085	-2.31637	-0.96302	C	-2.02951	-3.54803	-5.49515
C	-2.01367	-2.73421	2.54457	H	-4.01504	-3.99717	-4.78025
H	-2.83163	-0.7672	2.24944	H	0.0437	-3.1172	-5.90523
C	-1.23636	-3.76191	2.00621	H	-2.31712	-3.55162	-6.54301
H	-0.06405	-4.40544	0.31176	C	1.10718	0.04753	-0.54542
H	-2.45709	-2.84509	3.53065	O	1.71489	1.00264	-0.43439
H	-1.0712	-4.67472	2.5724	Thermal correction to Energy= 0.460172			
P	-1.92726	0.11201	-0.48688	Thermal correction to Enthalpy=0.461116			
Pd	-0.16956	0.63129	-2.18273	Thermal correction to Gibbs Free Energy=0.366641			
Cl	-1.19048	2.98847	-2.41801	Sum of electronic and zero-point Energies=-1586.043499			
H	-0.59842	1.10003	1.93742	Sum of electronic and thermal Energies= -1586.014386			
H	-1.09452	2.90936	3.52199	Sum of electronic and thermal Enthalpies= -1586.013442			
C	-0.82771	-0.65142	-3.54811	Sum of electronic and thermal Free Energies= -1586.107917			
O	-1.08834	-1.35302	-4.41694	SCF Done: E(RM06) = -1587.13571922			
H	0.81187	1.09002	-3.3068	Int3a			
Thermal correction to Energy= 0.315328				Number of imaginary frequencies=0			
Thermal correction to Enthalpy= 0.316272				Charge = 0 Multiplicity = 1			
Thermal correction to Gibbs Free Energy= 0.236184				P	3.02862	0.01578	-0.29479
Sum of electronic and zero-point Energies= -1736.922993				C	3.60354	-0.25645	1.43856
Sum of electronic and thermal Energies= -1736.900268				C	2.64352	-0.38304	2.46201
Sum of electronic and thermal Enthalpies= -1736.899324				C	4.96269	-0.36568	1.77358
Sum of electronic and thermal Free Energies= -1736.979411				C	3.03685	-0.61506	3.78047
SCF Done: E(RM06) = -1624.685194				C	5.35263	-0.60363	3.09509
TS2a				C	4.39365	-0.72282	4.10008
Number of imaginary frequencies=1				C	4.55984	0.17849	-1.28369
Charge = 0 Multiplicity = 1				C	5.30347	1.36962	-1.29806
C	-2.00478	2.51661	2.63956	C	4.99285	-0.91824	-2.04755
C	-2.30494	1.78548	1.48874	C	6.47511	1.45338	-2.04964
C	-1.75651	0.50781	1.3027	C	6.16746	-0.83117	-2.79511
C	-0.8965	-0.01699	2.28471	C	6.90644	0.35289	-2.79968
C	-0.60812	0.71288	3.43825	C	2.25646	1.68044	-0.26854
C	-1.16184	1.98265	3.6159	C	2.47131	2.59785	0.77257
H	-2.43035	3.50722	2.7702	C	1.44173	2.04181	-1.35762
H	-2.95471	2.21928	0.7366	C	1.8813	3.85926	0.72277
H	-0.93165	2.55603	4.50892	C	0.85959	3.3116	-1.40039
H	1.12089	-4.31193	-1.58531	C	1.07536	4.22093	-0.36235
C	-1.27969	-3.54712	-2.78616	H	2.04584	4.56127	1.5347
C	-2.61691	-3.78688	-3.16189	H	0.23586	3.58626	-2.24658

H	0.61925	5.20677	-0.39717	TS4a			
H	1.26846	1.33495	-2.16508	Number of imaginary frequencies=1			
H	3.0864	2.32568	1.62432	Charge = 0 Multiplicity = 1			
H	7.04798	2.37447	-2.06038	P	3.03775	0.00819	-0.25757
H	6.48853	-1.67925	-3.38999	C	3.62777	-0.23487	1.47039
H	7.8161	0.42137	-3.38952	C	2.67198	-0.37363	2.49209
H	4.39518	-1.82197	-2.07618	C	4.98834	-0.32581	1.79681
H	4.97035	2.22838	-0.72617	C	3.07029	-0.58281	3.81079
H	2.2831	-0.71124	4.5562	C	5.38377	-0.54701	3.11875
H	6.40935	-0.68426	3.33525	C	4.42882	-0.67303	4.12731
H	4.6993	-0.90922	5.12704	C	4.56079	0.17347	-1.26917
H	5.71886	-0.27081	1.00238	C	5.29554	1.36954	-1.30273
H	1.58561	-0.29979	2.22941	C	5.00632	-0.9286	-2.01314
Pd	1.55085	-1.72569	-1.03221	C	6.46476	1.4534	-2.05891
C	1.26286	-2.66242	0.57358	C	6.17864	-0.84163	-2.76497
O	1.03913	-3.23672	1.55145	C	6.9087	0.34779	-2.78848
C	-0.03505	-3.6205	-1.4021	C	2.26587	1.67945	-0.25627
C	0.4998	-4.99432	-0.99986	C	2.48462	2.60493	0.77693
H	1.52115	-5.13256	-1.35715	C	1.44956	2.03776	-1.3428
Cl	1.51078	-1.02359	-3.35371	C	1.89787	3.87081	0.72163
H	0.48354	-5.20345	0.08091	C	0.87085	3.30624	-1.39154
H	0.12489	-3.38194	-2.4526	C	1.09101	4.22349	-0.36141
H	-0.13211	-5.76847	-1.48809	H	2.07186	4.57893	1.52751
C	-1.35521	-3.2011	-0.88703	H	0.24159	3.57371	-2.23597
C	-2.04437	-3.83866	0.17214	H	0.63299	5.20828	-0.40067
C	-2.01781	-2.14545	-1.55592	H	1.27218	1.32455	-2.14365
C	-3.33916	-3.45057	0.51698	H	3.10542	2.34001	1.62684
H	-1.57253	-4.64954	0.72174	H	7.02475	2.38435	-2.08312
C	-3.30414	-1.77134	-1.21445	H	6.51081	-1.69872	-3.34389
H	-1.49286	-1.63889	-2.36271	H	7.81654	0.41749	-3.38173
C	-3.98633	-2.42239	-0.17889	H	4.42146	-1.84318	-2.0224
H	-3.85663	-3.9664	1.31956	H	4.95148	2.23647	-0.74646
H	-3.7957	-0.96638	-1.75973	H	2.31954	-0.68471	4.58951
H	-4.99839	-2.1339	0.08403	H	6.44176	-0.61846	3.35629
Thermal correction to Energy= 0.463027				H	4.73867	-0.84496	5.15448
Thermal correction to Enthalpy= 0.463971				H	5.74158	-0.22406	1.02284
Thermal correction to Gibbs Free Energy= 0.365065				H	1.6128	-0.31605	2.25614
Sum of electronic and zero-point Energies= -2046.461464				Pd	1.57945	-1.70718	-1.008
Sum of electronic and thermal Energies= -2046.430742				C	1.12863	-2.78804	0.4536
Sum of electronic and thermal Enthalpies= -2046.429797				O	0.98486	-3.29145	1.4872
Sum of electronic and thermal Free Energies= -2046.528703				C	-0.04591	-3.67599	-1.27516
SCF Done: E(RM06) = -2047.518759				C	0.43978	-5.08524	-1.00798
				H	1.46768	-5.21406	-1.35984
				Cl	1.52511	-1.02637	-3.33415

H	0.40237	-5.36949	0.04751	H	2.05654	4.55057	1.5347
H	0.19946	-3.34786	-2.28498	H	0.24656	3.57556	-2.24658
H	-0.19431	-5.79135	-1.56409	H	0.62995	5.19607	-0.39717
C	-1.40106	-3.25691	-0.86828	H	1.26846	1.32425	-2.16508
C	-2.108	-3.89225	0.17006	H	3.0757	2.30428	1.62432
C	-2.02716	-2.19087	-1.54841	H	7.01588	2.37447	-2.03898
C	-3.39616	-3.48071	0.51062	H	6.48853	-1.67925	-3.38999
H	-1.65214	-4.71383	0.71396	H	7.8054	0.43207	-3.37882
C	-3.31195	-1.78243	-1.20499	H	4.39518	-1.84337	-2.07618
H	-1.48699	-1.6866	-2.34651	H	4.93825	2.20698	-0.71547
C	-4.00364	-2.42529	-0.17262	H	2.2831	-0.73264	4.5669
H	-3.92726	-3.98772	1.31208	H	6.40935	-0.67356	3.34595
H	-3.7777	-0.96238	-1.74508	H	4.6993	-0.89852	5.13774
H	-5.00752	-2.1066	0.09481	H	5.71886	-0.26011	1.01308
Thermal correction to Energy= 0.462147				H	1.58561	-0.36399	2.22941
Thermal correction to Enthalpy= 0.463092				Pd	1.59365	-1.65079	-1.075
Thermal correction to Gibbs Free Energy= 0.365711				C	0.98466	-2.87642	0.25258
Sum of electronic and zero-point Energies= -2046.444761				O	0.99633	-3.23672	1.39095
Sum of electronic and thermal Energies= -2046.414720				C	0.09335	-3.5991	-0.9634
Sum of electronic and thermal Enthalpies= -2046.413776				C	0.4677	-5.09062	-0.89286
Sum of electronic and thermal Free Energies= -2046.511156				H	1.51045	-5.22886	-1.20735
SCF Done: E(RM06) = -2047.50546386				Cl	1.52148	-0.98079	-3.41791
Int5a				H	0.36584	-5.49235	0.12371
Number of imaginary frequencies=0				H	0.39239	-3.23214	-1.9604
Charge = 0 Multiplicity = 1				H	-0.17491	-5.67217	-1.57369
P	3.01792	-0.01632	-0.26269	C	-1.35521	-3.2225	-0.73723
C	3.60354	-0.26715	1.45996	C	-2.09787	-3.84936	0.26844
C	2.64352	-0.41514	2.47271	C	-1.95361	-2.19895	-1.49172
C	4.96269	-0.36568	1.78428	C	-3.41406	-3.46127	0.52768
C	3.03685	-0.62576	3.79117	H	-1.64743	-4.63884	0.86084
C	5.35263	-0.59293	3.10579	C	-3.27204	-1.80344	-1.22515
C	4.39365	-0.72282	4.11078	H	-1.38586	-1.70309	-2.27711
C	4.53844	0.15709	-1.28369	C	-3.99703	-2.43309	-0.21099
C	5.28207	1.34822	-1.28736	H	-3.97433	-3.9557	1.31956
C	4.98215	-0.92894	-2.04755	H	-3.7208	-1.00918	-1.81323
C	6.45371	1.44268	-2.03894	H	-5.01979	-2.1232	-0.00157
C	6.15676	-0.83117	-2.79511	Thermal correction to Energy= 0.464751			
C	6.89574	0.35289	-2.78898	Thermal correction to Enthalpy= 0.465695			
C	2.24576	1.65904	-0.26854	Thermal correction to Gibbs Free Energy= 0.368035			
C	2.46061	2.57645	0.77257	Sum of electronic and zero-point Energies= -2046.468021			
C	1.44173	2.03111	-1.35762	Sum of electronic and thermal Energies= -2046.437904			
C	1.8813	3.84856	0.72277	Sum of electronic and thermal Enthalpies= -2046.436960			
C	0.87029	3.3009	-1.40039	Sum of electronic and thermal Free Energies= -2046.534620			
C	1.08606	4.21023	-0.36235	SCF Done: E(M06) = -2047.532411			

				H	-0.98042	-4.59589	-1.30657	
TS6a				O	1.37483	-4.95169	-1.2115	
Number of imaginary frequencies=1				C	1.46434	-3.30616	0.59187	
Charge = 0 Multiplicity = 1				H	1.45619	-2.27154	0.15856	
P	2.94151	0.74298	-0.48641	C	0.60164	-3.27815	1.85361	
C	3.77414	0.1688	1.07188	C	0.54324	-4.38578	2.71475	
C	2.97812	0.03189	2.22268	C	-0.17104	-2.14627	2.1564	
C	5.13358	-0.16635	1.15526	C	-0.25992	-4.35745	3.85575	
C	3.52686	-0.41338	3.42445	H	1.13379	-5.27255	2.49797	
C	5.68167	-0.62469	2.35743	C	-0.97676	-2.12008	3.29819	
C	4.88297	-0.7474	3.49469	H	-0.12966	-1.28368	1.4925	
C	4.29747	0.62827	-1.7478	C	-1.02194	-3.22403	4.15106	
C	5.31258	1.58861	-1.88414	H	-0.29077	-5.2216	4.51407	
C	4.29726	-0.47886	-2.61086	H	-1.56486	-1.23348	3.51945	
C	6.30811	1.43684	-2.85145	H	-1.64669	-3.20335	5.03984	
C	5.29687	-0.63465	-3.57237	C	2.92458	-3.71413	0.82202	
C	6.30494	0.32367	-3.69491	H	3.00866	-4.74918	1.16846	
C	2.7988	2.56956	-0.19978	H	3.49099	-3.62825	-0.109	
C	3.58277	3.2748	0.72671	H	3.37548	-3.05469	1.56747	
C	1.85361	3.27658	-0.9607					Thermal correction to Energy= 0.500396
C	3.43072	4.6551	0.88025					Thermal correction to Enthalpy= 0.501340
C	1.70921	4.65625	-0.81334					Thermal correction to Gibbs Free Energy= 0.398039
C	2.49708	5.34924	0.10885					Sum of electronic and zero-point Energies= -2102.974310
H	4.04211	5.18639	1.60544					Sum of electronic and thermal Energies= -2102.942513
H	0.9732	5.18765	-1.41107					Sum of electronic and thermal Enthalpies= -2102.941569
H	2.37844	6.42277	0.23105					Sum of electronic and thermal Free Energies= -2103.044870
H	1.2233	2.73186	-1.65944					SCF Done: E(RM06) = -2104.07234932
H	4.30881	2.74676	1.33799					
H	7.08415	2.19197	-2.94836	TS2b				
H	5.28034	-1.49776	-4.23281	Number of imaginary frequencies=1				
H	7.07881	0.20934	-4.44961	Charge = 0 Multiplicity = 1				
H	3.49289	-1.20622	-2.53138	C	-2.20173	3.4875	-0.83507	
H	5.32187	2.46351	-1.24096	C	-2.50311	2.14152	-1.05917	
H	2.89413	-0.50964	4.30298	C	-2.01217	1.15815	-0.18889	
H	6.73645	-0.88436	2.40146	C	-1.22177	1.54164	0.90953	
H	5.3108	-1.10337	4.42829	C	-0.92863	2.88569	1.12979	
H	5.76982	-0.07359	0.28105	C	-1.41504	3.86137	0.25425	
H	1.91869	0.26855	2.16851	H	-2.58939	4.24219	-1.51305	
Pd	1.03556	-0.26919	-1.08976	H	-3.12514	1.86754	-1.90425	
C	0.83039	-4.15286	-0.48804	H	-1.18401	4.90856	0.42534	
H	-0.74355	-2.7748	-1.29707	C	-3.59965	-0.75966	-1.7618	
Cl	-1.0772	-1.24061	-1.98096	C	-4.93279	-1.10493	-1.49891	
N	-0.56669	-3.87385	-0.71225	C	-3.19885	-0.52797	-3.09103	
H	-1.09183	-3.76489	0.16082	C	-5.85021	-1.20753	-2.54801	

H	-5.25989	-1.29521	-0.48224	Sum of electronic and zero-point Energies=	-1586.005298
C	-4.1214	-0.62046	-4.13241	Sum of electronic and thermal Energies=	-1585.976934
H	-2.16671	-0.26357	-3.31196	Sum of electronic and thermal Enthalpies=	-1585.975990
C	-5.44945	-0.96376	-3.86169	Sum of electronic and thermal Free Energies=	-1586.069612
H	-6.87994	-1.4777	-2.33333	SCF Done: E(M06) =	-1587.09493
H	-3.8046	-0.42798	-5.15335		
H	-6.1664	-1.04282	-4.67345	Int3b	
C	-3.11301	-1.18631	1.12864	Number of imaginary frequencies=	0
C	-2.7741	-2.4299	1.68333	Charge = 0	Multiplicity = 1
C	-4.04963	-0.37053	1.78899	C	1.49672 1.52867 -3.00762
C	-3.36902	-2.85957	2.87066	C	1.07331 2.8242 -3.2766
H	-2.03484	-3.05848	1.19495	C	2.25974 1.26761 -1.85371
C	-4.64412	-0.80565	2.97274	C	1.39096 3.87206 -2.40183
H	-4.30767	0.60371	1.38444	C	2.57703 2.31136 -0.97725
C	-4.30582	-2.04926	3.51385	C	2.13957 3.61048 -1.25317
H	-3.09592	-3.8214	3.29442	H	1.0475 4.87722 -2.61282
H	-5.36691	-0.17044	3.47617	H	3.15493 2.12558 -0.07887
H	-4.7668	-2.38144	4.43934	H	2.38243 4.41592 -0.56738
P	-2.33995	-0.63394	-0.43519	P	2.8327 -0.45769 -1.57488
Pd	-0.34073	-1.9199	-0.97672	C	3.38723 -0.47512 0.19062
C	-1.43271	-3.53919	-1.83685	C	2.41955 -0.43395 1.20925
H	-2.06744	-3.15774	-2.6313	C	4.7435 -0.53629 0.54914
H	-1.96372	-4.03039	-1.02506	C	2.80156 -0.44749 2.55563
C	-0.11723	-4.02924	-2.15921	H	1.36382 -0.38345 0.96093
H	0.75759	-3.02097	-1.45346	C	5.12239 -0.55379 1.89386
H	0.24859	-4.83242	-1.51803	H	5.50532 -0.56674 -0.22257
H	-0.85313	0.79434	1.6082	C	4.1553 -0.51051 2.89808
H	-0.3239	3.17195	1.98524	H	2.0418 -0.41903 3.32547
C	0.46653	-4.03046	-3.52905	H	6.17669 -0.60727 2.1528
C	1.48338	-4.95339	-3.81587	H	4.45265 -0.53186 3.94308
C	0.02196	-3.16435	-4.5406	C	4.3574 -0.664 -2.55701
C	2.03741	-5.02145	-5.09393	C	4.70222 -1.94399 -3.01026
H	1.83654	-5.6272	-3.03877	C	5.18707 0.42605 -2.86868
C	0.57973	-3.23046	-5.81456	C	5.86825 -2.14006 -3.74186
H	-0.75832	-2.43646	-4.33606	H	4.03951 -2.78515 -2.80946
C	1.58743	-4.15926	-6.09471	C	6.35597 0.22649 -3.60595
H	2.81838	-5.74536	-5.3054	H	4.91734 1.42507 -2.53956
H	0.22957	-2.55802	-6.59202	C	6.69905 -1.05286 -4.03759
H	2.01946	-4.20778	-7.08974	H	6.12735 -3.13448 -4.09408
C	1.06233	-0.66772	-0.30673	H	6.98952 1.07688 -3.84303
O	1.89469	0.01707	0.05424	H	7.60667 -1.20636 -4.62291
Thermal correction to Energy=	0.454833			Cl	1.23961 -1.8173 -4.4216
Thermal correction to Enthalpy=	0.455777			H	1.24579 0.71991 -3.68301
Thermal correction to Gibbs Free Energy=	0.362155			H	0.48258 3.02084 -4.17113

Pd	1.13523	-2.11064	-2.02558	C	4.74678	-0.53331	0.55256
C	0.74247	-2.751	-0.30709	C	2.8056	-0.4486	2.55965
O	0.43171	-3.26949	0.68253	H	1.36736	-0.41016	0.96543
C	-0.51126	-3.69466	-2.2164	C	5.12616	-0.54965	1.89721
C	-0.00707	-5.14384	-2.08561	H	5.50836	-0.56453	-0.21937
H	0.92533	-5.26161	-2.65536	C	4.15948	-0.50536	2.90173
H	0.20244	-5.42478	-1.03625	H	2.04612	-0.41908	3.33594
H	-1.29118	-3.46445	-1.44816	H	6.18055	-0.59683	2.15581
H	-0.83001	-3.42322	-3.23358	H	4.45717	-0.51959	3.94665
C	-1.07327	-6.06688	-2.66149	C	4.34739	-0.67011	-2.55307
C	-1.23527	-6.13177	-4.05412	C	4.6998	-1.95083	-3.00324
C	-1.93695	-6.80749	-1.84974	C	5.17574	0.42009	-2.86145
C	-2.23482	-6.91301	-4.62588	C	5.87212	-2.14119	-3.73457
H	-0.56725	-5.5562	-4.69761	H	4.04427	-2.79225	-2.80037
C	-2.94442	-7.59637	-2.41926	C	6.34471	0.22625	-3.59852
H	-1.8244	-6.76894	-0.76787	H	4.90493	1.41961	-2.53477
C	-3.09622	-7.65407	-3.80671	C	6.6954	-1.05378	-4.0332
H	-2.34531	-6.95639	-5.7009	H	6.13229	-3.13619	-4.08436
H	-3.60707	-8.16711	-1.77302	H	6.97721	1.07679	-3.83788
H	-3.87348	-8.26933	-4.24592	H	7.60308	-1.20147	-4.61213
Thermal correction to Energy=	0.463272			Cl	1.25669	-1.81741	-4.4408
Thermal correction to Enthalpy=	0.464217			H	1.24204	0.71075	-3.68263
Thermal correction to Gibbs Free Energy=	0.364617			H	0.48265	3.01689	-4.16548
Sum of electronic and zero-point Energies=	-2046.457198			Pd	1.1581	-2.084	-2.03436
Sum of electronic and thermal Energies=	-2046.426656			C	0.56835	-2.88915	-0.45906
Sum of electronic and thermal Enthalpies=	-2046.425712			O	0.41269	-3.26714	0.62947
Sum of electronic and thermal Free Energies=	-2046.525311			C	-0.51101	-3.7291	-1.95181
SCF Done: E(RM06) = -2047.512617				C	-0.00472	-5.16813	-2.06302
				H	0.89506	-5.1869	-2.68766
TS4b				H	0.27519	-5.54801	-1.07333
Number of imaginary frequencies=1				H	-1.39523	-3.62246	-1.32126
Charge = 0 Multiplicity = 1				H	-0.72909	-3.28837	-2.92816
C	1.49461	1.52049	-3.00287	C	-1.07353	-6.0599	-2.66956
C	1.06995	2.8217	-3.27246	C	-1.23959	-6.12673	-4.0606
C	2.25507	1.25502	-1.85095	C	-1.9363	-6.80358	-1.85343
C	1.38996	3.86472	-2.40018	C	-2.242	-6.91905	-4.62057
C	2.57464	2.30639	-0.977	H	-0.57718	-5.55365	-4.70591
C	2.14216	3.60498	-1.25344	C	-2.94044	-7.59722	-2.41107
H	1.05177	4.87568	-2.61159	H	-1.81583	-6.765	-0.77261
H	3.15528	2.11586	-0.08007	C	-3.09621	-7.65681	-3.79713
H	2.39308	4.41148	-0.56957	H	-2.35416	-6.96256	-5.70078
P	2.82254	-0.46998	-1.55251	H	-3.59739	-8.17163	-1.76292
C	3.39047	-0.47862	0.20055	H	-3.87574	-8.27581	-4.2333
C	2.42321	-0.44244	1.21959	Thermal correction to Energy=	0.462271		



Thermal correction to Enthalpy= 0.463215		H	1.24579	0.70701	-3.69591			
Thermal correction to Gibbs Free Energy= 0.363767		H	0.49548	3.02084	-4.17113			
Sum of electronic and zero-point Energies= -2046.440913		Pd	1.18684	-2.04614	-2.06428			
Sum of electronic and thermal Energies= -2046.410929		C	0.39417	-3.0477	-0.64249			
Sum of electronic and thermal Enthalpies= -2046.409985		O	0.44461	-3.25659	0.56643			
Sum of electronic and thermal Free Energies= -		C	-0.49836	-3.77206	-1.62301			
2046.509434SCF Done: E(RM06) = -2047.501952		C	-0.00707	-5.20834	-1.98241			
		H	0.87373	-5.13262	-2.64246			
Int5b		H	0.31854	-5.69568	-1.04915			
Number of imaginary frequencies=0		H	-1.51048	-3.78695	-1.16436			
Charge =0 Multiplicity = 1		H	-0.58491	-3.15232	-2.56278			
C	1.49672	1.51577	-3.00762	C	-1.07327	-6.05398	-2.64859	
C	1.07331	2.8242	-3.2766	C	-1.22237	-6.10597	-4.04122	
C	2.24684	1.24181	-1.85371	C	-1.94985	-6.80749	-1.84974	
C	1.39096	3.85916	-2.40183	C	-2.22192	-6.90011	-4.61298	
C	2.56413	2.29846	-0.97725	H	-0.55435	-5.5304	-4.67181	
C	2.13957	3.59758	-1.25317	C	-2.94442	-7.59637	-2.41926	
H	1.0604	4.87722	-2.61282	H	-1.8373	-6.78184	-0.76787	
H	3.14203	2.09978	-0.07887	C	-3.08332	-7.64117	-3.80671	
H	2.39533	4.40302	-0.56738	H	-2.31951	-6.93059	-5.7009	
P	2.8069	-0.48349	-1.53618	H	-3.60707	-8.18001	-1.78592	
C	3.38723	-0.48802	0.20352	H		-3.86058	-8.25643	-4.25882
C	2.41955	-0.45975	1.22215	Thermal correction to Energy= 0.465042				
C	4.7435	-0.53629	0.54914	Thermal correction to Enthalpy= 0.465986				
C	2.80156	-0.46039	2.55563	Thermal correction to Gibbs Free Energy= 0.366443				
H	1.36382	-0.44795	0.96093	Sum of electronic and zero-point Energies= -2046.469473				
C	5.12239	-0.55379	1.89386	Sum of electronic and thermal Energies= -2046.439381				
H	5.50532	-0.56674	-0.22257	Sum of electronic and thermal Enthalpies= -2046.438437				
C	4.1553	-0.51051	2.89808	Sum of electronic and thermal Free Energies= -2046.537980				
H	2.0418	-0.43193	3.33837	SCF Done: E(RM06) = -2047.533801				
H	6.17669	-0.59437	2.1528					
H	4.45265	-0.51896	3.94308	TS6b				
C	4.3316	-0.6769	-2.55701	Number of imaginary frequencies=1				
C	4.68932	-1.95689	-3.01026	Charge =0 Multiplicity = 1				
C	5.16127	0.41315	-2.85578	P	-2.38032	0.67693	0.39211	
C	5.86825	-2.14006	-3.74186	C	-3.27615	0.46841	1.99878	
H	4.03951	-2.79805	-2.80946	C	-3.69067	-0.82206	2.37311	
C	6.33017	0.22649	-3.59305	C	-3.49261	1.5289	2.88878	
H	4.89154	1.41217	-2.52666	C	-4.30747	-1.04325	3.60366	
C	6.68615	-1.05286	-4.03759	C	-4.10589	1.30426	4.1246	
H	6.12735	-3.13448	-4.09408	C	-4.51426	0.02073	4.48652	
H	6.96372	1.07688	-3.83013	C	-3.55867	-0.02049	-0.83578	
H	7.59377	-1.19346	-4.61001	C	-3.0363	-0.67513	-1.96105	
Cl	1.25251	-1.8044	-4.4861	C	-4.9534	0.08935	-0.6871	

C	-3.89697	-1.19987	-2.92886	H	2.84052	-1.88548	4.15101
C	-5.80686	-0.43404	-1.6579	C	4.80594	-4.32174	2.8172
C	-5.27879	-1.07746	-2.78171	H	4.07719	-6.1321	1.89891
C	-2.38444	2.50264	0.10173	H	5.21692	-2.43993	3.78864
C	-3.39885	3.17118	-0.59997	H	5.8532	-4.56062	2.6549
C	-1.29877	3.24655	0.59572	Thermal correction to Energy= 0.500489			
C	-3.33239	4.55224	-0.79238	Thermal correction to Enthalpy= 0.501433			
C	-1.2389	4.62835	0.41026	Thermal correction to Gibbs Free Energy= 0.398354			
C	-2.25643	5.28382	-0.28583	Sum of electronic and zero-point Energies= -2102.956925			
H	-1.96367	-0.80945	-2.07636	Sum of electronic and thermal Energies= -2102.925392			
H	-5.37187	0.57264	0.1914	Sum of electronic and thermal Enthalpies= -2102.924447			
H	-4.1221	5.05581	-1.34359	Sum of electronic and thermal Free Energies= -2103.027526			
H	-0.39274	5.18845	0.79892	SCF Done: E(RM06) = -2104.05934004			
H	-2.20653	6.35824	-0.44072				
H	-0.4961	2.73623	1.1244	P1			
H	-4.23564	2.61418	-1.00857	Number of imaginary frequencies=0			
H	-3.4748	-1.71625	-3.78599	Charge = 0 Multiplicity = 1			
H	-6.88316	-0.34511	-1.53452	C	3.10644	-1.68151	-2.42024
H	-5.94643	-1.49026	-3.53367	C	4.46372	-2.35105	-2.69142
H	-3.54672	-1.65478	1.68867	C	1.94587	-2.66245	-2.48931
H	-3.18527	2.53474	2.62058	N	0.68395	-2.11054	-2.21226
H	-4.63113	-2.04562	3.87223	O	2.06152	-3.82829	-2.81991
H	-4.26757	2.13908	4.80152	H	4.42115	-2.85422	-3.66266
H	-4.99324	-0.15122	5.44656	H	-0.02353	-2.82265	-2.04202
Pd	-0.20684	-0.10657	0.41298	H	0.63033	-1.3537	-1.52079
C	0.58152	-1.90165	1.30429	H	3.10725	-1.19512	-1.43616
H	0.20626	-2.75127	-0.76612	C	5.60963	-1.36106	-2.66079
Cl	0.03183	-2.55237	-2.4581	C	6.12977	-0.90116	-1.44171
N	0.29926	-3.03318	0.4558	C	6.15929	-0.85915	-3.84771
H	-0.5664	-3.5166	0.70299	C	7.16265	0.03655	-1.40947
H	1.07408	-3.70631	0.50692	H	5.7196	-1.27842	-0.50729
O	1.58471	-1.21342	0.96212	C	7.19484	0.07792	-3.82182
C	0.13937	-2.04646	2.76035	H	5.77321	-1.20921	-4.80268
H	-0.95289	-2.00049	2.84056	C	7.69979	0.53073	-2.60132
C	0.62781	-3.35745	3.44307	H	7.55145	0.37657	-0.45285
H	0.5341	-1.17053	3.28091	H	7.61069	0.44862	-4.75542
H	0.41129	-3.25615	4.51486	H	8.50998	1.25499	-2.57835
H	0.01694	-4.20168	3.09714	H	2.92228	-0.87362	-3.14091
C	2.09182	-3.69133	3.2344	H	4.62259	-3.14058	-1.94737
C	2.46543	-4.885	2.60038	Thermal correction to Energy= 0.195103			
C	3.10454	-2.81854	3.65965	Thermal correction to Enthalpy= 0.196048			
C	3.81108	-5.20066	2.39122	Thermal correction to Gibbs Free Energy= 0.147765			
H	1.69549	-5.58845	2.28601	Sum of electronic and zero-point Energies= -479.382865			
C	4.44742	-3.13041	3.45435	Sum of electronic and thermal Energies= -479.372456			

Sum of electronic and thermal Enthalpies=	-479.371512		C	3.23199	-0.75345	2.92776	
Sum of electronic and thermal Free Energies=	-479.419795		C	5.10467	-0.20721	1.49493	
SCF Done: E(RM06) =	-479.384303608		C	4.09234	-0.83961	4.02096	
			C	5.96615	-0.30689	2.59214	
			C	5.46323	-0.61866	3.85519	
P2			C	3.56622	0.0436	-1.22141	
Number of imaginary frequencies=	0		C	3.8253	1.36108	-1.62992	
Charge =	0	Multiplicity =	1	4.11235	-1.0219	-1.95904	
C	3.46996	-1.64648	-1.00242	C	4.61937	1.60758	-2.75158
C	3.73481	-1.67771	0.50855	C	4.9137	-0.76988	-3.07365
C	1.96987	-1.66327	-1.30767	C	5.16657	0.54436	-3.473
N	1.71972	-1.50267	-2.80937	C	1.54266	1.1485	0.59222
O	1.13644	-2.45081	-0.75062	C	2.04139	2.22341	1.34582
H	3.32272	-0.78128	0.98287	C	0.23971	1.22339	0.07502
H	2.03254	-2.35503	-3.29031	C	1.25352	3.35392	1.5687
H	0.71271	-1.40415	-2.9638	C	-0.54287	2.35763	0.29557
H	3.27796	-2.55313	0.97935	C	-0.03846	3.42368	1.04293
C	4.14611	-2.80197	-1.74972	H	1.64851	4.17799	2.15683
C	4.95774	-2.53786	-2.86285	H	-1.55022	2.40188	-0.10924
C	3.94686	-4.13559	-1.35883	H	-0.65173	4.30287	1.22136
C	5.57719	-3.58356	-3.55293	H	-0.16477	0.39336	-0.49741
H	5.07964	-1.51319	-3.20613	H	3.04116	2.17465	1.76696
C	4.56716	-5.17799	-2.04795	H	4.80837	2.63202	-3.06146
H	3.29895	-4.35895	-0.51585	H	5.33088	-1.6045	-3.62988
C	5.38911	-4.90457	-3.14481	H	5.78363	0.73956	-4.34602
H	6.20241	-3.36011	-4.41322	H	3.91251	-2.0521	-1.67171
H	4.40705	-6.20495	-1.7293	H	3.40211	2.19512	-1.07869
H	5.87221	-5.71733	-3.68093	H	3.69348	-1.08959	5.00021
H	4.81265	-1.70589	0.69598	H	7.03066	-0.13731	2.4546
H	3.86914	-0.71256	-1.40993	H	6.13435	-0.69497	4.7063
Thermal correction to Energy=	0.775268		H	5.50771	0.04195	0.51859	
Thermal correction to Enthalpy=	0.776213		H	2.1713	-0.94833	3.0635	
Thermal correction to Gibbs Free Energy=	0.654251		Pd	1.28814	-2.40924	-0.11763	
Sum of electronic and zero-point Energies=	-2264.779669		C	1.98604	-3.59562	1.36851	
Sum of electronic and thermal Energies=	-2264.736129		O	1.38885	-4.09218	2.29564	
Sum of electronic and thermal Enthalpies=	-2264.735185		C	0.12914	-4.04584	-0.87677	
Sum of electronic and thermal Free Energies=	-2264.857147		C	-0.66225	-4.94426	0.04797	
SCF Done: E(RwB97XD) =	-2266.46875373		H	-0.0093	-5.69584	0.49726	
			H	-1.12739	-4.39416	0.87202	
TS4c			H	0.87117	-4.5764	-1.47673	
Number of imaginary frequencies=	1		H	-1.45456	-5.47584	-0.50118	
Charge =	0	Multiplicity =	1	C	-0.5233	-2.9432	-1.58154
P	2.52928	-0.36893	0.24591	C	-1.83569	-2.47957	-1.28178
C	3.72793	-0.42692	1.65166	C	0.23941	-2.18311	-2.51586

C	-2.35867	-1.36302	-1.91243	C	-2.54965	4.82777	-0.5768
H	-2.44	-3.02988	-0.56776	C	3.31332	1.92578	1.75679
C	-0.30192	-1.04549	-3.13892	C	2.41789	2.87166	2.28699
H	1.2109	-2.55575	-2.8325	C	4.49372	1.65125	2.46309
C	-1.5959	-0.63564	-2.84599	C	2.70628	3.53886	3.47606
H	-3.37446	-1.04794	-1.68643	C	4.77437	2.31027	3.66349
H	0.29671	-0.50173	-3.86467	C	3.88612	3.25823	4.17088
H	-2.02122	0.2354	-3.33671	C	4.37422	0.07971	-0.20314
H	3.66985	-4.5696	0.00224	C	5.51588	0.66334	-0.77681
Cl	4.04167	-5.08475	-1.34783	C	4.39301	-1.29088	0.09872
N	3.40092	-3.94243	1.22618	C	6.65276	-0.1045	-1.0315
H	3.71237	-4.50423	2.0261	C	5.53564	-2.05522	-0.14919
H	3.97761	-3.10305	1.14907	C	6.66692	-1.46494	-0.71402
Thermal correction to Energy=	0.498222			C	2.86371	2.39569	-1.06333
Thermal correction to Enthalpy=	0.499166			C	3.56453	3.60161	-0.89794
Thermal correction to Gibbs Free Energy=	0.395653			C	2.1377	2.19157	-2.24861
Sum of electronic and zero-point Energies=	-2102.952518			C	3.54717	4.57423	-1.8999
Sum of electronic and thermal Energies=	-2102.920196			C	2.1259	3.16264	-3.25119
Sum of electronic and thermal Enthalpies=	-2102.919252			C	2.83123	4.35581	-3.07926
Sum of electronic and thermal Free Energies=	-2104.04890550			H	4.09261	5.50369	-1.75679
2103.022765SCF SCF Done: E(RM06) =	-2104.04890550			H	1.55113	2.98838	-4.15644
				H	2.81687	5.1155	-3.85654
Int5c				H	-3.05268	0.04256	-1.04564
Number of imaginary frequencies=0				H	-2.70588	-0.91323	3.1438
Charge =0 Multiplicity = 1				H	1.55673	1.28198	-2.37779
P	-1.18035	0.69582	1.10382	H	4.11709	3.78657	0.01843
P	2.84116	1.04173	0.1976	H	7.52714	0.36042	-1.47988
C	-0.97933	1.04462	2.91809	H	5.5342	-3.1159	0.08826
C	0.1145	0.47575	3.58676	H	7.55286	-2.06209	-0.91438
C	-1.87646	1.83883	3.65169	H	3.50208	-1.76257	0.49942
C	0.30141	0.67858	4.95637	H	5.51726	1.71873	-1.03155
C	-1.68799	2.04632	5.01807	H	2.00281	4.26958	3.86602
C	-0.6005	1.46322	5.67478	H	5.69428	2.08336	4.19652
C	-2.73447	-0.31899	1.06616	H	4.10768	3.77292	5.10218
C	-3.40266	-0.48469	-0.16192	H	5.2001	0.9247	2.07575
C	-3.20442	-1.02214	2.18584	H	1.48791	3.08753	1.76853
C	-4.51712	-1.31768	-0.25768	H	-4.50952	4.34515	0.18703
C	-4.3173	-1.86286	2.08479	H	-0.50846	4.99615	-1.2611
C	-4.97948	-2.01163	0.86566	H	-2.85043	5.79759	-0.96449
C	-1.7761	2.31309	0.4217	H	0.15629	2.7802	-0.40826
C	-3.0995	2.76439	0.56389	H	-3.8419	2.13301	1.04267
C	-0.85641	3.13257	-0.24738	H	-5.02705	-1.42175	-1.21212
C	-3.48111	4.01269	0.07076	H	-4.66804	-2.3955	2.96516
C	-1.2373	4.38286	-0.7383	H	-5.85034	-2.65764	0.7903

H	0.82995	-0.11342	3.01918	C	3.41184	-0.41961	4.29959
H	-2.72162	2.30501	3.15577	C	5.52979	0.13818	3.28263
H	1.15783	0.23273	5.45478	C	4.78851	-0.20439	4.41348
H	-2.39033	2.66537	5.57049	C	3.92918	0.35787	-0.96443
H	-0.45539	1.62695	6.7395	C	4.57699	1.57521	-1.23096
Pd	0.75077	-0.28285	0.18917	C	4.29135	-0.78473	-1.69741
C	0.87906	-0.8392	-1.9458	C	5.57737	1.64568	-2.20177
N	-0.02917	-0.83868	-3.0865	C	5.29618	-0.7092	-2.66428
H	-0.89043	-1.34656	-2.88537	C	5.94071	0.50283	-2.91791
H	0.444	-1.29221	-3.86886	C	1.85927	1.88245	0.39844
O	2.11377	-0.86763	-2.20683	C	2.31506	2.88407	1.26936
C	-0.22823	-2.10928	0.28323	C	0.78172	2.16562	-0.45716
H	-1.20208	-1.63027	0.42344	C	1.71229	4.14419	1.27612
C	-0.47954	-3.49738	-0.31233	C	0.18705	3.42752	-0.4547
C	0.58482	-4.30063	-0.75092	C	0.65046	4.41946	0.41295
C	-1.78525	-3.99406	-0.42489	H	2.07302	4.9095	1.95851
C	0.34806	-5.56879	-1.28068	H	-0.64439	3.63213	-1.12389
H	1.60173	-3.92189	-0.6838	H	0.18147	5.39981	0.42094
C	-2.02379	-5.26544	-0.95436	H	0.40392	1.39186	-1.12151
H	-2.61943	-3.38185	-0.0887	H	3.13723	2.67956	1.94855
C	-0.95788	-6.05671	-1.38333	H	6.0682	2.59469	-2.40164
H	1.18409	-6.17716	-1.6162	H	5.56564	-1.59989	-3.2254
H	-3.04327	-5.63478	-1.03127	H	6.71724	0.55989	-3.67631
H	-1.14133	-7.04479	-1.79686	H	3.78068	-1.72827	-1.52405
C	0.47191	-2.20608	1.64539	H	4.29401	2.47239	-0.68833
H	1.47336	-2.63404	1.54296	H	2.82721	-0.68945	5.17532
H	0.5715	-1.21509	2.09788	H	6.60132	0.30207	3.36219
H	-0.11143	-2.84247	2.31868	H	5.27917	-0.30842	5.37754
Thermal correction to Energy=	0.783022			H	5.48997	0.54179	1.16954
Thermal correction to Enthalpy=	0.783966			H	1.71841	-0.48401	2.97063
Thermal correction to Gibbs Free Energy=	0.649454			Pd	1.13722	-1.56802	-0.08739
Sum of electronic and zero-point Energies=	-2678.165481			C	-0.13428	-3.37423	-0.32124
Sum of electronic and thermal Energies=	-2678.118040			C	1.91902	-3.47167	-0.12039
Sum of electronic and thermal Enthalpies=	-2678.117095			N	2.19238	-4.03918	1.11347
Sum of electronic and thermal Free Energies=	-2678.251607			O	2.48916	-3.84321	-1.13648
SCF Done: E(RM06) =	-2679.18710933			H	0.1038	-4.33531	-0.77171
				H	3.06745	-4.55619	1.14768
TS6c				H	1.99691	-3.46781	1.92528
Number of imaginary frequencies=	1			C	-0.91008	-3.59728	0.97569
Charge =0 Multiplicity =	1			H	-0.35537	-4.27453	1.63061
P	2.60623	0.19204	0.31344	H	-1.09882	-2.6734	1.53205
C	3.52198	0.05748	1.91565	H	-1.88566	-4.05986	0.76341
C	2.78658	-0.29865	3.05943	C	-0.77542	-2.51107	-1.36958
C	4.90145	0.27283	2.04088	C	-0.39636	-2.65982	-2.7264

C	-1.75862	-1.5415	-1.06802	H	3.55002	2.34053	1.8575
C	-0.97208	-1.87975	-3.72256	H	4.69882	2.84106	-3.02763
H	0.36715	-3.39156	-2.97558	H	4.67553	-1.39167	-3.81987
C	-2.33658	-0.7647	-2.07701	H	5.30067	0.92515	-4.49305
H	-2.09623	-1.41643	-0.04391	H	3.45589	-1.78907	-1.7227
C	-1.94956	-0.92754	-3.40633	H	3.49469	2.45503	-0.90759
H	-0.66392	-2.01871	-4.75591	H	4.08282	-1.07566	4.99071
H	-3.10125	-0.03673	-1.8166	H	7.17421	-0.94282	1.99923
H	-2.40534	-0.32772	-4.18945	H	6.48273	-1.29061	4.36299
Thermal correction to Energy= 0.488182				H	5.49369	-0.37564	0.28114
Thermal correction to Enthalpy= 0.489126				H	2.39447	-0.53477	3.27616
Thermal correction to Gibbs Free Energy= 0.394072				Pd	1.0113	-2.00758	0.05459
Sum of electronic and zero-point Energies= -1642.136947				C	1.50826	-3.37594	1.41213
Sum of electronic and thermal Energies= -1642.107267				O	0.85962	-3.87336	2.29322
Sum of electronic and thermal Enthalpies= -1642.106322				C	-0.26679	-3.50551	-0.60426
Sum of electronic and thermal Free Energies= -1642.201377				H	0.21201	-4.481	-0.70689
SCF Done: E(RM06) = -1643.21834393				C	-0.71098	-2.95167	-1.96488
				H	3.15192	-4.38101	-0.01053
TS4d				Cl	3.52696	-4.83463	-1.39397
Number of imaginary frequencies=1				N	2.91292	-3.82831	1.23887
Charge =0 Multiplicity = 1				H	3.16311	-4.4699	1.99845
P	2.49931	-0.07662	0.40844	H	3.5522	-3.03099	1.2359
C	3.82432	-0.40334	1.6537	H	-1.08411	-3.57084	0.12083
C	3.44086	-0.61361	2.99187	H	0.1342	-2.97243	-2.66353
C	5.1783	-0.52795	1.30835	H	-1.03376	-1.90151	-1.87496
C	4.3939	-0.92217	3.96102	C	-1.86466	-3.75727	-2.54639
C	6.12946	-0.84861	2.28243	C	-1.61313	-4.9318	-3.26953
C	5.74178	-1.04266	3.60808	C	-3.19457	-3.36935	-2.33917
C	3.40026	0.3074	-1.15215	C	-2.66512	-5.69618	-3.77544
C	3.75489	1.60982	-1.53711	H	-0.58511	-5.24573	-3.43646
C	3.7313	-0.77136	-1.99286	C	-4.24935	-4.13231	-2.84341
C	4.43438	1.82795	-2.73652	H	-3.40509	-2.45938	-1.78041
C	4.42179	-0.54756	-3.18517	C	-3.98762	-5.29922	-3.56388
C	4.77177	0.75125	-3.55984	H	-2.45126	-6.60154	-4.33787
C	1.76047	1.51258	0.96863	H	-5.27501	-3.81281	-2.67633
C	2.49993	2.50469	1.63365	H	-4.80714	-5.8935	-3.95936
C	0.39895	1.73599	0.71226	Thermal correction to Energy= 0.498597			
C	1.88963	3.69844	2.0205	Thermal correction to Enthalpy= 0.499541			
C	-0.20877	2.93248	1.09557	Thermal correction to Gibbs Free Energy= 0.393563			
C	0.53623	3.91513	1.74981	Sum of electronic and zero-point Energies= -2102.930709			
H	2.4707	4.45804	2.53643	Sum of electronic and thermal Energies= -2102.898319			
H	-1.26417	3.091	0.89241	Sum of electronic and thermal Enthalpies= -2102.897374			
H	0.06261	4.84409	2.05525	Sum of electronic and thermal Free Energies= -2103.003353			
H	-0.18958	0.96453	0.22132	SCF Done: E(RM06) = -2104.02624215			

				H	3.79962	6.37755	-0.09127
Int5d				H	-1.73631	-0.66831	-2.13517
Number of imaginary frequencies=0				H	-4.65733	-0.35871	1.01717
Charge = 0	Multiplicity = 1			H	1.57937	2.95969	-1.47628
P	-1.85321	0.57949	0.47691	H	4.84587	2.45179	1.29373
P	2.87787	0.69952	-0.14975	H	6.41815	0.76248	-3.67053
C	-2.46035	0.6455	2.22311	H	3.27256	-2.12631	-4.20128
C	-2.72039	-0.54714	2.91804	H	5.40029	-1.09565	-4.97304
C	-2.61307	1.86582	2.89892	H	2.16732	-1.296	-2.14635
C	-3.13513	-0.51761	4.2487	H	5.33123	1.56984	-1.60345
C	-3.02069	1.89133	4.23436	H	4.13293	0.09013	4.59779
C	-3.28569	0.70171	4.91254	H	6.78861	-1.78209	1.77599
C	-3.07796	-0.43354	-0.46006	H	6.16565	-1.27031	4.12953
C	-2.71351	-0.91438	-1.72903	H	5.41173	-0.9346	-0.08622
C	-4.35993	-0.7192	0.03786	H	2.73435	0.90901	2.74375
C	-3.6164	-1.66996	-2.47902	H	-4.73251	4.35183	-1.09708
C	-5.25666	-1.47854	-0.71628	H	-0.74778	5.39351	0.15469
C	-4.88635	-1.95735	-1.97438	H	-2.98421	6.07607	-0.70628
C	-2.23917	2.33003	0.04595	H	-0.26843	3.01213	0.6026
C	-3.49436	2.71922	-0.44068	H	-4.26496	1.97603	-0.61868
C	-1.25336	3.30667	0.25202	H	-3.32425	-2.03091	-3.46158
C	-3.75822	4.06329	-0.71153	H	-6.24441	-1.69516	-0.3178
C	-1.5235	4.65002	-0.00756	H	-5.58576	-2.54907	-2.55938
C	-2.77643	5.03088	-0.49265	H	-2.60673	-1.50587	2.42346
C	3.97782	0.05972	1.18938	H	-2.41967	2.80129	2.3857
C	3.63002	0.3375	2.52344	H	-3.33138	-1.45332	4.76424
C	5.12414	-0.7083	0.9349	H	-3.13528	2.84649	4.74017
C	4.41743	-0.13306	3.57321	H	-3.60551	0.72358	5.95104
C	5.9051	-1.18647	1.99027	Pd	0.49448	0.20057	-0.03139
C	5.5565	-0.89842	3.30994	C	0.52626	-0.51571	1.84149
C	3.69297	0.16153	-1.70975	C	0.11331	-1.78435	-0.22027
C	4.88506	0.75118	-2.16068	H	0.16353	-1.44904	-1.26139
C	3.11651	-0.87321	-2.45898	C	-1.21306	-2.49933	-0.01998
C	5.49753	0.29694	-3.32876	H	0.95084	-2.4226	-0.03032
C	3.73358	-1.32887	-3.62509	H	-1.9348	-1.81042	0.36654
C	4.9247	-0.74655	-4.06029	H	-1.55509	-2.88571	-0.95733
C	3.17982	2.52809	-0.08783	C	-0.80789	-3.59359	0.98502
C	4.21102	3.08651	0.6855	C	0.29734	-4.40447	0.72539
C	2.37562	3.37821	-0.86698	C	-1.54575	-3.77399	2.15489
C	4.43	4.46611	0.68344	C	0.66416	-5.39594	1.63514
C	2.60421	4.75507	-0.86671	H	0.87838	-4.26251	-0.19737
C	3.62756	5.30427	-0.09112	C	-1.17836	-4.76507	3.06549
H	5.23135	4.88154	1.28902	H	-2.41676	-3.13486	2.35977
H	1.97656	5.39736	-1.47898	C	-0.07369	-5.5761	2.80576

H	1.53493	-6.03554	1.43026	H	5.86104	-1.12857	-3.18926
H	-1.76006	-4.9068	3.98799	H	6.80889	1.15321	-3.49803
H	0.21576	-6.35787	3.52294	H	4.09342	-1.52381	-1.51762
O	0.52448	-1.9278	2.06707	H	4.20953	2.64606	-0.42057
N	0.55138	0.41085	2.98244	H	3.03882	-1.08321	5.20001
H	-0.0531	0.06965	3.7023	H	6.64647	0.59139	3.55918
H	1.48445	0.47963	3.3355	H	5.39981	-0.35141	5.49046
Thermal correction to Energy= 0.783151				H	5.5415	0.82444	1.35657
Thermal correction to Enthalpy= 0.784095				H	1.93994	-0.87353	2.99212
Thermal correction to Gibbs Free Energy= 0.648185				Pd	1.33997	-1.67742	-0.18544
Sum of electronic and zero-point Energies= -2678.165077				C	0.15666	-3.22506	-0.70389
Sum of electronic and thermal Energies= -2678.117599				C	-0.96123	-2.32729	-1.36644
Sum of electronic and thermal Enthalpies=-2678.116655				C	2.07473	-3.57855	-0.53108
Sum of electronic and thermal Free Energies= -2678.252565				N	2.14892	-4.37	0.60579
SCF Done: E(RM06) = -2679.18370651				O	2.7264	-3.8046	-1.52793
TS6d				H	-0.60308	-1.95033	-2.33148
Number of imaginary frequencies=1				H	-1.20775	-1.45243	-0.74748
Charge = 0 Multiplicity = 1				C	-2.231	-3.13037	-1.57982
P	2.74228	0.15484	0.43313	C	-3.25525	-3.13007	-0.62238
C	3.65713	0.013	2.02551	C	-2.39466	-3.92106	-2.72654
C	2.96547	-0.53512	3.11947	C	-4.40887	-3.89465	-0.80286
C	4.98947	0.41404	2.19567	H	-3.14844	-2.51815	0.27111
C	3.58606	-0.659	4.36247	C	-3.54655	-4.68698	-2.91219
C	5.6116	0.28128	3.44022	H	-1.61146	-3.93267	-3.48159
C	4.91232	-0.25031	4.52449	C	-4.55882	-4.67702	-1.95001
C	4.04972	0.5251	-0.82041	H	-5.19255	-3.87524	-0.05021
C	4.57945	1.81225	-1.01034	H	-3.65517	-5.28838	-3.81078
C	4.51862	-0.52977	-1.61968	H	-5.45716	-5.27042	-2.0948
C	5.57005	2.03448	-1.96778	H	0.28854	-3.99959	-1.46843
C	5.5124	-0.30309	-2.57493	H	2.99375	-4.93652	0.66528
C	6.04118	0.97671	-2.74922	H	1.83367	-3.94757	1.46987
C	1.80685	1.7435	0.59136	H	-0.26839	-3.73339	0.16785
C	2.22693	2.82734	1.37632	Thermal correction to Energy= 0.488028			
C	0.61843	1.85979	-0.14823	Thermal correction to Enthalpy= 0.488972			
C	1.47992	4.0092	1.40822	Thermal correction to Gibbs Free Energy= 0.390760			
C	-0.11996	3.04293	-0.12334	Sum of electronic and zero-point Energies= -1642.135412			
C	0.30987	4.11975	0.65638	Sum of electronic and thermal Energies= -1642.105702			
H	1.81244	4.84012	2.02502	Sum of electronic and thermal Enthalpies= -1642.104758			
H	-1.03684	3.11946	-0.70153	Sum of electronic and thermal Free Energies= -1642.202970			
H	-0.27015	5.03822	0.68459	SCF Done: E(RM06) = -1643.21041174			
H	0.27303	1.01493	-0.73989	Cat0'			
H	3.13008	2.74658	1.97324	Number of imaginary frequencies=0			
H	5.96887	3.03606	-2.10691				



Charge = 0 Multiplicity = 1

C	-1.70028	-2.60097	2.83976	C	-1.70028	-2.60097	2.83976
C	-3.70702	3.58013	-0.34376	H	-0.80818	-2.44227	0.88166
C	-3.57843	2.20484	-0.53601	C	-3.3887	-0.95298	3.35946
C	-2.36629	1.55875	-0.25805	H	-3.82776	0.4739	1.81207
C	-1.317	2.34224	0.23269	C	-2.62327	-2.06013	3.7355
C	-1.41184	3.72194	0.44051	H	-1.08945	-3.45142	3.13029
C	-2.63256	4.33138	0.13375	H	-4.10398	-0.52283	4.05576
H	-4.64841	4.07063	-0.57422	H	-2.74136	-2.49265	4.72561
H	-4.41474	1.63592	-0.92614	C	2.35843	-0.96062	1.01385
H	-2.75444	5.4009	0.26858	C	2.8378	-0.25189	2.1241
O	-0.13539	1.68586	0.51652	C	2.19969	-2.35274	1.11666
C	-0.19437	4.4398	1.03539	C	3.14874	-0.92094	3.31111
C	-0.22218	5.95093	0.75247	H	2.97092	0.82362	2.06456
H	-1.1119	6.41066	1.19359	C	2.52602	-3.02135	2.29551
H	0.64109	6.44677	1.2069	H	1.81613	-2.90872	0.2645
H	-0.21884	6.16289	-0.32179	C	2.99735	-2.30483	3.39933
C	-0.19834	4.22109	2.57621	H	3.51308	-0.35663	4.16554
H	-0.17987	3.15604	2.8267	H	2.40675	-4.10014	2.35543
H	0.67975	4.69548	3.02985	H	3.24246	-2.8233	4.32243
H	-1.09944	4.6604	3.01959	C	3.41274	-0.47185	-1.6525
C	1.01854	2.38531	0.23911	C	3.28181	-0.24422	-3.03405
C	1.05641	3.76937	0.45263	C	4.64105	-0.91035	-1.13774
C	2.10535	1.65179	-0.25103	C	4.37116	-0.45547	-3.87963
C	2.25259	4.43055	0.16083	H	2.32938	0.09311	-3.44144
C	3.29114	2.35306	-0.5167	C	5.72437	-1.12818	-1.99356
C	3.36286	3.72913	-0.3112	H	4.75565	-1.089	-0.07293
H	2.32696	5.50355	0.302	C	5.59135	-0.90067	-3.36403
H	4.1521	1.82297	-0.90736	H	4.25877	-0.28154	-4.94619
H	4.2846	4.25995	-0.53102	H	6.66987	-1.47699	-1.58605
P	1.93017	-0.15595	-0.5933	H	6.43421	-1.0728	-4.02853
C	-3.59477	-0.7418	-1.4368	P	-2.06818	-0.24513	-0.52069
C	-4.60418	-1.54058	-0.8816	Pd	-0.01248	-1.07294	-1.67391
C	-3.70718	-0.32551	-2.77767	H	1.12198	-1.96334	-2.33574
C	-5.71386	-1.91083	-1.64779	Cl	-0.31025	0.76005	-3.71909
H	-4.53236	-1.87483	0.14842				
C	-4.82313	-0.68944	-3.53127	Thermal correction to Energy=	0.647634		
H	-2.9094	0.26364	-3.22902	Thermal correction to Enthalpy=	0.648578		
C	-5.8287	-1.48259	-2.97016	Thermal correction to Gibbs Free Energy=	0.532682		
H	-6.48829	-2.53206	-1.20501	Sum of electronic and zero-point Energies=	-2850.331544		
H	-4.90094	-0.35817	-4.56347	Sum of electronic and thermal Energies=	-2850.291724		
H	-6.69357	-1.76864	-3.56318	Sum of electronic and thermal Enthalpies=	-2850.290780		
C	-2.31347	-0.93336	1.17941	Sum of electronic and thermal Free Energies=	-2850.406676		
C	-1.54523	-2.03862	1.57096	SCF Done: E(RM06) =	-2851.344145		
C	-3.23448	-0.39191	2.09153	TS1a'			

Number of imaginary frequencies=1				C	-3.22602	-0.38577	2.09315
Charge = 0 Multiplicity = 1				C	-1.68936	-2.59401	2.83874
C	-3.7062	3.58406	-0.34908	H	-0.80374	-2.43765	0.87771
C	-3.57864	2.20855	-0.54086	C	-3.37609	-0.94547	3.36219
C	-2.36732	1.56177	-0.26142	H	-3.82022	0.47972	1.81464
C	-1.31785	2.34455	0.22996	C	-2.60938	-2.05218	3.73693
C	-1.41169	3.72421	0.43775	H	-1.07744	-3.44404	3.12819
C	-2.6317	4.33452	0.12959	H	-4.0891	-0.51459	4.06037
H	-4.6469	4.07534	-0.58068	H	-2.72419	-2.4836	4.72791
H	-4.41498	1.64008	-0.93164	C	2.35233	-0.9661	1.01132
H	-2.75299	5.40413	0.26428	C	2.8257	-0.26008	2.12584
O	-0.13717	1.68666	0.51459	C	2.19539	-2.3588	1.10887
C	-0.19449	4.44084	1.03453	C	3.13262	-0.93245	3.31201
C	-0.22019	5.95191	0.75101	H	2.95725	0.81584	2.07036
H	-1.11052	6.41258	1.18988	C	2.51797	-3.03065	2.28691
H	0.64243	6.44719	1.20727	H	1.81609	-2.91255	0.25333
H	-0.2142	6.16345	-0.32332	C	2.98333	-2.31688	3.39507
C	-0.20155	4.22265	2.57542	H	3.49224	-0.37028	4.16984
H	-0.18484	3.15765	2.82627	H	2.4004	-4.10984	2.3428
H	0.67628	4.69612	3.03052	H	3.22543	-2.83792	4.31751
H	-1.10294	4.66317	3.017	C	3.41763	-0.46835	-1.64921
C	1.01798	2.38492	0.23997	C	3.29393	-0.2311	-3.02984
C	1.05679	3.76891	0.45443	C	4.64308	-0.91071	-1.13128
C	2.1052	1.65048	-0.24821	C	4.3874	-0.43681	-3.87134
C	2.25442	4.42903	0.16631	H	2.34359	0.10849	-3.44001
C	3.2925	2.35093	-0.50981	C	5.7306	-1.12343	-1.98319
C	3.36524	3.72671	-0.30297	H	4.75229	-1.09648	-0.06715
H	2.32952	5.50185	0.30837	C	5.60475	-0.88634	-3.35263
H	4.15413	1.82052	-0.89843	H	4.28063	-0.25513	-4.93719
H	4.28826	4.25658	-0.5197	H	6.67378	-1.47572	-1.57329
P	1.93025	-0.15701	-0.59506	H	6.45087	-1.05432	-4.01402
C	-3.59588	-0.74243	-1.43432	P	-2.0677	-0.24179	-0.52291
C	-4.60394	-1.53945	-0.8741	Pd	-0.0094	-1.06103	-1.68416
C	-3.71133	-0.33089	-2.77638	C	-1.20012	-2.61187	-2.80777
C	-5.71514	-1.91275	-1.63655	H	-1.69558	-2.05611	-3.59552
H	-4.52975	-1.87015	0.15689	H	-1.82797	-2.98225	-2.003
C	-4.82884	-0.69779	-3.52627	C	0.02651	-3.23416	-3.04066
H	-2.91455	0.25664	-3.2316	H	1.13398	-1.91573	-2.36382
C	-5.83293	-1.48925	-2.9602	H	0.34689	-3.9783	-2.31307
H	-6.4884	-2.53268	-1.18991	Cl	-0.32228	0.75279	-3.73142
H	-4.90897	-0.37023	-4.55947	C	0.74267	-3.293	-4.33461
H	-6.69897	-1.77772	-3.55035	C	1.57803	-4.39524	-4.57993
C	-2.30797	-0.92815	1.17863	C	0.58653	-2.31579	-5.334
C	-1.53854	-2.03306	1.56881	C	2.22376	-4.54063	-5.80725

H	1.71149	-5.1494	-3.80687	H	1.8185	5.28218	0.05261
C	1.24203	-2.46237	-6.5546	H	3.63456	1.46739	0.72557
H	0.00451	-1.41978	-5.13046	H	3.81125	3.93186	0.5683
C	2.05428	-3.57406	-6.80016	P	1.38091	-0.44048	0.32801
H	2.85924	-5.40419	-5.98492	C	-4.05497	-1.18932	-2.16503
H	1.12288	-1.69658	-7.31642	C	-5.20435	-1.71819	-1.56273
H	2.55866	-3.68149	-7.75704	C	-3.92347	-1.25857	-3.56519
Thermal correction to Energy=	0.788986			C	-6.21084	-2.29267	-2.34606
Thermal correction to Enthalpy=	0.789931			H	-5.31969	-1.68929	-0.48455
Thermal correction to Gibbs Free Energy=	0.655705			C	-4.93535	-1.82107	-4.34211
Sum of electronic and zero-point Energies=	-3159.820147			H	-3.02504	-0.8734	-4.04175
Sum of electronic and thermal Energies=	-3159.772427			C	-6.08162	-2.34159	-3.73395
Sum of electronic and thermal Enthalpies=	-3159.771483			H	-7.09664	-2.69954	-1.86543
Sum of electronic and thermal Free Energies=	-3159.905709			H	-4.82309	-1.86131	-5.42206
SCF Done: E(RM06) =	-3160.81922			H	-6.86567	-2.78764	-4.33973
				C	-3.10188	-0.55731	0.55845
Int2a'				C	-2.30415	-1.25188	1.47648
Number of imaginary frequencies=	0			C	-4.2246	0.14802	1.02669
Charge = 0 Multiplicity =	1			C	-2.62968	-1.25984	2.83481
C	-3.70075	3.26897	-2.58787	H	-1.41357	-1.76604	1.13504
C	-3.67851	1.89134	-2.37852	C	-4.55389	0.13059	2.38145
C	-2.69863	1.313	-1.56416	H	-4.83479	0.72122	0.33432
C	-1.75044	2.15908	-0.96252	C	-3.75751	-0.57566	3.28755
C	-1.77894	3.54956	-1.12085	H	-1.98859	-1.78943	3.53337
C	-2.76245	4.08496	-1.96045	H	-5.42635	0.67648	2.73061
H	-4.45756	3.70664	-3.23222	H	-4.0111	-0.58099	4.34431
H	-4.42006	1.26444	-2.86002	C	1.37136	-0.84132	2.13713
H	-2.80901	5.15656	-2.12016	C	1.39276	0.11428	3.16404
O	-0.80244	1.55851	-0.16755	C	1.24411	-2.19783	2.49219
C	-0.81623	4.40232	-0.28919	C	1.29648	-0.27388	4.5031
C	-0.5431	5.76573	-0.95164	H	1.48587	1.1676	2.91966
H	-1.46991	6.33487	-1.06937	C	1.16481	-2.58744	3.82928
H	0.11422	6.37833	-0.3279	H	1.21217	-2.95657	1.71279
H	-0.07861	5.64959	-1.93626	C	1.18679	-1.62319	4.84151
C	-1.47153	4.64713	1.10177	H	1.31355	0.48309	5.28326
H	-1.6873	3.70129	1.60898	H	1.08025	-3.64178	4.08017
H	-0.80032	5.23231	1.74119	H	1.11812	-1.92296	5.88392
H	-2.41375	5.19621	0.98902	C	3.09443	-0.92336	-0.19449
C	0.40542	2.20572	0.01532	C	3.39932	-0.78098	-1.5617
C	0.47453	3.60428	-0.07544	C	4.06883	-1.45682	0.66221
C	1.5252	1.4074	0.30618	C	4.65128	-1.15434	-2.05004
C	1.72227	4.20415	0.12113	H	2.65584	-0.36996	-2.24178
C	2.7506	2.05896	0.5107	C	5.31809	-1.84036	0.16558
C	2.85295	3.44363	0.41545	H	3.85823	-1.5747	1.7206

C	5.61384	-1.68908	-1.18935	H	-4.53786	1.38336	-2.58282
H	4.87139	-1.03245	-3.10747	H	-2.8807	5.28218	-1.94582
H	6.06124	-2.2528	0.84373	O	-0.81644	1.69403	-0.04249
H	6.58624	-1.98655	-1.57328	C	-0.77346	4.51146	-0.22211
P	-2.6312	-0.49317	-1.22209	C	-0.54682	5.88217	-0.88414
Pd	-0.71715	-1.70122	-1.99874	H	-1.47568	6.4598	-0.9093
C	-1.48929	-3.45729	-1.09918	H	0.17055	6.47738	-0.31127
C	-1.95826	-4.49623	-2.12958	H	-0.17381	5.78021	-1.90855
H	-2.69915	-4.04304	-2.79864	C	-1.29351	4.73811	1.22734
Cl	0.08886	0.2179	-3.36216	H	-1.47094	3.78627	1.73777
H	-1.1191	-4.81493	-2.75993	H	-0.55992	5.3075	1.80994
H	-0.67808	-3.85044	-0.47638	H	-2.23638	5.29717	1.21134
H	-2.32013	-3.19647	-0.44048	C	0.42448	2.29818	-0.03073
C	-2.56142	-5.7125	-1.44859	C	0.52092	3.69196	-0.14568
C	-1.75457	-6.79512	-1.06976	C	1.54205	1.46057	0.11118
C	-3.93018	-5.7668	-1.14875	C	1.80154	4.25223	-0.11454
C	-2.29655	-7.90003	-0.41149	C	2.80444	2.07089	0.15712
H	-0.69123	-6.77376	-1.30098	C	2.93382	3.45275	0.04298
C	-4.47672	-6.86941	-0.4901	H	1.92445	5.32593	-0.20724
H	-4.57135	-4.93783	-1.44096	H	3.69112	1.45485	0.25997
C	-3.66139	-7.94067	-0.11843	H	3.91919	3.90905	0.07116
H	-1.65411	-8.73159	-0.13251	P	1.32518	-0.37759	0.12366
H	-5.54158	-6.89485	-0.27166	C	-3.93261	-1.1125	-2.09006
H	-4.0865	-8.80151	0.39103	C	-5.11114	-1.68193	-1.58651
Thermal correction to Energy= 0.794939				C	-3.6802	-1.17398	-3.47445
Thermal correction to Enthalpy= 0.795883				C	-6.02553	-2.29422	-2.44969
Thermal correction to Gibbs Free Energy= 0.660677				H	-5.32096	-1.65057	-0.52239
Sum of electronic and zero-point Energies= -3159.852608				C	-4.6025	-1.77529	-4.3309
Sum of electronic and thermal Energies= -3159.805044				H	-2.75891	-0.75481	-3.87321
Sum of electronic and thermal Enthalpies= -3159.804100				C	-5.77576	-2.33946	-3.82146
Sum of electronic and thermal Free Energies= -3159.939306SCF Done: E(RM06) = -3160.84587				H	-6.93462	-2.73197	-2.04534
				H	-4.39814	-1.80981	-5.39764
				H	-6.48809	-2.81503	-4.49037
				C	-3.25442	-0.50334	0.69951
TS4a'				C	-2.57701	-1.32282	1.6126
Number of imaginary frequencies=1				C	-4.38077	0.21379	1.13884
Charge = 1 Multiplicity = 1				C	-3.02133	-1.43966	2.93181
C	-3.80781	3.39271	-2.34366	H	-1.68032	-1.85005	1.30282
C	-3.7811	2.01481	-2.12974	C	-4.82751	0.09314	2.45441
C	-2.76764	1.439	-1.35524	H	-4.90299	0.87525	0.45321
C	-1.80007	2.29031	-0.80342	C	-4.14944	-0.73591	3.35291
C	-1.8144	3.67767	-0.97783	H	-2.47271	-2.0679	3.62766
C	-2.83488	4.21242	-1.77241	H	-5.70039	0.65253	2.78076
H	-4.59122	3.82956	-2.95621	H	-4.49521	-0.82287	4.37958

C	1.2253	-0.79729	1.92255	Thermal correction to Energy= 0.804321
C	1.18305	0.1626	2.94405	Thermal correction to Enthalpy= 0.805265
C	1.10913	-2.15498	2.27469	Thermal correction to Gibbs Free Energy= 0.663002
C	1.03114	-0.2232	4.27857	Sum of electronic and zero-point Energies= -3273.146629
H	1.27183	1.21637	2.69954	Sum of electronic and thermal Energies= -3273.096458
C	0.97353	-2.54084	3.60786	Sum of electronic and thermal Enthalpies= -3273.095513
H	1.13688	-2.91783	1.49965	Sum of electronic and thermal Free Energies= -
C	0.92958	-1.57301	4.61611	3273.237777SCF Done: E(RM06) = -3274.12806
H	0.99911	0.53633	5.05554	
H	0.89942	-3.59585	3.85905	Int5a'
H	0.81815	-1.87094	5.65528	Number of imaginary frequencies=0
C	3.01743	-0.94937	-0.35751	Charge =0 Multiplicity = 1
C	3.32473	-0.93415	-1.73056	C -3.80396 3.40023 -2.35353
C	3.98573	-1.40222	0.55129	C -3.78081 2.02172 -2.14012
C	4.57685	-1.35701	-2.17676	C -2.77207 1.44369 -1.36222
H	2.58342	-0.58831	-2.44778	C -1.8017 2.29342 -0.80969
C	5.23424	-1.83558	0.09725	C -1.8131 3.67772 -0.97949
H	3.76908	-1.41941	1.61484	C -2.83236 4.21832 -1.77418
C	5.53313	-1.81275	-1.26571	H -4.58656 3.84244 -2.96594
H	4.79978	-1.33866	-3.24014	H -4.53685 1.39529 -2.59246
H	5.97344	-2.18723	0.81271	H -2.87469 5.28863 -1.94396
H	6.50472	-2.15056	-1.61685	O -0.81944 1.69135 -0.04892
P	-2.61853	-0.36569	-1.02896	C -0.77515 4.51026 -0.21839
Pd	-0.50641	-1.5181	-1.67087	C -0.54709 5.8827 -0.87648
C	0.49404	-2.94672	-2.33105	H -1.47618 6.45985 -0.90366
O	1.24749	-3.61354	-2.91184	H 0.16779 6.47708 -0.29966
C	-0.88114	-3.81722	-1.15302	H -0.17029 5.78332 -1.89975
C	-1.6555	-4.69512	-2.14197	C -1.30034 4.73334 1.22976
H	-2.38562	-4.08017	-2.67842	H -1.47889 3.78023 1.73746
Cl	-0.05938	0.1206	-3.47218	H -0.56911 5.30185 1.81617
H	-0.96932	-5.10973	-2.88908	H -2.24352 5.29182 1.2118
H	-0.10208	-4.3577	-0.61199	C 0.42063 2.29736 -0.02881
H	-1.54935	-3.36536	-0.41843	C 0.51955 3.69163 -0.1392
C	-2.36033	-5.82333	-1.41153	C 1.5388 1.46107 0.1133
C	-1.70289	-7.03746	-1.16666	C 1.79925 4.25355 -0.10038
C	-3.6701	-5.66424	-0.93673	C 2.80007 2.06934 0.17034
C	-2.33513	-8.06572	-0.46614	C 2.93196 3.45162 0.06017
H	-0.68944	-7.1801	-1.5365	H 1.92106 5.3277 -0.18932
C	-4.30531	-6.69053	-0.23587	H 3.68703 1.45411 0.27221
H	-4.19747	-4.73217	-1.12899	H 3.91654 3.90924 0.09413
C	-3.63928	-7.89469	0.00308	P 1.32759 -0.38108 0.12219
H	-1.81147	-9.00233	-0.29222	C -3.93397 -1.10463 -2.10631
H	-5.32355	-6.55187	0.11885	C -5.10914 -1.68455 -1.60268
H	-4.13466	-8.69557	0.54563	C -3.68559 -1.16087 -3.4918

C	-6.02426	-2.29445	-2.46681	O	1.20447	-3.61801	-2.90273
H	-5.31947	-1.65665	-0.53777	C	-0.77025	-3.87575	-1.23857
C	-4.60861	-1.75974	-4.34911	C	-1.66541	-4.72195	-2.1545
H	-2.76672	-0.73322	-3.89096	H	-2.39875	-4.06599	-2.64396
C	-5.7786	-2.33056	-3.83955	Cl	-0.05077	0.12112	-3.47287
H	-6.93069	-2.73755	-2.06234	H	-1.04336	-5.16016	-2.94769
H	-4.40732	-1.7873	-5.41663	H	-0.06976	-4.47738	-0.64445
H	-6.49148	-2.80427	-4.50918	H	-1.38165	-3.28433	-0.5305
C	-3.25488	-0.50258	0.68459	C	-2.37187	-5.82693	-1.39301
C	-2.57076	-1.31921	1.59846	C	-1.70912	-7.03953	-1.15482
C	-4.38539	0.2044	1.12753	C	-3.67422	-5.6644	-0.90687
C	-3.00889	-1.43619	2.91853	C	-2.33266	-8.06635	-0.44619
H	-1.67087	-1.83714	1.28868	H	-0.70215	-7.1828	-1.53336
C	-4.82972	0.08337	2.44385	C	-4.3045	-6.69298	-0.20158
H	-4.91271	0.86486	0.44128	H	-4.20558	-4.73723	-1.09757
C	-4.14124	-0.73927	3.3395	C	-3.63326	-7.89925	0.03058
H	-2.45501	-2.05914	3.61495	H	-1.80877	-9.00543	-0.27758
H	-5.70221	0.63759	2.77386	H	-5.32004	-6.55732	0.16192
H	-4.48518	-0.82642	4.37047	H	-4.12552	-8.69824	0.57659
C	1.23095	-0.7997	1.92452				
C	1.188	0.15822	2.9479	Thermal correction to Energy=	0.807184		
C	1.11605	-2.15815	2.27439	Thermal correction to Enthalpy=	0.808128		
C	1.03685	-0.23013	4.28177	Thermal correction to Gibbs Free Energy=	0.668800		
H	1.27567	1.21253	2.70162	Sum of electronic and zero-point Energies=	-3273.195006		
C	0.98108	-2.54658	3.6069	Sum of electronic and thermal Energies=	-3273.145363		
H	1.14425	-2.9196	1.49797	Sum of electronic and thermal Enthalpies=	-3273.144419		
C	0.93657	-1.58066	4.61695	Sum of electronic and thermal Free Energies=	-3273.2837475CF Done: E(RM06) = -3274.18088		
H	1.00443	0.52796	5.06014				
H	0.90792	-3.60212	3.85617	TS6a'			
H	0.82573	-1.88057	5.65561	Number of imaginary frequencies=	1		
C	3.02024	-0.95029	-0.3577	Charge =	0 Multiplicity =	1	
C	3.32219	-0.93292	-1.73113	C	-4.44972	2.73225	-1.199
C	3.98988	-1.40088	0.54898	C	-4.12705	1.38694	-1.05362
C	4.5775	-1.35122	-2.17967	C	-2.85464	0.98735	-0.6169
H	2.58002	-0.59317	-2.45055	C	-1.9221	1.99889	-0.31522
C	5.23787	-1.83336	0.09265	C	-2.23046	3.3629	-0.43874
H	3.77458	-1.42	1.61278	C	-3.50354	3.71008	-0.89757
C	5.53505	-1.80833	-1.27064	H	-5.43649	3.0189	-1.55079
H	4.79912	-1.33467	-3.24331	H	-4.86435	0.63204	-1.30363
H	5.97804	-2.18606	0.80661	H	-3.76838	4.75484	-1.01717
H	6.50622	-2.14544	-1.62357	O	-0.66716	1.6347	0.13544
P	-2.62185	-0.35476	-1.0408	C	-1.17457	4.38329	0.00029
Pd	-0.51052	-1.50378	-1.6884	C	-1.41777	5.77021	-0.61846
C	0.39534	-3.0454	-2.25529	H	-2.38781	6.16958	-0.30753

H	-0.66486	6.48457	-0.27214	H	0.71828	-1.21204	2.31309
H	-1.3892	5.73853	-1.71265	C	2.92022	0.24182	4.45662
C	-1.2381	4.51811	1.55017	H	4.53367	1.55534	3.87586
H	-1.0714	3.55437	2.04066	H	1.23093	-1.07214	4.71948
H	-0.47061	5.217	1.90232	H	3.14578	0.30183	5.51822
H	-2.22061	4.89486	1.85787	C	3.44999	-0.40348	-0.97102
C	0.39903	2.43985	-0.22912	C	3.4513	-0.29549	-2.37514
C	0.19842	3.81804	-0.37617	C	4.56872	-0.95322	-0.32669
C	1.65413	1.83589	-0.42073	C	4.56559	-0.70275	-3.10711
C	1.28411	4.59688	-0.78814	H	2.57254	0.09093	-2.88643
C	2.71775	2.65574	-0.81986	C	5.67747	-1.36911	-1.06973
C	2.53311	4.02229	-1.01618	H	4.58169	-1.05806	0.75328
H	1.16083	5.66491	-0.93008	C	5.68183	-1.23939	-2.45829
H	3.69238	2.21501	-1.00154	H	4.55676	-0.60765	-4.18967
H	3.36481	4.64089	-1.34089	H	6.53739	-1.79232	-0.55703
P	1.89715	0.03555	-0.08323	H	6.54619	-1.56039	-3.03369
C	-3.62436	-1.59355	-1.70799	P	-2.46436	-0.82046	-0.49916
C	-4.8711	-2.12667	-1.34604	Pd	-0.11266	-1.05412	-0.85765
C	-3.22296	-1.6336	-3.0545	C	1.12844	-2.62011	-1.0951
C	-5.7027	-2.69275	-2.31512	H	0.65306	-3.06711	-3.1348
H	-5.19375	-2.10651	-0.31007	Cl	0.33973	-2.02493	-4.45709
C	-4.06356	-2.19178	-4.01765	N	0.80815	-3.66297	-2.0384
H	-2.26189	-1.21281	-3.34133	H	-0.03682	-4.1264	-1.77144
C	-5.30171	-2.72544	-3.65154	H	1.56081	-4.31832	-2.10173
H	-6.6643	-3.10637	-2.0223	O	2.38564	-2.79945	-0.81105
H	-3.74616	-2.21126	-5.05691	C	0.60141	-3.32678	0.16762
H	-5.95112	-3.16517	-4.4042	H	0.78714	-2.71256	1.02386
C	-3.53267	-0.89948	0.99899	H	-0.45096	-3.49373	0.06994
C	-3.88182	-2.15604	1.52374	C	1.32171	-4.67716	0.33858
C	-3.96574	0.25575	1.66697	H	2.35373	-4.50506	0.56267
C	-4.66404	-2.25015	2.6737	H	1.24266	-5.24079	-0.5675
H	-3.54685	-3.06579	1.0347	C	0.67045	-5.46405	1.49108
C	-4.73744	0.15737	2.82662	C	-0.3911	-6.33124	1.23117
H	-3.70769	1.23571	1.27958	C	1.14189	-5.30991	2.79475
C	-5.09234	-1.09413	3.33057	C	-0.98147	-7.04359	2.27485
H	-4.92962	-3.22973	3.06179	H	-0.76304	-6.45196	0.2034
H	-5.06545	1.06272	3.33065	C	0.55209	-6.02314	3.83871
H	-5.6963	-1.16957	4.23096	H	1.97866	-4.6266	2.99975
C	2.34012	0.08412	1.71216	C	-0.50952	-6.88978	3.57901
C	3.41052	0.87221	2.17385	H	-1.81861	-7.72666	2.07016
C	1.55518	-0.60884	2.64416	H	0.92428	-5.90171	4.86643
C	3.70184	0.9447	3.53448	H	-0.97512	-7.45159	4.40174
H	4.01401	1.43725	1.46975				
C	1.84814	-0.52843	4.00941				
					Thermal correction to Energy=	0.843529	
					Thermal correction to Enthalpy=	0.844473	

Thermal correction to Gibbs Free Energy= 0.703702				C	-5.16118	0.15197	-3.0556
Sum of electronic and zero-point Energies= -3329.698200				H	-3.15974	0.9095	-2.86649
Sum of electronic and thermal Energies= -3329.647355				C	-6.20531	-0.54137	-2.43501
Sum of electronic and thermal Enthalpies= -3329.646411				H	-6.85286	-1.54573	-0.64105
Sum of electronic and thermal Free Energies= -3329.787182				H	-5.28254	0.53137	-4.06628
SCF Done: E(RM06) = -3330.71575794				H	-7.13975	-0.70576	-2.96361
				C	-2.35413	-0.55835	1.43512
TS1b'				C	-2.23847	-1.95442	1.54452
Number of imaginary frequencies=1				C	-2.63221	0.19698	2.58309
Charge = 0 Multiplicity = 1				C	-2.41841	-2.58164	2.77708
C	-3.51582	4.12258	0.08972	H	-2.02331	-2.55513	0.66524
C	-3.49315	2.73777	-0.06088	C	-2.7941	-0.43402	3.81836
C	-2.28677	2.02873	0.05851	H	-2.72746	1.27586	2.51684
C	-1.13751	2.76467	0.37427	C	-2.69246	-1.82229	3.91739
C	-1.12131	4.15752	0.51619	H	-2.34191	-3.66326	2.84557
C	-2.34009	4.82482	0.35987	H	-3.0066	0.16186	4.70144
H	-4.45408	4.65956	-0.01037	H	-2.82726	-2.31096	4.87818
H	-4.41219	2.21016	-0.28696	C	1.84918	-0.5994	1.29576
H	-2.38274	5.90379	0.4591	C	2.42199	0.15418	2.33152
O	0.02295	2.04198	0.5498	C	1.34151	-1.87745	1.57437
C	0.20149	4.83903	0.89578	C	2.48581	-0.36697	3.62483
C	0.22891	6.31715	0.46806	H	2.824	1.14222	2.13075
H	-0.56961	6.87959	0.96008	C	1.41589	-2.39739	2.86627
H	1.16783	6.78991	0.77032	H	0.88812	-2.46665	0.78146
H	0.1163	6.43055	-0.61519	C	1.986	-1.64256	3.89353
C	0.36863	4.75981	2.44128	H	2.93008	0.22399	4.42067
H	0.35604	3.72284	2.7915	H	1.02161	-3.38818	3.07172
H	1.31961	5.21237	2.74338	H	2.03937	-2.04656	4.90041
H	-0.4452	5.29878	2.93875	C	3.352	-0.69398	-1.19201
C	1.19042	2.65175	0.14659	C	3.54633	-0.5915	-2.57991
C	1.33817	4.0373	0.24817	C	4.35145	-1.28832	-0.40848
C	2.18456	1.79888	-0.3467	C	4.71438	-1.07145	-3.17041
C	2.55407	4.5749	-0.18976	H	2.78693	-0.12577	-3.20354
C	3.39621	2.3733	-0.75651	C	5.51533	-1.78138	-1.00531
C	3.57143	3.75476	-0.68235	H	4.22673	-1.37292	0.66552
H	2.72076	5.64536	-0.14044	C	5.70015	-1.67396	-2.38328
H	4.19327	1.74631	-1.13937	H	4.85308	-0.97924	-4.24386
H	4.50857	4.19616	-1.00717	H	6.27653	-2.24894	-0.38738
P	1.81513	0.00257	-0.43822	H	6.60577	-2.05746	-2.8442
C	-3.78677	-0.11573	-1.06354	P	-2.16677	0.20538	-0.22838
C	-4.84183	-0.80178	-0.44749	Pd	-0.19735	-0.68044	-1.56728
C	-3.96099	0.3594	-2.37689	C	-1.54657	-2.12555	-2.86863
C	-6.04289	-1.01438	-1.13292	H	-2.43491	-1.51544	-2.99928
H	-4.7342	-1.1695	0.56731	C	-0.43564	-1.8208	-3.64939



H	0.9112	-1.18221	-2.57077	H	-0.25487	5.51271	1.54711
H	0.31796	-2.5728	-3.86418	H	-2.01422	5.23853	1.53974
C	-1.72933	-3.38369	-2.12612	C	0.50274	2.48401	-0.32571
C	-3.03291	-3.78527	-1.77912	C	0.35908	3.85501	-0.56527
C	-0.64965	-4.21734	-1.77019	C	1.73026	1.81814	-0.43904
C	-3.25206	-4.98707	-1.10722	C	1.49046	4.5557	-0.99312
H	-3.87582	-3.15593	-2.04962	C	2.84466	2.55858	-0.85487
C	-0.87191	-5.4136	-1.09301	C	2.72278	3.91503	-1.14227
H	0.36709	-3.92665	-2.01918	H	1.42161	5.61746	-1.20375
C	-2.17349	-5.80365	-0.7601	H	3.80527	2.06808	-0.96474
H	-4.26564	-5.28762	-0.85814	H	3.58768	4.48115	-1.47298
H	-0.02975	-6.04669	-0.82853	P	1.80493	0.0324	-0.01997
H	-2.3442	-6.74077	-0.23821	C	-3.58593	-1.46571	-1.48778
H	-0.48041	-0.98851	-4.34546	C	-4.73693	-2.10015	-0.9965
Cl	-0.4437	1.31372	-2.62347	C	-3.35216	-1.45641	-2.87629
Thermal correction to Energy= 0.789636				C	-5.6353	-2.71836	-1.87335
Thermal correction to Enthalpy= 0.790581				H	-4.93302	-2.11893	0.0711
Thermal correction to Gibbs Free Energy= 0.655863				C	-4.25799	-2.06597	-3.74726
Sum of electronic and zero-point Energies= -3159.820701				H	-2.45647	-0.98162	-3.26665
Sum of electronic and thermal Energies= -3159.772895				C	-5.39922	-2.70055	-3.24905
Sum of electronic and thermal Enthalpies= -3159.771951				H	-6.52227	-3.20749	-1.47823
Sum of electronic and thermal Free Energies= -3159.906669				H	-4.06539	-2.04967	-4.81677
SCF Done: E(RM06) = -3160.823429				H	-6.09549	-3.18034	-3.92893
				C	-2.82629	-1.11678	1.2932
Int2b'				C	-2.57141	-2.43008	1.7303
Number of imaginary frequencies=0				C	-3.39249	-0.20831	2.19742
Charge =0 Multiplicity = 1				C	-2.8885	-2.8246	3.02921
C	-4.35299	2.85729	-1.21564	H	-2.13115	-3.15242	1.04557
C	-4.05757	1.51369	-1.00028	C	-3.69719	-0.60011	3.50375
C	-2.77874	1.11384	-0.58089	H	-3.60104	0.80913	1.88467
C	-1.82518	2.12181	-0.37155	C	-3.44901	-1.90745	3.92309
C	-2.09064	3.48261	-0.58054	H	-2.69689	-3.84665	3.34109
C	-3.37333	3.82946	-1.01534	H	-4.13447	0.11927	4.19441
H	-5.34579	3.14846	-1.54675	H	-3.69062	-2.21166	4.93816
H	-4.81834	0.76178	-1.17692	C	1.7342	0.06118	1.82589
H	-3.61947	4.87011	-1.19936	C	2.40537	1.05193	2.56289
O	-0.57841	1.72416	0.06906	C	0.97421	-0.89533	2.51112
C	-0.99617	4.50218	-0.25445	C	2.33234	1.06661	3.95525
C	-1.19025	5.82105	-1.02384	H	2.98165	1.81676	2.04694
H	-2.14511	6.28662	-0.7626	C	0.8999	-0.87507	3.9052
H	-0.41262	6.54358	-0.75852	H	0.42335	-1.64592	1.96091
H	-1.16471	5.66542	-2.10739	C	1.57921	0.10387	4.62898
C	-1.04514	4.80456	1.27167	H	2.85795	1.83884	4.51355
H	-0.9066	3.89285	1.86124	H	0.2932	-1.61824	4.41803

H	1.51745	0.12127	5.71661	TS4b'				
C	3.53532	-0.44366	-0.4472	Number of imaginary frequencies=1				
C	3.83878	-0.60867	-1.81289	Charge =0	Multiplicity = 1			
C	4.52969	-0.69309	0.50806	C	-4.37283	2.83295	-1.19354	
C	5.11915	-0.99365	-2.20717	C	-4.07359	1.48987	-0.98121	
H	3.06509	-0.437	-2.5584	C	-2.79078	1.09155	-0.57524	
C	5.80732	-1.09595	0.10578	C	-1.83687	2.10059	-0.36955	
H	4.31177	-0.58284	1.56522	C	-2.10647	3.46121	-0.57588	
C	6.10713	-1.24157	-1.2491	C	-3.39292	3.80629	-1.00057	
H	5.34234	-1.10935	-3.26443	H	-5.3687	3.12277	-1.51644	
H	6.5684	-1.29019	0.85912	H	-4.83471	0.73699	-1.15483	
H	7.10162	-1.55152	-1.55617	H	-3.64198	4.84668	-1.17908	
P	-2.29751	-0.6681	-0.42335	O	-0.58666	1.70497	0.06214	
Pd	0.37382	-1.55779	-1.1475	C	-1.00951	4.48333	-0.2567	
C	0.86181	-3.10038	-0.20708	C	-1.21052	5.80107	-1.02643	
O	1.28932	-3.95078	0.45019	H	-2.16498	6.26489	-0.76075	
C	-0.0801	-3.73823	-2.34289	H	-0.43319	6.52558	-0.76579	
C	1.21161	-3.93921	-3.10966	H	-1.19016	5.64438	-2.10993	
H	1.5324	-2.99794	-3.56121	C	-1.05395	4.78715	1.26937	
Cl	0.20807	-0.18341	-3.20995	H	-0.91051	3.87632	1.85914	
H	2.03159	-4.32107	-2.49034	H	-0.26353	5.497	1.53996	
H	-0.79137	-3.09552	-2.86043	H	-2.02243	5.22249	1.5421	
H	1.04669	-4.67151	-3.91879	C	0.4907	2.46545	-0.33616	
C	-0.73255	-4.9178	-1.72735	C	0.34273	3.83635	-0.57379	
C	-0.02923	-6.10089	-1.41079	C	1.7197	1.80042	-0.45706	
C	-2.12611	-4.90932	-1.50195	C	1.4737	4.54058	-1.00157	
C	-0.69407	-7.22145	-0.91066	C	2.83092	2.54445	-0.87193	
H	1.04216	-6.15226	-1.56909	C	2.70446	3.90365	-1.15492	
C	-2.7855	-6.02551	-0.99427	H	1.40128	5.60238	-1.21075	
H	-2.69194	-4.01418	-1.74266	H	3.79264	2.05696	-0.98547	
C	-2.07271	-7.19269	-0.69772	H	3.56972	4.4696	-1.4876	
H	-0.12678	-8.12113	-0.68514	P	1.80758	0.01366	-0.02584	
H	-3.86207	-5.98594	-0.84435	C	-3.60316	-1.48235	-1.48378	
H		-2.58837	-8.06605	-0.3106	C	-4.74548	-2.13291	-0.99437
Thermal correction to Energy=	0.805017			C	-3.37921	-1.44869	-2.87361	
Thermal correction to Enthalpy=	0.805961			C	-5.64607	-2.74002	-1.8747	
Thermal correction to Gibbs Free Energy=	0.663378			H	-4.93359	-2.17093	0.07408	
Sum of electronic and zero-point Energies=	-3273.173716			C	-4.28721	-2.0473	-3.74775	
Sum of electronic and thermal Energies=	-3273.122887			H	-2.48849	-0.96063	-3.26525	
Sum of electronic and thermal Enthalpies=	-3273.121942			C	-5.42058	-2.69781	-3.25162	
Sum of electronic and thermal Free Energies=	-3273.264525			H	-6.52671	-3.24157	-1.48102	
SCF Done: E(RM06) =	-3160.852904			H	-4.10241	-2.01249	-4.81818	
				H	-6.12176	-3.17077	-3.93423	
				C	-2.83729	-1.13729	1.30008	

C	-2.59022	-2.45283	1.73497	C	-0.03438	-6.09263	-1.23487
C	-3.39524	-0.22509	2.20756	C	-2.0781	-4.8745	-1.6303
C	-2.90601	-2.84552	3.0355	C	-0.77654	-7.20887	-0.85119
H	-2.15697	-3.17843	1.05035	H	1.0494	-6.14678	-1.22208
C	-3.69608	-0.61539	3.51518	C	-2.81998	-5.98944	-1.24085
H	-3.59775	0.79406	1.89363	H	-2.59307	-3.97538	-1.95296
C	-3.45493	-1.92465	3.93269	C	-2.17264	-7.16269	-0.84802
H	-2.71711	-3.86901	3.34877	H	-0.26113	-8.11812	-0.55237
H	-4.12462	0.10679	4.20548	H	-3.9055	-5.93888	-1.25462
H	-3.69321	-2.22753	4.94894	H	-2.7489	-8.03398	-0.54805
C	1.76243	0.05897	1.81741	Thermal correction to Energy= 0.804087			
C	2.48501	1.02585	2.53869	Thermal correction to Enthalpy= 0.805031			
C	0.96969	-0.8591	2.51837	Thermal correction to Gibbs Free Energy= 0.664348			
C	2.42745	1.05659	3.93151	Sum of electronic and zero-point Energies= -3273.159267			
H	3.08619	1.76022	2.01019	Sum of electronic and thermal Energies= -3273.109034			
C	0.90751	-0.82197	3.91323	Sum of electronic and thermal Enthalpies= -3273.108090			
H	0.38728	-1.59425	1.97486	Sum of electronic and thermal Free Energies= -3273.248773			
C	1.63812	0.1319	4.6214	SCF Done: E(RM06) = -3274.140596			
H	2.99243	1.80738	4.47773				
H	0.27665	-1.53323	4.43864	Int5b'			
H	1.58824	0.16249	5.70667	Number of imaginary frequencies=0			
C	3.53032	-0.45613	-0.48337	Charge =0 Multiplicity = 1			
C	3.8221	-0.57435	-1.85574	C	-4.35299	2.85039	-1.21564
C	4.52409	-0.75824	0.45713	C	-4.05757	1.50679	-1.00028
C	5.09382	-0.9669	-2.26985	C	-2.77874	1.10694	-0.58779
H	3.04863	-0.36413	-2.59163	C	-1.82518	2.11491	-0.37155
C	5.79284	-1.16548	0.03415	C	-2.09064	3.47571	-0.58054
H	4.31297	-0.68348	1.51873	C	-3.37333	3.82256	-1.01534
C	6.08166	-1.26642	-1.32641	H	-5.34579	3.14156	-1.54675
H	5.3102	-1.04811	-3.33174	H	-4.81834	0.75488	-1.18382
H	6.5534	-1.40299	0.77333	H	-3.61947	4.86321	-1.19246
H	7.06933	-1.58171	-1.65236	O	-0.57841	1.71726	0.06906
P	-2.31334	-0.69167	-0.41676	C	-0.98927	4.49528	-0.25445
Pd	0.34689	-1.5265	-1.12366	C	-1.18335	5.81415	-1.02384
C	0.78846	-3.12742	-0.27526	H	-2.13821	6.27972	-0.7626
O	1.23243	-3.87897	0.49981	H	-0.40572	6.53668	-0.75852
C	0.10496	-3.70149	-2.07523	H	-1.15781	5.65852	-2.10739
C	1.38602	-3.95607	-2.86686	C	-1.04514	4.79766	1.27167
H	1.77139	-3.01792	-3.27258	H	-0.9066	3.88595	1.86124
Cl	0.1798	-0.17811	-3.21947	H	-0.25487	5.50581	1.54711
H	2.17385	-4.41821	-2.26309	H	-2.01422	5.23853	1.53974
H	-0.55849	-3.03363	-2.63039	C	0.50274	2.47021	-0.32571
H	1.1686	-4.6315	-3.70565	C	0.35908	3.84121	-0.56527
C	-0.67262	-4.90407	-1.63244	C	1.73026	1.79744	-0.44594

C	1.49736	4.5419	-0.98622	H	3.072	-0.437	-2.5584
C	2.84466	2.53788	-0.85487	C	5.82112	-1.09595	0.10578
C	2.72278	3.90123	-1.13537	H	4.32557	-0.58974	1.56522
H	1.42851	5.60366	-1.19685	C	6.11403	-1.24157	-1.2491
H	3.80527	2.04739	-0.96474	H	5.34924	-1.10935	-3.26443
H	3.59458	4.46045	-1.46608	H	6.5822	-1.29709	0.85222
P	1.81873	0.0048	-0.01307	H	7.10852	-1.55152	-1.56307
C	-3.58593	-1.47261	-1.48778	P	-2.29751	-0.675	-0.42335
C	-4.73693	-2.10705	-0.9965	Pd	0.36002	-1.46809	-1.1406
C	-3.35216	-1.46331	-2.87629	C	0.75831	-3.18318	-0.47618
C	-5.6353	-2.71836	-1.87335	O	1.24102	-3.90938	0.31909
H	-4.93302	-2.12583	0.0711	C	0.051	-3.80033	-2.12209
C	-4.25799	-2.06597	-3.74726	C	1.25991	-4.00131	-3.03376
H	-2.45647	-0.98162	-3.27355	H	1.5876	-3.03934	-3.43701
C	-5.39922	-2.70055	-3.24905	Cl	0.20117	-0.12821	-3.23755
H	-6.52227	-3.20749	-1.47823	H	2.10749	-4.47287	-2.51794
H	-4.06539	-2.04967	-4.81677	H	-0.63957	-3.06792	-2.54993
H	-6.1024	-3.18034	-3.92893	H	0.97769	-4.65081	-3.87739
C	-2.81939	-1.11678	1.2932	C	-0.69805	-5.0006	-1.65835
C	-2.56451	-2.43008	1.7303	C	-0.02923	-6.19749	-1.36249
C	-3.39249	-0.20831	2.19742	C	-2.09161	-4.94382	-1.48125
C	-2.8885	-2.8246	3.02921	C	-0.72857	-7.30425	-0.88996
H	-2.11735	-3.15242	1.05247	H	1.04906	-6.25576	-1.48629
C	-3.69719	-0.60011	3.50375	C	-2.7924	-6.05311	-1.00807
H	-3.60104	0.80913	1.87777	H	-2.62984	-4.03488	-1.72886
C	-3.44901	-1.90745	3.92309	C	-2.11411	-7.23409	-0.70462
H	-2.68999	-3.84665	3.34799	H	-0.19578	-8.22463	-0.66444
H	-4.13447	0.11927	4.18751	H	-3.86897	-5.99284	-0.87885
H	-3.69062	-2.21166	4.93816	H	-2.65737	-8.10055	-0.3313
C	1.7411	0.04738	1.82589	Thermal correction to Energy= 0.807052			
C	2.40537	1.04503	2.56289	Thermal correction to Enthalpy= 0.807996			
C	0.98801	-0.91603	2.51112	Thermal correction to Gibbs Free Energy= 0.669418			
C	2.32544	1.06661	3.95525	Sum of electronic and zero-point Energies= -3273.189118			
H	2.97475	1.80986	2.04694	Sum of electronic and thermal Energies= -3273.139469			
C	0.8999	-0.88887	3.9052	Sum of electronic and thermal Enthalpies= -3273.138525			
H	0.45785	-1.68042	1.94711	Sum of electronic and thermal Free Energies= -3273.277103			
C	1.57231	0.09697	4.62898	SCF Done: E(RM06) = -3274.173117			
H	2.84415	1.83884	4.51355				
H	0.3001	-1.63204	4.41803				
H	1.50365	0.12127	5.70971	TS6b'			
C	3.54912	-0.45056	-0.4472	Number of imaginary frequencies=1			
C	3.84568	-0.60867	-1.81289	Charge = 0 Multiplicity = 1			
C	4.54349	-0.69999	0.50806	C	-4.04544	2.60483	-2.11812
C	5.12605	-0.99365	-2.20717	C	-3.6718	1.33002	-1.69372

C	-2.49905	1.13899	-0.94901	H	-4.53761	0.63262	0.58812
C	-1.74119	2.27789	-0.64139	C	-3.96087	-0.19038	3.83737
C	-2.09956	3.57299	-1.03393	H	-2.17804	-1.15878	4.57212
C	-3.2658	3.71498	-1.79185	H	-5.59637	0.77805	2.81447
H	-4.95012	2.73371	-2.70539	H	-4.42488	-0.11662	4.81745
H	-4.28707	0.47724	-1.95814	C	2.31739	0.40595	1.91804
H	-3.57749	4.69774	-2.12925	C	2.43176	1.51536	2.76629
O	-0.59055	2.08628	0.09515	C	2.45564	-0.88377	2.46337
C	-1.22116	4.73238	-0.54584	C	2.6793	1.34164	4.13127
C	-1.41613	6.00033	-1.3935	H	2.3301	2.51823	2.36284
H	-2.45428	6.3431	-1.34396	C	2.71559	-1.05321	3.82251
H	-0.79967	6.81979	-1.0115	H	2.3629	-1.75269	1.81529
H	-1.15625	5.83172	-2.44388	C	2.82425	0.05983	4.66186
C	-1.60849	5.05433	0.92682	H	2.76233	2.21203	4.77717
H	-1.48663	4.1783	1.57076	H	2.82941	-2.05531	4.22829
H	-0.97428	5.85818	1.31838	H	3.02003	-0.07336	5.72264
H	-2.65441	5.37768	0.98227	C	3.58182	0.16953	-0.68319
C	0.47504	2.90524	-0.22472	C	3.56682	-0.22988	-2.03022
C	0.23165	4.24072	-0.57218	C	4.80944	0.27168	-0.01042
C	1.75707	2.33815	-0.19426	C	4.76474	-0.5009	-2.69296
C	1.33784	5.03752	-0.88008	H	2.62396	-0.34197	-2.56128
C	2.83889	3.17956	-0.49714	C	6.00398	-0.01079	-0.67657
C	2.63169	4.51568	-0.83296	H	4.83397	0.56618	1.03479
H	1.19652	6.07596	-1.16031	C	5.98347	-0.39358	-2.01936
H	3.84546	2.77506	-0.49603	H	4.7384	-0.80814	-3.73484
H	3.4797	5.15073	-1.07297	H	6.94903	0.0673	-0.14484
P	1.95313	0.52306	0.1106	H	6.91403	-0.61459	-2.53614
C	-3.09441	-1.66573	-1.18669	P	-1.91813	-0.51145	-0.33794
C	-4.04131	-2.44146	-0.50262	Pd	0.31017	-1.21245	-0.53005
C	-2.95334	-1.83902	-2.57894	C	0.30619	-3.29092	-0.98895
C	-4.83024	-3.37054	-1.18982	H	0.22983	-2.47169	-3.0851
H	-4.16657	-2.32623	0.56899	Cl	0.40274	-1.1213	-4.12401
C	-3.75162	-2.7591	-3.26112	N	-0.0382	-3.47578	-2.37718
H	-2.20852	-1.26693	-3.13043	H	-1.04162	-3.62408	-2.51544
C	-4.691	-3.53095	-2.56799	H	0.47304	-4.26026	-2.79592
H	-5.5563	-3.96523	-0.64145	O	1.53805	-3.00297	-0.77838
H	-3.63697	-2.86984	-4.33645	C	-0.44802	-4.20537	-0.02407
H	-5.30869	-4.24925	-3.10061	C	-0.00027	-5.67407	-0.14247
C	-2.76053	-0.3723	1.30371	C	-0.46091	-6.46074	-1.19861
C	-2.10605	-0.86729	2.44051	C	0.86586	-6.21786	0.80604
C	-4.02263	0.22644	1.45407	C	-0.05601	-7.79108	-1.30576
C	-2.70286	-0.77799	3.70022	H	-1.14435	-6.03196	-1.9458
H	-1.1168	-1.30444	2.33336	C	1.27177	-7.5483	0.69845
C	-4.61952	0.31256	2.71192	H	1.22916	-5.59793	1.63841

C	0.8109	-8.33497	-0.35715	H	-4.63765	-1.29617	0.22757
H	-0.41955	-8.41138	-2.13784	C	-4.77329	-0.54201	-3.56942
H	1.955	-7.97666	1.44623	H	-2.70417	0.03981	-3.39538
H	1.13006	-9.3839	-0.44187	C	-5.9009	-1.04194	-2.91505
H	-0.25039	-3.86071	0.96944	H	-6.70747	-1.7144	-1.0304
C	-1.96846	-4.10504	-0.24717	H	-4.80419	-0.33932	-4.63673
H	-2.38265	-3.39167	0.43434	H	-6.81808	-1.22752	-3.46807
H	-2.16163	-3.7922	-1.25202	C	-2.15282	-0.94432	1.07291
H	-2.41753	-5.06155	-0.07885	C	-1.3963	-2.07259	1.42165
Thermal correction to Energy=	0.843004			C	-3.0571	-0.42151	2.01556
Thermal correction to Enthalpy=	0.843948			C	-1.54855	-2.67676	2.67225
Thermal correction to Gibbs Free Energy=	0.703853			H	-0.67126	-2.46304	0.71131
Sum of electronic and zero-point Energies=	-3329.700465			C	-3.20784	-1.02373	3.26451
Sum of electronic and thermal Energies=	-3329.650321			H	-3.63779	0.4642	1.7755
Sum of electronic and thermal Enthalpies=	-3329.649377			C	-2.45618	-2.15544	3.59411
Sum of electronic and thermal Free Energies=	-3329.789472			H	-0.94867	-3.54632	2.92637
SCF Done: E(RM06) =	-3330.71821400			H	-3.91094	-0.60805	3.98154
				H	-2.5739	-2.62195	4.56869
<b>cat0</b>				C	2.42667	-0.90894	0.70065
Number of imaginary frequencies=	0			C	1.90504	-0.38803	1.89601
Charge = 0	Multiplicity = 1			C	3.18224	-2.09248	0.75824
C	-2.57529	3.86152	-0.97033	C	2.14921	-1.02035	3.1162
C	-2.57441	2.48617	-1.20914	H	1.31082	0.52024	1.87655
C	-1.99361	1.60395	-0.28607	C	3.42394	-2.72379	1.97882
C	-1.39517	2.13532	0.86862	H	3.58984	-2.51897	-0.15346
C	-1.39965	3.50956	1.10569	C	2.91094	-2.18891	3.16279
C	-1.9929	4.37785	0.18772	H	1.74071	-0.59752	4.03012
H	-3.03692	4.52795	-1.69408	H	4.01832	-3.63346	2.00343
H	-3.032	2.10559	-2.11512	H	3.10266	-2.6798	4.11312
H	-1.99837	5.4487	0.37282	C	3.44493	-0.42501	-2.0054
C	1.24817	2.42391	-1.60831	C	3.24881	-0.64518	-3.37695
C	1.32736	3.81728	-1.56182	C	4.75286	-0.30512	-1.50769
C	1.98453	1.65157	-0.69611	C	4.34897	-0.76526	-4.23007
C	2.12668	4.44902	-0.60842	H	2.23998	-0.69057	-3.78009
C	2.79753	2.2908	0.25447	C	5.84663	-0.43574	-2.3628
C	2.86101	3.68358	0.30073	H	4.92181	-0.11974	-0.4509
H	2.18237	5.53418	-0.57434	C	5.6462	-0.66909	-3.72608
H	3.38229	1.70788	0.9596	H	4.18351	-0.93472	-5.29036
H	3.49067	4.16923	1.04204	H	6.8547	-0.35296	-1.96467
P	1.96433	-0.17715	-0.92798	H	6.49977	-0.76903	-4.39163
C	-3.52921	-0.56058	-1.48155	P	-1.92801	-0.21761	-0.61257
C	-4.66339	-1.07351	-0.83336	Pd	0.00986	-1.23209	-1.78371
C	-3.58961	-0.31137	-2.86556	H	1.09742	-2.26504	-2.34436
C	-5.83956	-1.31339	-1.54775	Cl	-0.3382	0.30786	-4.13862

H	0.63244	1.9368	-2.36261	H	-5.66987	0.92371	-3.99696
H	-0.93858	1.47375	1.59856	H	-6.80287	-1.26772	-3.66731
H	-0.93611	3.90026	2.00755	C	-1.53677	-1.53731	0.06731
H	0.75575	4.40558	-2.2738	C	-0.77405	-2.53498	-0.56462
Thermal correction to Energy= 0.598628				C	-1.9538	-1.74141	1.38994
Thermal correction to Enthalpy= 0.599573				C	-0.44395	-3.71202	0.10844
Thermal correction to Gibbs Free Energy= 0.484100				H	-0.43375	-2.38378	-1.58614
Sum of electronic and zero-point Energies= -2659.624959				C	-1.61657	-2.91733	2.0654
Sum of electronic and thermal Energies= -2659.587262				H	-2.5359	-0.98047	1.89965
Sum of electronic and thermal Enthalpies= -2659.586318				C	-0.86237	-3.90438	1.42796
Sum of electronic and thermal Free Energies=-2659.701790				H	0.14452	-4.47385	-0.39562
SCF Done: E(RM06) = -2660.652892				H	-1.94625	-3.06079	3.09131
				H	-0.60154	-4.81816	1.95532
<b>cat0'</b>				C	3.23774	2.04911	-3.25913
Number of imaginary frequencies=0				C	3.29985	3.43374	-3.03432
Charge = 0 Multiplicity = 1				C	4.27072	1.23665	-2.7609
C	-4.23271	2.10475	1.79532	C	4.37178	3.99221	-2.33499
C	-3.80873	1.14186	0.87935	H	2.51479	4.08119	-3.41078
C	-2.52776	1.21835	0.30559	C	5.3429	1.79951	-2.06859
C	-1.69393	2.28972	0.6553	H	4.24565	0.16286	-2.91652
C	-2.11914	3.25338	1.57186	C	5.39693	3.17812	-1.85249
C	-3.38799	3.16167	2.14473	H	4.40544	5.06657	-2.17439
H	-5.22664	2.0345	2.22945	H	6.13235	1.15434	-1.69377
H	-4.47973	0.33581	0.59767	H	6.2322	3.61401	-1.31104
H	-3.7227	3.91462	2.85346	C	2.55128	0.19444	-5.39077
C	-0.17726	3.21342	-4.67152	C	1.82402	-0.91242	-5.85781
C	-0.72628	4.30979	-5.34072	C	3.81905	0.45325	-5.93953
C	1.07212	2.70196	-5.05118	C	2.34665	-1.73143	-6.86008
C	-0.03834	4.89824	-6.40226	H	0.85042	-1.13201	-5.42949
C	1.75822	3.30193	-6.11948	C	4.33958	-0.37013	-6.93881
C	1.2036	4.3901	-6.79256	H	4.41033	1.28911	-5.57883
H	-0.46968	5.74502	-6.92946	C	3.60395	-1.46242	-7.4032
H	2.72105	2.91407	-6.43746	H	1.77028	-2.58347	-7.2099
H	1.73969	4.83852	-7.62476	H	5.32215	-0.15786	-7.35193
P	1.78566	1.28026	-4.1079	H	4.01192	-2.10355	-8.18007
C	-3.47903	-0.48152	-1.79562	P	-1.91992	-0.02274	-0.92029
C	-4.11807	-1.71722	-1.6206	Pd	0.04803	0.64078	-2.35456
C	-4.04911	0.46503	-2.6636	H	-0.72637	2.73667	-3.86424
C	-5.31032	-1.99775	-2.29309	H	-0.71188	2.37147	0.20116
H	-3.69193	-2.46456	-0.95961	H	-1.45999	4.07742	1.83109
C	-5.24318	0.18388	-3.32534	H	-1.69649	4.693	-5.03698
H	-3.54917	1.41144	-2.83726	Cl	1.90946	0.80513	-1.00777
C	-5.87626	-1.04786	-3.14341	H	-0.79215	0.66958	-3.69234
H	-5.79427	-2.96025	-2.14842	Thermal correction to Energy= 0.598761			

Thermal correction to Enthalpy=	0.599705		C	-1.54118	4.57138	0.75568		
Thermal correction to Gibbs Free Energy=	0.482809		H	-2.56639	5.0729	-1.07479		
Sum of electronic and zero-point Energies=	-2659.641204		H	-2.79508	2.73992	-1.81762		
Sum of electronic and thermal Energies=	-2659.603422		H	-1.44528	5.60281	1.0841		
Sum of electronic and thermal Enthalpies=	-2659.602478		C	1.42652	2.77377	-1.4021		
Sum of electronic and thermal Free Energies=	-2659.719374		C	1.62241	4.1468	-1.23445		
SCF Done: E(RM06) =	-2660.65538393		C	2.15929	1.86381	-0.62538		
			C	2.53757	4.62128	-0.29465		
<b>R1</b>			C	3.093	2.34591	0.3077		
Number of imaginary frequencies=	0		C	3.27346	3.71808	0.47708		
Charge =0	Multiplicity = 1		H	2.68437	5.69078	-0.16625		
C	-1.27585	-2.85002	-2.61046	H	3.68324	1.65421	0.90113	
H	-1.78885	-2.40907	-3.45794	H	3.99569	4.08082	1.20415	
H	-1.88906	-3.1113	-1.7532	P	1.97473	0.06862	-1.00554	
C	-0.05955	-3.52671	-2.79305	C	-3.53243	0.08931	-1.56044	
H	0.25626	-4.18485	-1.98501	C	-4.74068	-0.34679	-0.99444	
C	0.57952	-3.81875	-4.1004	C	-3.52225	0.52498	-2.89799	
C	1.3633	-4.97864	-4.20908	C	-5.92111	-0.31708	-1.74027	
C	0.39359	-3.00814	-5.2334	H	-4.77166	-0.71532	0.02486	
C	1.9307	-5.34255	-5.43004	C	-4.71032	0.56878	-3.62991	
H	1.51749	-5.60644	-3.33371	H	-2.58358	0.80696	-3.37317	
C	0.97084	-3.37218	-6.44833	C	-5.91173	0.15249	-3.05466	
H	-0.15299	-2.07233	-5.14578	H	-6.84862	-0.65964	-1.28821	
C	1.73289	-4.53994	-6.55486	H	-4.68514	0.91022	-4.66092	
H	2.52702	-6.24837	-5.50044	H	-6.8334	0.18046	-3.63034	
H	0.82902	-2.7335	-7.316	C	-2.24581	-0.74374	0.95153	
H		2.17603	-4.81802	-7.50759	C	-1.53791	-1.92023	1.23547
Thermal correction to Energy=	0.140555		C	-3.16386	-0.26493	1.90464		
Thermal correction to Enthalpy=	0.141499		C	-1.75802	-2.61869	2.42578		
Thermal correction to Gibbs Free Energy=	0.102415		H	-0.79185	-2.27504	0.53016		
Sum of electronic and zero-point Energies=	-309.508005		C	-3.385	-0.96225	3.09169		
Sum of electronic and thermal Energies=	-309.501251		H	-3.69786	0.6628	1.72247		
Sum of electronic and thermal Enthalpies=	-309.500307		C	-2.68584	-2.14452	3.35246		
Sum of electronic and thermal Free Energies=	-309.539391		H	-1.19389	-3.52453	2.62999		
SCF Done: E(RM06) =	-309.4762247		H	-4.09965	-0.5801	3.81586		
			H	-2.85743	-2.68522	4.27948		
<b>TS2a''</b>			C	2.32903	-0.83176	0.56614		
Number of imaginary frequencies=	1		C	1.95182	-0.31076	1.81446		
Charge =0	Multiplicity = 1		C	2.83869	-2.14206	0.51576		
C	-2.16924	4.27402	-0.45417	C	2.09606	-1.06912	2.97836	
C	-2.29914	2.94971	-0.87676	H	1.55134	0.69563	1.88103	
C	-1.80446	1.89995	-0.08941	C	2.98409	-2.89701	1.67952	
C	-1.1607	2.21069	1.12003	H	3.13394	-2.57053	-0.43785	
C	-1.03456	3.53431	1.54082	C	2.61437	-2.36301	2.91676	



H	1.80287	-0.64358	3.93445	Sum of electronic and thermal Free Energies=-2969.192847
H	3.39101	-3.90316	1.61907	SCF Done: E(RM06) = -2970.127145
H	2.73017	-2.95085	3.82329	
C	3.46841	-0.22802	-2.05905	
C	3.31566	-0.16777	-3.45376	<b>Int3a''</b>
C	4.74941	-0.41608	-1.51629	Number of imaginary frequencies=0
C	4.42901	-0.31037	-4.28556	Charge =0 Multiplicity = 1
H	2.33252	0.01508	-3.88423	C -2.18955 4.26198 -0.37995
C	5.85517	-0.56904	-2.35366	C -2.30903 2.94522 -0.82893
H	4.8885	-0.45432	-0.43992	C -1.79008 1.88517 -0.0717
C	5.69697	-0.51797	-3.74048	C -1.13825 2.17767 1.13786
H	4.29922	-0.25633	-5.36317	C -1.02298 3.49342 1.58554
H	6.84013	-0.72529	-1.92107	C -1.54967 4.54118 0.82795
H	6.55965	-0.63458	-4.39141	H -2.60428 5.06912 -0.97805
P	-1.92532	0.1354	-0.64481	H -2.81565 2.74824 -1.76729
Pd	-0.0807	-0.85554	-1.96972	H -1.46108 5.56654 1.17682
C	-1.35362	-2.61875	-2.53983	C 1.41711 2.74607 -1.45067
H	-1.97235	-2.72643	-1.65184	C 1.58824 4.12688 -1.32491
C	-0.03735	-3.09739	-2.44914	C 2.16873 1.87303 -0.65029
H	1.04149	-1.64153	-2.77869	C 2.49929 4.64488 -0.40447
H	0.3411	-3.50369	-1.5162	C 3.10072 2.39889 0.26071
Cl	-0.17515	0.90302	-4.06233	C 3.25722 3.77842 0.38807
H	0.72922	2.40683	-2.15222	H 2.62693 5.72017 -0.30812
H	-0.76946	1.4154	1.74705	H 3.70828 1.73538 0.869
H	-0.53901	3.75364	2.48283	H 3.97764 4.17586 1.09857
H	1.05257	4.84301	-1.84304	P 2.00904 0.06413 -0.97271
H	0.47007	-3.43913	-3.34668	C -3.47008 0.10253 -1.61759
C	-2.1043	-2.55359	-3.81257	C -4.69865 -0.29629 -1.06884
C	-3.4632	-2.91083	-3.81142	C -3.42363 0.52656 -2.95795
C	-1.49854	-2.21181	-5.03456	C -5.86411 -0.24368 -1.83603
C	-4.19123	-2.95885	-4.99927	H -4.75601 -0.6538 -0.04664
H	-3.94953	-3.15747	-2.8707	C -4.59687 0.59257 -3.71202
C	-2.22949	-2.25498	-6.21916	H -2.47036 0.78415 -3.41809
H	-0.47372	-1.85753	-5.04696	C -5.81836 0.2118 -3.15464
C	-3.5746	-2.63515	-6.20919	H -6.80836 -0.55772 -1.39811
H	-5.23985	-3.24362	-4.9775	H -4.54477 0.92363 -4.7453
H	-1.74979	-1.97337	-7.15256	H -6.72831 0.25693 -3.74762
H	-4.14028	-2.66611	-7.13686	C -2.21716 -0.7914 0.89445
Thermal correction to Energy= 0.740602				C -1.52578 -1.98685 1.13862
Thermal correction to Enthalpy= 0.741546				C -3.13191 -0.33399 1.86058
Thermal correction to Gibbs Free Energy= 0.610298				C -1.76015 -2.72392 2.30237
Sum of electronic and zero-point Energies= -2969.108044				H -0.78118 -2.32512 0.42311
Sum of electronic and thermal Energies= -2969.062543				C -3.36676 -1.06988 3.02169
Sum of electronic and thermal Enthalpies= -2969.061599				H -3.65195 0.60724 1.71002

C	-2.68491	-2.27001	3.24251
H	-1.20931	-3.64415	2.47662
H	-4.07871	-0.70382	3.75678
H	-2.86697	-2.84066	4.14936
C	2.32762	-0.7816	0.63903
C	1.96852	-0.20422	1.8674
C	2.80198	-2.10624	0.63734
C	2.09445	-0.92307	3.05849
H	1.59737	0.81479	1.8976
C	2.93027	-2.82101	1.82771
H	3.0853	-2.57735	-0.29978
C	2.57724	-2.23168	3.04475
H	1.81552	-0.45425	3.9985
H	3.31025	-3.83915	1.80411
H	2.67836	-2.78845	3.97237
C	3.53457	-0.25365	-1.97159
C	3.42724	-0.17929	-3.3702
C	4.79283	-0.47001	-1.38826
C	4.56853	-0.32933	-4.16545
H	2.45902	0.01812	-3.83036
C	5.92368	-0.63377	-2.18998
H	4.89495	-0.5221	-0.30846
C	5.81381	-0.56525	-3.5804
H	4.47572	-0.26244	-5.24614
H	6.89037	-0.81251	-1.726
H	6.69572	-0.69091	-4.20323
P	-1.87819	0.13307	-0.67208
Pd	-0.0142	-0.78425	-1.97803
C	-1.25008	-2.73295	-2.69206
H	-1.71378	-2.97208	-1.73871
C	0.13631	-3.00585	-2.8064
H	0.96144	-1.83658	-2.79922
H	0.62596	-3.53326	-1.98772
Cl	-0.07435	0.80706	-4.21103
H	0.72676	2.34479	-2.18919
H	-0.73118	1.37331	1.7429
H	-0.52061	3.69871	2.5272
H	1.00372	4.79447	-1.95136
H	0.52434	-3.25935	-3.80027
C	-2.16988	-2.61823	-3.83133
C	-3.50018	-3.05077	-3.67556
C	-1.75815	-2.14949	-5.0937
C	-4.38383	-3.0441	-4.75272
H	-3.83719	-3.39836	-2.70305

C	-2.6465	-2.13772	-6.16591
H	-0.76248	-1.73252	-5.21291
C	-3.9592	-2.59203	-6.00607
H	-5.40585	-3.38654	-4.6143
H	-2.31488	-1.75755	-7.12831
H	-4.64683	-2.58187	-6.84788

Thermal correction to Energy= 0.746086

Thermal correction to Enthalpy= 0.747030

Thermal correction to Gibbs Free Energy= 0.614918

Sum of electronic and zero-point Energies= -2969.140720

Sum of electronic and thermal Energies= -2969.095121

Sum of electronic and thermal Enthalpies= -2969.094177

Sum of electronic and thermal Free Energies= -2969.226290

SCF Done: E(RM06) = -2970.155785

#### TS4a''

Number of imaginary frequencies=1

Charge = 0 Multiplicity = 1

P	-1.90158	0.80639	0.28512
P	2.51669	0.71545	-0.17966
C	-2.14806	0.36476	2.06345
C	-2.3497	-0.98708	2.4003
C	-2.02171	1.30177	3.10101
C	-2.44228	-1.38347	3.73363
C	-2.10169	0.8991	4.4376
C	-2.31491	-0.44173	4.75855
C	-3.49875	0.34135	-0.52465
C	-3.52727	0.36458	-1.93106
C	-4.66316	-0.00742	0.17574
C	-4.70232	0.04972	-2.61519
C	-5.8343	-0.32887	-0.51552
C	-5.85762	-0.30007	-1.91091
C	-2.00426	2.65116	0.27154
C	-3.1913	3.33565	0.58582
C	-0.86605	3.38968	-0.07367
C	-3.22732	4.72903	0.57046
C	-0.903	4.78664	-0.09025
C	-2.08168	5.45735	0.23423
C	2.96967	0.58498	1.60483
C	1.94469	0.63474	2.56154
C	4.29979	0.46465	2.04138
C	2.23997	0.57371	3.92428
C	4.59297	0.39872	3.4042
C	3.56433	0.45393	4.34801

C	3.89771	-0.1724	-1.031	O	0.77503	-2.4781	1.33685
C	4.69147	0.42775	-2.01771	C	-0.23407	-2.66543	-1.44872
C	4.12586	-1.52175	-0.70719	C	1.04711	-3.28681	-1.97348
C	5.68959	-0.30484	-2.6663	H	1.69235	-2.52446	-2.41487
C	5.12965	-2.24595	-1.34722	Cl	0.00682	0.64583	-2.97692
C	5.91354	-1.63996	-2.33327	H	1.61788	-3.81402	-1.20228
C	2.81207	2.4943	-0.58525	H	-0.66378	-1.95766	-2.15584
C	3.46056	3.36655	0.30418	H	0.79756	-4.02	-2.75502
C	2.36982	2.98713	-1.8263	C	-1.26307	-3.54785	-0.85387
C	3.67394	4.70124	-0.04505	C	-0.93103	-4.7308	-0.16445
C	2.5958	4.32118	-2.17217	C	-2.6278	-3.22664	-0.99566
C	3.24789	5.18104	-1.28512	C	-1.92393	-5.55814	0.3567
H	4.1759	5.3645	0.6546	H	0.11075	-5.00446	-0.03233
H	2.24999	4.68705	-3.13517	C	-3.61963	-4.05313	-0.4713
H	3.41881	6.21968	-1.55631	H	-2.90815	-2.32385	-1.52996
H	-2.62578	0.61644	-2.48557	C	-3.27262	-5.22384	0.20877
H	-4.65897	-0.03617	1.26076	H	-1.6433	-6.46785	0.88139
H	1.82745	2.33535	-2.50607	H	-4.66388	-3.78119	-0.59911
H	3.79955	3.00932	1.27043	H	-4.04489	-5.87093	0.61615
H	6.29298	0.17584	-3.43172	Thermal correction to Energy= 0.755393			
H	5.29655	-3.28588	-1.07914	Thermal correction to Enthalpy= 0.756337			
H	6.69112	-2.20705	-2.83778	Thermal correction to Gibbs Free Energy= 0.616511			
H	3.52222	-2.00741	0.05469	Sum of electronic and zero-point Energies= -3082.449752			
H	4.53522	1.46703	-2.28545	Sum of electronic and thermal Energies= -3082.401582			
H	1.43011	0.60684	4.64767	Sum of electronic and thermal Enthalpies= -3082.400638			
H	5.62599	0.30205	3.72791	Sum of electronic and thermal Free Energies= -3082.540463			
H	3.79526	0.39739	5.40849	SCF Done: E(RM06) = -3083.440538			
H	5.10663	0.41715	1.31652	Int5a''			
H	0.90988	0.70971	2.24151	Number of imaginary frequencies=0			
H	-4.15117	5.2473	0.81438	Charge =0 Multiplicity = 1			
H	-0.01041	5.34093	-0.36638	P	-1.8964	0.64305	0.35019
H	-2.11406	6.54376	0.21811	P	2.85629	0.68152	-0.18015
H	0.04458	2.87141	-0.35118	C	-2.5639	0.44332	2.06421
H	-4.0901	2.77879	0.83481	C	-2.68976	-0.84914	2.59878
H	-4.71076	0.07195	-3.70174	C	-2.91377	1.54066	2.86437
H	-6.72912	-0.5979	0.04031	C	-3.16126	-1.04211	3.89585
H	-6.76981	-0.54967	-2.44667	C	-3.38125	1.34589	4.16672
H	-2.44351	-1.73503	1.617	C	-3.50844	0.05736	4.68501
H	-1.86626	2.35029	2.86889	C	-3.07653	-0.32379	-0.68879
H	-2.60553	-2.43132	3.97055	C	-2.65749	-0.76194	-1.95638
H	-2.00555	1.64091	5.22654	C	-4.37923	-0.62399	-0.25707
H	-2.38068	-0.75249	5.79784	C	-3.52811	-1.48771	-2.77074
Pd	0.32915	-0.3156	-0.6909	C	-5.24424	-1.35219	-1.07612
C	0.50968	-1.79965	0.42979				

C	-4.81993	-1.7874	-2.33308	H	-2.89929	6.20475	-0.61516
C	-2.23433	2.41627	-0.01799	H	-0.31983	3.05035	0.75275
C	-3.43889	2.84201	-0.59344	H	-4.19129	2.11596	-0.88427
C	-1.2683	3.3715	0.33204	H	-3.19372	-1.81588	-3.75135
C	-3.6743	4.20156	-0.80812	H	-6.24835	-1.57979	-0.72785
C	-1.51095	4.72942	0.12745	H	-5.49346	-2.35597	-2.96904
C	-2.71435	5.14733	-0.4453	H	-2.45311	-1.80205	2.138
C	3.94163	-0.06022	1.11791	H	-2.82627	2.54948	2.47641
C	3.6654	0.22152	2.46785	H	-3.24334	-2.0516	4.28802
C	5.00779	-0.92021	0.81256	H	-3.64826	2.20741	4.77326
C	4.44369	-0.33551	3.48167	H	-3.87153	-0.09015	5.69873
C	5.77921	-1.48451	1.83169	Pd	0.46006	0.25129	-0.06512
C	5.50153	-1.19253	3.1673	C	0.61417	-1.01478	1.49077
C	3.66171	0.20079	-1.76251	O	0.788	-0.72062	2.64499
C	4.85589	0.80117	-2.19102	Cl	0.18061	1.28389	-2.35873
C	3.07985	-0.8035	-2.54931	C	0.51196	-2.50454	1.01841
C	5.46314	0.39145	-3.3782	H	0.03553	-2.50118	0.0311
C	3.69201	-1.21465	-3.73439	C	1.94356	-3.06538	0.84459
C	4.88387	-0.61908	-4.14964	H	2.49262	-3.03313	1.79019
C	3.20213	2.49649	-0.02356	H	1.89036	-4.10676	0.5085
C	4.27649	2.98471	0.74011	H	2.50804	-2.49432	0.10195
C	2.38839	3.41067	-0.71415	C	-0.31052	-3.38657	1.94769
C	4.52552	4.3568	0.8168	C	-1.38359	-4.13138	1.43607
C	2.64658	4.77999	-0.63548	C	0.0006	-3.51487	3.3112
C	3.71052	5.25855	0.13141	C	-2.12608	-4.98368	2.25743
H	5.3599	4.71675	1.41315	H	-1.64644	-4.04345	0.38489
H	2.00893	5.47205	-1.17932	C	-0.7409	-4.36469	4.1319
H	3.90507	6.32621	0.19302	H	0.81235	-2.93175	3.73068
H	-1.66409	-0.50304	-2.31167	C	-1.80626	-5.10368	3.61026
H	-4.71789	-0.3007	0.72226	H	-2.95304	-5.55035	1.83783
H	1.56292	3.04692	-1.31934	H	-0.4852	-4.45002	5.18499
H	4.92166	2.301	1.28035	H	-2.38035	-5.76613	4.25264
H	6.38543	0.86581	-3.70291	Thermal correction to Energy= 0.758191			
H	3.22722	-1.98758	-4.34018	Thermal correction to Enthalpy= 0.759135			
H	5.35545	-0.93307	-5.07712	Thermal correction to Gibbs Free Energy= 0.621440			
H	2.13108	-1.23529	-2.24826	Sum of electronic and zero-point Energies=-3082.490590			
H	5.30844	1.59362	-1.60202	Sum of electronic and thermal Energies=-3082.442969			
H	4.21682	-0.10459	4.51895	Sum of electronic and thermal Enthalpies=-3082.442025			
H	6.60061	-2.14903	1.57682	Sum of electronic and thermal Free Energies=-3082.579720			
H	6.10397	-1.62999	3.95898	SCF Done: E(RM06) = -3083.491696			
H	5.24377	-1.1488	-0.2212				
H	2.83637	0.87049	2.72884	TS6a''			
H	-4.60882	4.51906	-1.26309	Number of imaginary frequencies=1			
H	-0.7523	5.4572	0.40252	Charge =0 Multiplicity = 1			

P	-1.15994	0.70969	1.08963	H	4.12392	3.77581	-0.10854
P	2.76577	1.07056	0.11582	H	7.64824	0.45783	-0.83276
C	-0.94001	0.96027	2.91248	H	5.34509	-3.14597	-0.36044
C	0.23396	0.47529	3.50626	H	7.5272	-2.02663	-0.77496
C	-1.88457	1.61239	3.72349	H	3.29871	-1.79358	-0.01951
C	0.45885	0.62683	4.87675	H	5.61764	1.80694	-0.46829
C	-1.6612	1.76389	5.09142	H	1.97863	4.59991	3.52713
C	-0.4894	1.26956	5.67174	H	5.0442	1.74802	4.51784
C	-2.7303	-0.26778	0.97097	H	3.69178	3.74912	5.1216
C	-3.38126	-0.3336	-0.2778	H	4.70447	0.62647	2.34904
C	-3.23832	-1.02432	2.0371	H	1.61691	3.47025	1.37247
C	-4.51176	-1.13547	-0.44424	H	-4.32696	4.54192	0.44455
C	-4.37172	-1.82679	1.86454	H	-0.45099	4.94027	-1.38615
C	-5.01124	-1.88594	0.62623	H	-2.69907	5.88655	-0.8706
C	-1.70471	2.35752	0.45215	H	0.15801	2.69349	-0.57413
C	-2.98268	2.88365	0.70803	H	-3.7183	2.2964	1.24951
C	-0.80688	3.11176	-0.31392	H	-5.00664	-1.16634	-1.41159
C	-3.33436	4.14922	0.23971	H	-4.75481	-2.40008	2.70495
C	-1.15927	4.37894	-0.7833	H	-5.89433	-2.50542	0.49476
C	-2.42026	4.90334	-0.50085	H	0.97967	-0.0061	2.87998
C	3.14098	1.96529	1.69249	H	-2.79646	2.009	3.28991
C	2.37435	3.08852	2.05123	H	1.37959	0.25238	5.315
C	4.09919	1.49123	2.60154	H	-2.40168	2.27077	5.70473
C	2.57674	3.72888	3.27287	H	-0.31684	1.39146	6.73789
C	4.29296	2.12833	3.83019	Pd	0.69603	-0.3237	0.06624
C	3.53668	3.25062	4.16843	C	0.02243	-2.26936	-0.55772
C	4.31616	0.10066	-0.18556	H	-0.8376	-1.09509	-2.31473
C	5.55173	0.72392	-0.43114	Cl	-0.99675	0.33584	-3.24202
C	4.2541	-1.30007	-0.16533	N	-0.93192	-2.14688	-1.63205
C	6.70017	-0.0378	-0.64034	H	-1.89486	-2.13201	-1.28378
C	5.40866	-2.06101	-0.37316	H	-0.84582	-2.93121	-2.28782
C	6.63143	-1.43382	-0.60842	O	1.25156	-2.20915	-0.91287
C	2.83968	2.39351	-1.17105	C	-0.43759	-3.24793	0.54584
C	3.58306	3.57775	-1.02933	H	-1.37507	-2.86226	0.96402
C	2.12297	2.17547	-2.35931	C	-0.73759	-4.61639	-0.07029
C	3.61635	4.51789	-2.06011	C	0.23881	-5.30484	-0.80856
C	2.1608	3.11864	-3.3888	C	-1.99885	-5.20725	0.08592
C	2.90796	4.28867	-3.24291	C	-0.03979	-6.5528	-1.36714
H	4.19339	5.43101	-1.93708	H	1.2158	-4.85091	-0.95322
H	1.58873	2.93531	-4.29369	C	-2.27787	-6.45847	-0.46968
H	2.93252	5.0246	-4.04259	H	-2.76781	-4.68261	0.64936
H	-2.99763	0.23603	-1.12256	C	-1.29873	-7.13539	-1.19789
H	-2.75618	-0.98585	3.00889	H	0.72735	-7.0704	-1.93726
H	1.50385	1.28932	-2.47887	H	-3.26143	-6.90134	-0.33502

H	-1.51462	-8.10726	-1.63346	H	-6.70611	-1.70223	-1.03212
C	0.59123	-3.35149	1.68037	H	-4.80399	-0.32784	-4.63933
H	1.55866	-3.69277	1.30155	H	-6.81756	-1.21558	-3.46979
H	0.73641	-2.37545	2.15451	C	-2.15084	-0.93332	1.06876
H	0.24492	-4.06211	2.43818	C	-1.39638	-2.06353	1.41586
Thermal correction to Energy=	0.794638			C	-3.05325	-0.4096	2.01269
Thermal correction to Enthalpy=	0.795582			C	-1.54893	-2.66862	2.66601
Thermal correction to Gibbs Free Energy=	0.654032			H	-0.67251	-2.45492	0.70479
Sum of electronic and zero-point Energies=	-3138.993738			C	-3.20424	-1.01269	3.2612
Sum of electronic and thermal Energies=	-3138.944534			H	-3.63229	0.47752	1.77387
Sum of electronic and thermal Enthalpies=	-3138.943590			C	-2.45474	-2.14632	3.5891
Sum of electronic and thermal Free Energies=	-3139.085140			H	-0.95067	-3.53971	2.91878
SCF Done: E(RM06) =	-3140.01654884			H	-3.90591	-0.59623	3.97919
				H	-2.57271	-2.61357	4.5633
TS2b''				C	2.43448	-0.9263	0.69318
Number of imaginary frequencies=	1			C	1.90786	-0.41636	1.89102
Charge =0	Multiplicity =	1		C	3.20024	-2.10352	0.74434
C	-2.58746	3.87233	-0.96497	C	2.15735	-1.05299	3.10785
C	-2.58412	2.4973	-1.2058	H	1.30536	0.4865	1.87618
C	-1.99452	1.61533	-0.28814	C	3.447	-2.73928	1.96155
C	-1.39011	2.14685	0.86338	H	3.61137	-2.52152	-0.16967
C	-1.39731	3.52064	1.10276	C	2.92922	-2.21513	3.14826
C	-1.99909	4.38863	0.19003	H	1.74486	-0.63871	4.02387
H	-3.05601	4.53845	-1.68455	H	4.04902	-3.64401	1.98141
H	-3.0473	2.11665	-2.10895	H	3.12494	-2.70948	4.09597
H	-2.00664	5.45917	0.37688	C	3.44883	-0.42099	-2.01092
C	1.24422	2.41109	-1.60753	C	3.25497	-0.63781	-3.38324
C	1.3184	3.80453	-1.55746	C	4.7554	-0.29035	-1.51233
C	1.97732	1.63921	-0.69216	C	4.35652	-0.74426	-4.23639
C	2.10916	4.43682	-0.59723	H	2.24675	-0.69147	-3.78678
C	2.78183	2.27894	0.26519	C	5.8506	-0.40775	-2.3675
C	2.84005	3.67188	0.31502	H	4.92228	-0.10684	-0.45487
H	2.16082	5.52208	-0.56034	C	5.65268	-0.63792	-3.73169
H	3.36449	1.69651	0.97243	H	4.19296	-0.91109	-5.29738
H	3.46311	4.15799	1.06159	H	6.85772	-0.31712	-1.96871
P	1.96768	-0.18865	-0.93102	H	6.50731	-0.7274	-4.39737
C	-3.52778	-0.54908	-1.4846	P	-1.9258	-0.20601	-0.61671
C	-4.66182	-1.06171	-0.83592	Pd	0.01787	-1.23297	-1.78881
C	-3.58873	-0.29985	-2.86857	C	-1.2956	-2.85817	-2.61813
C	-5.83832	-1.30143	-1.54982	H	-1.80123	-2.40601	-3.46402
H	-4.63567	-1.28423	0.22503	H	-1.90652	-3.09056	-1.75119
C	-4.77273	-0.53033	-3.57199	C	-0.09418	-3.54873	-2.79443
H	-2.7032	0.05053	-3.39878	H	1.11881	-2.23729	-2.3463
C	-5.90014	-1.03006	-2.91713	H	0.22594	-4.19183	-1.97618

Cl	-0.33799	0.29414	-4.14684	H	4.09714	2.85522	-0.08513
H	0.63471	1.92368	-2.36677	H	4.49374	5.12849	-0.9143
H	-0.92661	1.48562	1.58929	P	1.99462	0.74836	-0.86155
H	-0.92899	3.91129	2.00217	C	-3.16842	-0.74348	-1.49754
H	0.74933	4.39251	-2.27171	C	-4.29597	-1.36398	-0.94112
C	0.56199	-3.83772	-4.0913	C	-3.29454	-0.1235	-2.74815
C	1.35578	-4.99225	-4.18798	C	-5.51653	-1.35266	-1.62349
C	0.38383	-3.03156	-5.22916	H	-4.22658	-1.87726	0.00933
C	1.94017	-5.35529	-5.401	C	-4.50807	-0.10129	-3.41955
H	1.50424	-5.61636	-3.30899	H	-2.41801	0.31872	-3.19763
C	0.97816	-3.39448	-6.43598	C	-5.62757	-0.71789	-2.86122
H	-0.16898	-2.09872	-5.15066	H	-6.38134	-1.84841	-1.18496
C	1.74978	-4.55709	-6.53029	H	-4.58023	0.38488	-4.38858
H	2.544	-6.25681	-5.46192	H	-6.57414	-0.71052	-3.39066
H	0.84255	-2.75891	-7.30691	C	-1.54126	-2.03885	0.5977
H	2.20631	-4.83432	-7.47693	C	-0.63643	-3.08896	0.40951
Thermal correction to Energy= 0.740150				C	-2.4112	-2.08814	1.7061
Thermal correction to Enthalpy= 0.741094				C	-0.60907	-4.17851	1.28379
Thermal correction to Gibbs Free Energy= 0.609154				H	0.05598	-3.05168	-0.42552
Sum of electronic and zero-point Energies= -2969.112775				C	-2.38353	-3.17348	2.57964
Sum of electronic and thermal Energies= -2969.067355				H	-3.10435	-1.27464	1.89744
Sum of electronic and thermal Enthalpies= -2969.066411				C	-1.48703	-4.22531	2.36846
Sum of electronic and thermal Free Energies= -2969.198351				H	0.10232	-4.98424	1.11697
SCF Done: E(RM06) = -2970.124833				H	-3.06342	-3.20259	3.42757
				H	-1.46117	-5.06496	3.05531
Int3b''				C	1.97672	0.76479	0.99263
Number of imaginary frequencies=0				C	1.94373	1.945	1.74931
Charge =0 Multiplicity = 1				C	1.94559	-0.46872	1.67734
C	-2.57361	3.16879	0.58301	C	1.92696	1.89777	3.14408
C	-2.3845	2.00285	-0.15266	H	1.94661	2.91105	1.24941
C	-1.7878	0.86694	0.4255	C	1.91593	-0.51322	3.0719
C	-1.36939	0.95439	1.77	H	1.96174	-1.39686	1.11983
C	-1.57005	2.12691	2.50932	C	1.91354	0.67151	3.81141
C	-2.1715	3.23379	1.91994	H	1.92306	2.82327	3.71012
H	-3.04186	4.02898	0.11133	H	1.90051	-1.47809	3.5797
H	-2.719	1.97457	-1.18507	H	1.9042	0.63884	4.89645
H	-2.32531	4.14276	2.49834	C	3.58528	-0.17386	-1.175
C	1.56877	3.00225	-2.34783	C	3.80304	-0.63417	-2.48141
C	1.82353	4.33733	-2.84628	C	4.5771	-0.37279	-0.20548
C	2.39733	2.48377	-1.34673	C	4.99427	-1.28241	-2.80802
C	2.859	5.104	-2.3229	H	3.0527	-0.4633	-3.24538
C	3.44101	3.25505	-0.84248	C	5.76421	-1.02928	-0.53899
C	3.66876	4.55531	-1.32097	H	4.42766	-0.02955	0.81179
H	3.0563	6.10968	-2.70269	C	5.9765	-1.48645	-1.84184

H	5.14874	-1.63071	-3.82519	C	-3.6892	4.53835	1.94855
H	6.52527	-1.18032	0.21932	H	-5.20056	3.95112	0.52647
H	6.90231	-1.99754	-2.09564	H	-4.26152	1.69265	0.17355
P	-1.53437	-0.65302	-0.61366	H	-4.1031	5.53155	2.10195
Pd	0.22042	-0.54265	-2.17785	C	1.55185	1.64193	-3.00184
C	-0.83011	-2.01204	-3.18458	C	1.16941	2.96071	-3.24886
H	-1.22813	-1.53093	-4.07677	C	2.26388	1.32468	-1.83182
H	-1.66211	-2.48425	-2.63087	C	1.484	3.97065	-2.33647
C	0.25098	-3.09077	-3.51659	C	2.5778	2.34281	-0.91776
H	1.34243	-2.60658	-3.72652	C	2.18795	3.65937	-1.17235
H	0.33363	-3.72859	-2.62632	H	1.17785	4.99529	-2.52988
Cl	0.86094	0.19463	-4.38982	H	3.1189	2.11208	-0.00592
H	0.84209	2.46294	-2.93591	H	2.43305	4.43941	-0.4565
H	-0.87428	0.1211	2.2434	P	2.7809	-0.4229	-1.56811
H	-1.24129	2.15972	3.54679	C	-2.61019	-0.34894	-0.1983
H	1.21772	4.73225	-3.65994	C	-3.77636	-1.13096	-0.20537
C	-0.02128	-3.94181	-4.75762	C	-1.97634	-0.07466	-1.42329
C	-0.64233	-5.19618	-4.69479	C	-4.2973	-1.61752	-1.40725
C	0.38967	-3.43292	-6.02314	H	-4.27696	-1.36422	0.72964
C	-0.87701	-5.94076	-5.85459	C	-2.4993	-0.55641	-2.62522
H	-0.9383	-5.59325	-3.72725	H	-1.06433	0.51748	-1.43893
C	0.14592	-4.1811	-7.17657	C	-3.66211	-1.33083	-2.6178
H	0.80145	-2.5383	-5.91892	H	-5.20002	-2.22327	-1.39597
C	-0.48835	-5.42581	-7.09502	H	-1.98214	-0.35086	-3.55805
H	-1.36013	-6.91239	-5.788	H	-4.06464	-1.71722	-3.55035
H	0.45688	-3.79505	-8.13967	C	-2.58428	-0.69948	2.67465
H	-0.66481	-6.00265	-7.99919	C	-1.98022	-1.93431	2.97122
Thermal correction to Energy= 0.746533				C	-3.70028	-0.30036	3.42631
Thermal correction to Enthalpy= 0.747477				C	-2.49058	-2.75505	3.97712
Thermal correction to Gibbs Free Energy= 0.614457				H	-1.10563	-2.25669	2.41097
Sum of electronic and zero-point Energies= -2969.147750				C	-4.20324	-1.11798	4.44149
Sum of electronic and thermal Energies= -2969.102402				H	-4.17798	0.65292	3.22148
Sum of electronic and thermal Enthalpies= -2969.101458				C	-3.60283	-2.34741	4.71769
Sum of electronic and thermal Free Energies= -2969.234479				H	-2.01322	-3.70844	4.18854
SCF Done: E(RM06) = -2970.156387				H	-5.06748	-0.79249	5.01518
				H	-3.99566	-2.98193	5.50788
TS4b''				C	3.34486	-0.48873	0.18305
Number of imaginary frequencies=1				C	2.37865	-0.38628	1.19923
Charge =0 Multiplicity = 1				C	4.69106	-0.66271	0.53521
C	-4.30429	3.65101	1.06355	C	2.75808	-0.44284	2.53922
C	-3.77417	2.37409	0.86416	H	1.32799	-0.25527	0.95175
C	-2.61595	1.96717	1.54414	C	5.0641	-0.72988	1.88003
C	-1.99887	2.87524	2.42167	H	5.44988	-0.74556	-0.23568
C	-2.53482	4.1461	2.63034	C	4.10123	-0.61821	2.88322



H	1.99985	-0.35845	3.31281	Sum of electronic and thermal Energies=	-3082.404831
H	6.11022	-0.86872	2.13954	Sum of electronic and thermal Enthalpies=	-3082.403887
H	4.3939	-0.67105	3.92846	Sum of electronic and thermal Free Energies=	-3082.551189
C	4.29766	-0.63643	-2.57964	SCF Done: E(RM06) =	-3083.43051
C	4.57263	-1.8914	-3.14132		
C	5.19572	0.42258	-2.78818	Int5b''	
C	5.73629	-2.08935	-3.8854	Number of imaginary frequencies=	0
H	3.86361	-2.70387	-3.01473	Charge =	0 Multiplicity = 1
C	6.35618	0.22161	-3.53595	C	-4.28184 3.65831 1.08986
H	4.98559	1.40439	-2.37417	C	-3.76323 2.37665 0.89073
C	6.62879	-1.0345	-4.08317	C	-2.6077 1.96004 1.56955
H	5.93601	-3.06379	-4.32213	C	-1.98145 2.86333 2.44544
H	7.04339	1.048	-3.69604	C	-2.50584 4.1391 2.6537
H	7.53026	-1.18725	-4.67049	C	-3.65769 4.54093 1.97324
P	-1.80657	0.31483	1.33287	H	-5.17623 3.96583 0.55384
Cl	1.03742	-1.62003	-4.48572	H	-4.25754 1.69908 0.20123
H	1.30138	0.85719	-3.71133	H	-4.06262 5.53784 2.12644
H	-1.08907	2.58414	2.94198	C	1.5511 1.6024 -3.0323
H	-2.04603	4.83314	3.31638	C	1.16506 2.91582 -3.29792
H	0.61932	3.196	-4.1559	C	2.25776 1.30162 -1.85542
Pd	1.10429	-2.00648	-2.08245	C	1.47068 3.93912 -2.39736
C	0.63469	-2.8911	-0.50935	C	2.56503 2.33314 -0.95355
O	0.58009	-3.27217	0.59043	C	2.17156 3.64658 -1.22659
C	-0.51024	-3.7558	-1.9158	H	1.16235 4.95957 -2.60527
C	-0.00576	-5.1976	-1.97356	H	3.10395 2.11706 -0.03683
H	0.9127	-5.23759	-2.57006	H	2.41206 4.43712 -0.51996
H	0.24338	-5.55081	-0.96608	P	2.78319 -0.4406 -1.56073
H	-1.39887	-3.6122	-1.29986	C	-2.62351 -0.35489 -0.17265
H	-0.70614	-3.34179	-2.90777	C	-3.78783 -1.13957 -0.17979
C	-1.05845	-6.10348	-2.58739	C	-1.99619 -0.07035 -1.39875
C	-1.17324	-6.22279	-3.98002	C	-4.31341 -1.61896 -1.38254
C	-1.95699	-6.81024	-1.77701	H	-4.28362 -1.38038 0.75581
C	-2.15974	-7.02993	-4.5472	C	-2.52482 -0.54372 -2.60136
H	-0.48309	-5.67911	-4.62178	H	-1.08524 0.52343 -1.41493
C	-2.94539	-7.61852	-2.34151	C	-3.68548 -1.32136 -2.59413
H	-1.87724	-6.73029	-0.69476	H	-5.2144 -2.22724 -1.3711
C	-3.04955	-7.73062	-3.72921	H	-2.01495 -0.32758 -3.53582
H	-2.23131	-7.11424	-5.62847	H	-4.09201 -1.70141 -3.52753
H	-3.63045	-8.16362	-1.69713	C	-2.60358 -0.7057 2.70131
H	-3.81637	-8.36173	-4.17058	C	-2.00824 -1.94295 3.00514
Thermal correction to Energy=	0.755534			C	-3.72092 -0.29751 3.44621
Thermal correction to Enthalpy=	0.756478			C	-2.52825 -2.75721 4.0114
Thermal correction to Gibbs Free Energy=	0.609176			H	-1.13294 -2.27237 2.44797
Sum of electronic and zero-point Energies=	-3082.453196			C	-4.23354 -1.10859 4.46175

H	-4.19212	0.65777	3.23573	C	-1.91493	-6.81487	-1.81886	
C	-3.64164	-2.34055	4.74511	C	-2.1578	-6.99324	-4.5881	
H	-2.05753	-3.71263	4.22843	H	-0.49796	-5.62186	-4.66571	
H	-5.0986	-0.77607	5.03012	C	-2.90368	-7.62602	-2.37868	
H	-4.04195	-2.97	5.53559	H	-1.81758	-6.7549	-0.73699	
C	3.34729	-0.47712	0.1881	C	-3.02793	-7.71633	-3.76825	
C	2.3787	-0.36966	1.2016	H	-2.24677	-7.06006	-5.66919	
C	4.69419	-0.63272	0.54257	H	-3.57139	-8.19091	-1.73339	
C	2.75608	-0.4042	2.54054	H		-3.79265	-8.34965	-4.20612
H	1.32503	-0.25653	0.94907	Thermal correction to Energy= 0.757760				
C	5.06546	-0.68012	1.88882	Thermal correction to Enthalpy= 0.758704				
H	5.45499	-0.71886	-0.226	Thermal correction to Gibbs Free Energy= 0.611320				
C	4.10006	-0.5642	2.889	Sum of electronic and zero-point Energies= -3082.470900				
H	1.99575	-0.31842	3.31399	Sum of electronic and thermal Energies= -3082.422410				
H	6.11226	-0.8047	2.1517	Sum of electronic and thermal Enthalpies= -3082.421466				
H	4.39135	-0.60167	3.93529	Sum of electronic and thermal Free Energies= -3082.568850				
C	4.30106	-0.65803	-2.5727	SCF Done: E(RM06) = -3083.455298				
C	4.58784	-1.92002	-3.1148					
C	5.19423	0.40208	-2.79347	TS6b''				
C	5.75389	-2.12122	-3.8536	Number of imaginary frequencies=1				
H	3.88231	-2.73378	-2.97771	Charge =0 Multiplicity = 1				
C	6.35928	0.19792	-3.53621	P	-1.29077	0.73497	1.04284	
H	4.97849	1.38894	-2.39466	P	2.74459	0.91727	0.20464	
C	6.63918	-1.06502	-4.06595	C	-1.11773	1.02711	2.86656	
H	5.95925	-3.10117	-4.27514	C	-0.21272	0.21888	3.5728	
H	7.04033	1.02522	-3.70777	C	-1.84168	2.00077	3.57298	
H	7.54476	-1.21987	-4.64702	C	-0.04895	0.36393	4.95157	
P	-1.81433	0.29974	1.35959	C	-1.67104	2.15246	4.95007	
Cl	1.08127	-1.6853	-4.47463	C	-0.77848	1.33176	5.64363	
H	1.30847	0.80713	-3.73271	C	-2.89299	-0.19651	0.92674	
H	-1.07362	2.56464	2.96488	C	-3.47411	-0.36562	-0.34518	
H	-2.01006	4.82237	3.33848	C	-3.49732	-0.81861	2.02878	
H	0.61998	3.13893	-4.21024	C	-4.62808	-1.13336	-0.50254	
Pd	1.11522	-2.02596	-2.06245	C	-4.65097	-1.59329	1.86621	
C	0.54982	-2.94673	-0.53187	C	-5.21968	-1.75392	0.60319	
O	0.51551	-3.28569	0.59285	C	-1.78247	2.38468	0.36202	
C	-0.49685	-3.75459	-1.83211	C	-3.07762	2.91331	0.50356	
C	0.01925	-5.19067	-2.00618	C	-0.81929	3.13928	-0.32203	
H	0.91587	-5.17762	-2.63512	C	-3.38764	4.17562	-0.00372	
H	0.30814	-5.59373	-1.02947	C	-1.12957	4.40309	-0.82849	
H	-1.42105	-3.67581	-1.25333	C	-2.41281	4.92572	-0.66657	
H	-0.67798	-3.27122	-2.80144	C	3.1913	1.73559	1.80555	
C	-1.03839	-6.08342	-2.63115	C	2.29435	2.67282	2.34825	
C	-1.17324	-6.18098	-4.02331	C	4.35054	1.42065	2.52955	

C	2.56005	3.29184	3.56818	H	-0.64651	1.45271	6.71568
C	4.60919	2.03239	3.75963	Pd	0.59862	-0.32157	0.14292
C	3.7193	2.9714	4.28034	C	-0.04788	-2.3765	-0.43868
C	4.23559	-0.11637	-0.16927	H	-0.91397	-1.0216	-2.49618
C	5.444	0.43164	-0.63165	Cl	-1.03247	0.04298	-3.39111
C	4.14897	-1.50329	0.02645	N	-0.92236	-2.33936	-1.60487
C	6.54434	-0.38963	-0.87877	H	-1.8993	-2.50656	-1.36773
C	5.25412	-2.32242	-0.21809	H	-0.61531	-3.0282	-2.29315
C	6.45268	-1.76833	-0.66861	O	1.19422	-2.31261	-0.67307
C	2.88024	2.29379	-1.02416	C	-0.58836	-3.12638	0.77587
C	3.58836	3.4828	-0.78746	H	-1.59215	-2.76707	1.02642
C	2.23353	2.12247	-2.26011	C	-0.64812	-4.66739	0.56832
C	3.65562	4.47417	-1.76907	H	0.06553	-2.89942	1.62273
C	2.30773	3.11232	-3.2413	H	-1.15888	-5.09077	1.44321
C	3.01851	4.29014	-2.99822	H	-1.28509	-4.89391	-0.29665
H	4.20595	5.39066	-1.5713	C	0.70096	-5.33276	0.39822
H	1.79742	2.96405	-4.18895	C	1.13261	-5.79368	-0.85144
H	3.07052	5.06355	-3.76026	C	1.55555	-5.49917	1.49813
H	-3.02426	0.10765	-1.21469	C	2.38421	-6.3933	-1.00562
H	-3.07167	-0.69844	3.02007	H	0.48017	-5.68609	-1.7158
H	1.65138	1.22383	-2.44919	C	2.80722	-6.09607	1.3511
H	4.08087	3.63965	0.16757	H	1.23443	-5.15974	2.48103
H	7.47202	0.04698	-1.24019	C	3.22744	-6.54446	0.09571
H	5.16443	-3.39554	-0.07111	H	2.69823	-6.74232	-1.98583
H	7.31	-2.40678	-0.86683	H	3.45256	-6.21782	2.21735
H	3.20627	-1.94596	0.32944	H	4.20025	-7.01498	-0.02002
H	5.52523	1.50026	-0.80708	Thermal correction to Energy= 0.795161			
H	1.8544	4.01489	3.96839	Thermal correction to Enthalpy= 0.796105			
H	5.51269	1.77431	4.3064	Thermal correction to Gibbs Free Energy= 0.652486			
H	3.92329	3.44792	5.23569	Sum of electronic and zero-point Energies= -3138.990755			
H	5.05667	0.69858	2.13353	Sum of electronic and thermal Energies= -3138.941505			
H	1.38038	2.91917	1.81514	Sum of electronic and thermal Enthalpies= -3138.940561			
H	-4.39391	4.56996	0.11261	Sum of electronic and thermal Free Energies= -3139.084179			
H	-0.36872	4.96564	-1.36243	SCF Done: E(RM06) = -3140.01527462			
H	-2.65843	5.90636	-1.06573				
H	0.17007	2.72549	-0.48204	TS4c''			
H	-3.85241	2.33241	0.99546	Number of imaginary frequencies=1			
H	-5.06945	-1.24093	-1.4903	Charge =0 Multiplicity = 1			
H	-5.10571	-2.06536	2.73351	P	-1.1617	0.60218	1.30611
H	-6.11816	-2.35252	0.47898	P	2.48352	1.38427	-0.0464
H	0.37796	-0.51319	3.02749	C	-0.37045	0.60701	2.97877
H	-2.53283	2.65297	3.04899	C	0.58511	-0.39206	3.22871
H	0.6588	-0.26932	5.47977	C	-0.67607	1.5181	4.00151
H	-2.23578	2.91473	5.48083	C	1.19202	-0.50055	4.48154

C	-0.05479	1.41904	5.24731	H	0.94818	5.02272	2.98021	
C	0.87277	0.40486	5.49411	H	5.14333	5.07696	2.02141	
C	-2.62309	-0.51258	1.57184	H	3.19683	6.0637	3.21675	
C	-3.76984	-0.34652	0.776	H	4.84736	3.07876	0.60488	
C	-2.60821	-1.54698	2.51921	H	0.65569	3.0214	1.56996	
C	-4.87917	-1.17624	0.94325	H	-4.46623	4.22901	2.3365	
C	-3.71633	-2.38251	2.67849	H	-1.89685	4.87397	-1.06613	
C	-4.85708	-2.19693	1.89706	H	-3.72631	5.66613	0.44617	
C	-1.99095	2.23574	1.08894	H	-0.81196	2.71924	-0.66206	
C	-3.04464	2.67131	1.91529	H	-3.40493	2.03735	2.72021	
C	-1.59537	3.04733	0.01496	H	-5.76154	-1.02212	0.32784	
C	-3.65601	3.90369	1.68912	H	-3.6872	-3.17326	3.42336	
C	-2.21669	4.27726	-0.21733	H	-5.72235	-2.84078	2.02918	
C	-3.24056	4.71033	0.62437	H	0.86581	-1.08183	2.43732	
C	2.72967	2.88664	1.00627	H	-1.3904	2.31521	3.82779	
C	1.64142	3.45549	1.67821	H	1.92859	-1.27999	4.65253	
C	3.99409	3.48998	1.13556	H	-0.29832	2.13663	6.02643	
C	1.80724	4.59257	2.47278	H	1.35127	0.32801	6.46677	
C	4.16039	4.62198	1.93176	Pd	0.31411	0.14232	-0.64719	
C	3.06652	5.17624	2.60304	C	1.08649	-0.11383	-2.50341	
C	3.35074	0.02862	0.869	H	0.28449	2.01295	-3.42211	
C	3.34961	-1.2583	0.29536	Cl	-0.05437	3.51009	-3.39179	
C	3.96773	0.21525	2.11355	N	0.35407	0.67552	-3.54359	
C	3.96026	-2.32501	0.95586	H	-0.64168	0.45306	-3.5018	
C	4.57552	-0.8579	2.77154	H	0.72121	0.4466	-4.47399	
C	4.57265	-2.12921	2.19713	O	2.043	-0.74308	-2.89371	
C	3.63757	1.76197	-1.44485	C	-0.72876	-1.65748	-1.14285	
C	4.84973	1.08859	-1.65012	H	-1.09442	-2.00986	-0.17387	
C	3.2732	2.79374	-2.32481	C	-1.87673	-1.69689	-2.16373	
C	5.68099	1.44195	-2.71615	H	-1.55824	-1.28103	-3.12777	
C	4.10646	3.14372	-3.38674	H	-2.7137	-1.08147	-1.81332	
C	5.31338	2.46909	-3.58569	H	0.07474	-2.32872	-1.46257	
H	6.61662	0.90886	-2.86429	C	-2.35311	-3.11899	-2.41426	
H	3.80192	3.9396	-4.06073	C	-3.30516	-3.72353	-1.581	
H	5.96093	2.73965	-4.4157	C	-1.81816	-3.87394	-3.46797	
H	-3.80809	0.44788	0.03666	C	-3.71132	-5.04146	-1.79626	
H	-1.7387	-1.69539	3.15119	H	-3.73174	-3.15494	-0.75892	
H	2.33168	3.3205	-2.20062	C	-2.22112	-5.19222	-3.68674	
H	5.1495	0.28519	-0.98613	H	-1.07864	-3.42126	-4.12596	
H	3.95788	-3.31011	0.49687	C	-3.1713	-5.78155	-2.85034	
H	5.05239	-0.69464	3.73471	H	-4.45465	-5.49003	-1.14146	
H	5.04711	-2.9621	2.70953	H	-1.7961	-5.75707	-4.51278	
H	3.97456	1.19596	2.5766	H		-3.48975	-6.80682	-3.02011
H	2.88921	-1.41848	-0.67591	Thermal correction to Energy=	0.792789			

Thermal correction to Enthalpy=	0.793733			C	4.21102	3.08651	0.6855
Thermal correction to Gibbs Free Energy=	0.652021			C	2.37562	3.37821	-0.86698
Sum of electronic and zero-point Energies=	-3138.958056			C	4.43	4.46611	0.68344
Sum of electronic and thermal Energies=	-3138.908715			C	2.60421	4.75507	-0.86671
Sum of electronic and thermal Enthalpies=	-3138.907771			C	3.62756	5.30427	-0.09112
Sum of electronic and thermal Free Energies=	-3139.049483			H	5.23135	4.88154	1.28902
SCF Done: E(RM06) =	-3139.98918438			H	1.97656	5.39736	-1.47898
				H	3.79962	6.37755	-0.09127
Int5c''				H	-1.73631	-0.66831	-2.13517
Number of imaginary frequencies=	0			H	-4.65733	-0.35871	1.01717
Charge =0	Multiplicity =	1		H	1.57937	2.95969	-1.47628
P	-1.85321	0.57949	0.47691	H	4.84587	2.45179	1.29373
P	2.87787	0.69952	-0.14975	H	6.41815	0.76248	-3.67053
C	-2.46035	0.6455	2.22311	H	3.27256	-2.12631	-4.20128
C	-2.72039	-0.54714	2.91804	H	5.40029	-1.09565	-4.97304
C	-2.61307	1.86582	2.89892	H	2.16732	-1.296	-2.14635
C	-3.13513	-0.51761	4.2487	H	5.33123	1.56984	-1.60345
C	-3.02069	1.89133	4.23436	H	4.13293	0.09013	4.59779
C	-3.28569	0.70171	4.91254	H	6.78861	-1.78209	1.77599
C	-3.07796	-0.43354	-0.46006	H	6.16565	-1.27031	4.12953
C	-2.71351	-0.91438	-1.72903	H	5.41173	-0.9346	-0.08622
C	-4.35993	-0.7192	0.03786	H	2.73435	0.90901	2.74375
C	-3.6164	-1.66996	-2.47902	H	-4.73251	4.35183	-1.09708
C	-5.25666	-1.47854	-0.71628	H	-0.74778	5.39351	0.15469
C	-4.88635	-1.95735	-1.97438	H	-2.98421	6.07607	-0.70628
C	-2.23917	2.33003	0.04595	H	-0.26843	3.01213	0.6026
C	-3.49436	2.71922	-0.44068	H	-4.26496	1.97603	-0.61868
C	-1.25336	3.30667	0.25202	H	-3.32425	-2.03091	-3.46158
C	-3.75822	4.06329	-0.71153	H	-6.24441	-1.69516	-0.3178
C	-1.5235	4.65002	-0.00756	H	-5.58576	-2.54907	-2.55938
C	-2.77643	5.03088	-0.49265	H	-2.60673	-1.50587	2.42346
C	3.97782	0.05972	1.18938	H	-2.41967	2.80129	2.3857
C	3.63002	0.3375	2.52344	H	-3.33138	-1.45332	4.76424
C	5.12414	-0.7083	0.9349	H	-3.13528	2.84649	4.74017
C	4.41743	-0.13306	3.57321	H	-3.60551	0.72358	5.95104
C	5.9051	-1.18647	1.99027	Pd	0.49448	0.20057	-0.03139
C	5.5565	-0.89842	3.30994	C	0.52626	-0.51571	1.84149
C	3.69297	0.16153	-1.70975	C	0.11331	-1.78435	-0.22027
C	4.88506	0.75118	-2.16068	H	0.16353	-1.44904	-1.26139
C	3.11651	-0.87321	-2.45898	C	-1.21306	-2.49933	-0.01998
C	5.49753	0.29694	-3.32876	H	0.95084	-2.4226	-0.03032
C	3.73358	-1.32887	-3.62509	H	-1.9348	-1.81042	0.36654
C	4.9247	-0.74655	-4.06029	H	-1.55509	-2.88571	-0.95733
C	3.17982	2.52809	-0.08783	C	-0.80789	-3.59359	0.98502

C	0.29734	-4.40447	0.72539	C	-1.00461	3.99283	3.30668
C	-1.54575	-3.77399	2.15489	C	-1.36206	5.19263	2.68712
C	0.66416	-5.39594	1.63514	C	3.66725	-0.40062	0.1395
H	0.87838	-4.26251	-0.19737	C	4.15494	0.01668	1.39084
C	-1.17836	-4.76507	3.06549	C	4.4199	-1.32088	-0.60368
H	-2.41676	-3.13486	2.35977	C	5.37106	-0.46125	1.87639
C	-0.07369	-5.5761	2.80576	C	5.63688	-1.80398	-0.11215
H	1.53493	-6.03554	1.43026	C	6.11648	-1.37447	1.12562
H	-1.76006	-4.9068	3.98799	C	1.83595	-0.45065	-2.1067
H	0.21576	-6.35787	3.52294	C	2.25175	0.16103	-3.29913
O	0.52448	-1.9278	2.06707	C	1.18982	-1.69782	-2.17935
N	0.55138	0.41085	2.98244	C	2.03302	-0.46219	-4.53091
H	-0.0531	0.06965	3.7023	C	0.98509	-2.32525	-3.40826
H	1.48445	0.47963	3.3355	C	1.40427	-1.70708	-4.58882
Thermal correction to Energy= 0.783151				C	2.53438	2.05218	-0.76167
Thermal correction to Enthalpy= 0.784095				C	3.81753	2.40612	-1.21587
Thermal correction to Gibbs Free Energy= 0.648185				C	1.59559	3.06969	-0.54113
Sum of electronic and zero-point Energies= -2678.165077				C	4.14058	3.74109	-1.46001
Sum of electronic and thermal Energies= -2678.117599				C	1.91973	4.40648	-0.78343
Sum of electronic and thermal Enthalpies= -2678.116655				C	3.19147	4.74453	-1.24601
Sum of electronic and thermal Free Energies= -2678.252565				H	5.13691	3.99853	-1.81017
SCF Done: E(RM06) = -2679.18370651				H	1.17779	5.17786	-0.59642
				H	3.44791	5.78461	-1.42991
TS6c''				H	-0.40923	0.95558	-2.05039
Number of imaginary frequencies=1				H	-4.35546	2.09292	-0.77005
Charge =0 Multiplicity = 1				H	0.61197	2.82071	-0.15948
P	-1.82705	1.09887	0.50182	H	4.56963	1.63751	-1.36805
P	2.04556	0.29669	-0.42303	H	2.35932	0.02702	-5.44519
C	-3.4115	0.3866	1.14943	H	0.48904	-3.29156	-3.44399
C	-3.97876	-0.70477	0.46723	H	1.23715	-2.19065	-5.54761
C	-4.01048	0.82003	2.33888	H	0.83805	-2.17098	-1.26604
C	-5.11892	-1.3387	0.9583	H	2.74206	1.12864	-3.27086
C	-5.14925	0.17842	2.83468	H	5.73292	-0.12644	2.84472
C	-5.70692	-0.90078	2.14906	H	6.21021	-2.51323	-0.70369
C	-2.32579	1.50492	-1.23596	H	7.06252	-1.75009	1.50603
C	-1.39746	1.34051	-2.27193	H	4.06368	-1.6585	-1.57164
C	-3.61357	1.97447	-1.55411	H	3.58091	0.72326	1.9857
C	-1.73598	1.646	-3.59263	H	-2.16369	6.10041	0.90151
C	-3.95182	2.28092	-2.87196	H	-0.59474	3.99862	4.31321
C	-3.01277	2.11841	-3.89486	H	-1.23147	6.13758	3.20817
C	-1.69914	2.74796	1.33729	H	-0.86774	1.85008	3.12651
C	-2.05525	3.95813	0.72182	H	-2.4617	3.96148	-0.28406
C	-1.15903	2.77738	2.63782	H	-1.00045	1.50274	-4.37938
C	-1.88392	5.17189	1.39303	H	-4.95087	2.64265	-3.10119

H	-3.28042	2.35301	-4.92185	C	0.28604	0.07663	3.4491
H	-3.53016	-1.05613	-0.45912	C	-1.08446	2.03723	3.78874
H	-3.58825	1.65485	2.88749	C	0.64485	0.0928	4.79832
H	-5.5476	-2.17577	0.41296	C	-0.71788	2.05726	5.13467
H	-5.59931	0.52816	3.76008	C	0.14189	1.08169	5.64436
H	-6.59309	-1.39685	2.53589	C	-2.7613	0.07712	1.294
Pd	0.126	-0.22662	1.08335	C	-3.59807	0.0746	0.16351
C	-0.80322	-1.00692	2.74887	C	-3.19468	-0.58135	2.45331
C	1.2365	-1.87206	2.51351	C	-4.83937	-0.55809	0.19902
H	2.16729	-1.30138	2.51036	C	-4.43788	-1.22042	2.48465
C	1.35761	-3.2003	1.76555	C	-5.26326	-1.20976	1.36098
O	-0.89399	-0.3152	3.75782	C	-1.55757	2.57081	0.59648
N	-1.60671	-2.126	2.58295	C	-2.71967	3.22195	1.0495
H	-2.44658	-2.12233	3.1562	C	-0.74281	3.22535	-0.33866
H	-1.75255	-2.43309	1.63046	C	-3.03229	4.50559	0.60256
H	0.94122	-2.0225	3.54877	C	-1.05888	4.50885	-0.79024
H	0.35752	-3.60478	1.56911	C	-2.20028	5.15371	-0.31477
H	1.8417	-3.04229	0.79478	C	2.981	1.63468	1.56585
C	2.14506	-4.22764	2.56221	C	2.31498	2.7626	2.07639
C	3.51636	-4.42227	2.34863	C	3.89789	0.96636	2.39019
C	1.51279	-4.98412	3.56066	C	2.57341	3.21838	3.36786
C	4.23586	-5.34775	3.10778	C	4.14872	1.42016	3.6878
H	4.0233	-3.84236	1.58069	C	3.49251	2.54818	4.17893
C	2.22807	-5.90871	4.32202	C	4.0157	-0.07297	-0.51219
H	0.44888	-4.84041	3.73858	C	5.2271	0.3483	-1.07947
C	3.59451	-6.09504	4.09742	C	3.86167	-1.423	-0.16217
H	5.29873	-5.48663	2.92388	C	6.2672	-0.56146	-1.27833
H	1.71845	-6.48753	5.08868	C	4.90847	-2.32592	-0.34584
H	4.153	-6.81714	4.68767	C	6.11327	-1.89789	-0.9063
Thermal correction to Energy=	0.782103			C	3.03347	2.60316	-1.13348
Thermal correction to Enthalpy=	0.783048			C	3.9656	3.55598	-0.68376
Thermal correction to Gibbs Free Energy=	0.646225			C	2.41366	2.7994	-2.37457
Sum of electronic and zero-point Energies=	-2678.149026			C	4.26483	4.67262	-1.46446
Sum of electronic and thermal Energies=	-2678.101867			C	2.71273	3.91766	-3.15586
Sum of electronic and thermal Enthalpies=	-2678.100922			C	3.63926	4.85619	-2.7012
Sum of electronic and thermal Free Energies=	-2678.237746			H	4.98706	5.40097	-1.10453
SCF Done: E(RM06) =	-2679.16414721			H	2.20756	4.03822	-4.10928
				H	3.87256	5.73001	-3.30408
TS4d''				H	-3.28037	0.57818	-0.74583
Number of imaginary frequencies=	1			H	-2.56845	-0.59127	3.33955
Charge =0 Multiplicity =	1			H	1.68184	2.09135	-2.74437
P	-1.09154	0.8716	1.1572	H	4.45438	3.42921	0.27688
P	2.61814	1.084	-0.16846	H	7.19785	-0.22244	-1.72583
C	-0.59302	1.04049	2.93107	H	4.76826	-3.36662	-0.06801

H	6.92482	-2.60409	-1.06162	H	2.57151	-5.35315	-0.45865
H	2.91735	-1.77679	0.23993	H	2.41317	-5.61163	2.01452
H	5.36194	1.38365	-1.37373	Thermal correction to Energy=	0.792788		
H	2.05243	4.09546	3.74159	Thermal correction to Enthalpy=	0.793732		
H	4.86804	0.89251	4.30893	Thermal correction to Gibbs Free Energy=	0.653297		
H	3.69363	2.90399	5.18587	Sum of electronic and zero-point Energies=	-3138.955839		
H	4.42952	0.09709	2.01872	Sum of electronic and thermal Energies=	-3138.906326		
H	1.60013	3.29925	1.45879	Sum of electronic and thermal Enthalpies=	-3138.905382		
H	-3.93338	4.99533	0.96234	Sum of electronic and thermal Free Energies=	-3139.045817		
H	-0.41768	4.98775	-1.52428	SCF Done: E(RM06) =	-3139.99016956		
H	-2.45168	6.15003	-0.66823				
H	0.13119	2.72226	-0.73623	Int5d''			
H	-3.39391	2.71752	1.73502	Number of imaginary frequencies=	0		
H	-5.47621	-0.5426	-0.68145	Charge =	0	Multiplicity =	1
H	-4.75879	-1.72292	3.3933	P	-1.18035	0.69582	1.10382
H	-6.23007	-1.70496	1.38731	P	2.84116	1.04173	0.1976
H	0.6955	-0.68756	2.79464	C	-0.97933	1.04462	2.91809
H	-1.74741	2.80712	3.40848	C	0.1145	0.47575	3.58676
H	1.32677	-0.66098	5.18186	C	-1.87646	1.83883	3.65169
H	-1.10598	2.83642	5.7857	C	0.30141	0.67858	4.95637
H	0.4241	1.09787	6.69376	C	-1.68799	2.04632	5.01807
Pd	0.43734	-0.23251	-0.54303	C	-0.6005	1.46322	5.67478
C	1.08042	-0.85032	-2.38308	C	-2.73447	-0.31899	1.06616
H	0.17215	0.82122	-4.03346	C	-3.40266	-0.48469	-0.16192
Cl	-0.07783	2.09822	-4.80859	C	-3.20442	-1.02214	2.18584
N	0.17379	-0.43646	-3.4831	C	-4.51712	-1.31768	-0.25768
H	-0.79938	-0.51866	-3.19205	C	-4.3173	-1.86286	2.08479
H	0.3445	-1.02978	-4.30185	C	-4.97948	-2.01163	0.86566
O	2.06518	-1.46289	-2.72379	C	-1.7761	2.31309	0.4217
C	-0.77684	-2.05636	-0.54387	C	-3.0995	2.76439	0.56389
H	-1.56744	-1.77276	0.14837	C	-0.85641	3.13257	-0.24738
C	-1.45026	-2.58763	-1.80953	C	-3.48111	4.01269	0.07076
H	-0.74955	-2.86944	-2.60101	C	-1.2373	4.38286	-0.7383
H	-2.03507	-3.48895	-1.56994	C	-2.54965	4.82777	-0.5768
H	-2.15858	-1.85664	-2.21944	C	3.31332	1.92578	1.75679
C	0.1365	-3.02476	0.13604	C	2.41789	2.87166	2.28699
C	0.05786	-3.19781	1.53457	C	4.49372	1.65125	2.46309
C	1.06587	-3.82501	-0.5608	C	2.70628	3.53886	3.47606
C	0.87054	-4.11009	2.20694	C	4.77437	2.31027	3.66349
H	-0.67599	-2.62206	2.09356	C	3.88612	3.25823	4.17088
C	1.87111	-4.7452	0.10919	C	4.37422	0.07971	-0.20314
H	1.17428	-3.71228	-1.63381	C	5.51588	0.66334	-0.77681
C	1.78473	-4.89178	1.49686	C	4.39301	-1.29088	0.09872
H	0.77653	-4.22328	3.28446	C	6.65276	-0.1045	-1.0315



C	5.53564	-2.05522	-0.14919	C	-0.22823	-2.10928	0.28323
C	6.66692	-1.46494	-0.71402	H	-1.20208	-1.63027	0.42344
C	2.86371	2.39569	-1.06333	C	-0.47954	-3.49738	-0.31233
C	3.56453	3.60161	-0.89794	C	0.58482	-4.30063	-0.75092
C	2.1377	2.19157	-2.24861	C	-1.78525	-3.99406	-0.42489
C	3.54717	4.57423	-1.8999	C	0.34806	-5.56879	-1.28068
C	2.1259	3.16264	-3.25119	H	1.60173	-3.92189	-0.6838
C	2.83123	4.35581	-3.07926	C	-2.02379	-5.26544	-0.95436
H	4.09261	5.50369	-1.75679	H	-2.61943	-3.38185	-0.0887
H	1.55113	2.98838	-4.15644	C	-0.95788	-6.05671	-1.38333
H	2.81687	5.1155	-3.85654	H	1.18409	-6.17716	-1.6162
H	-3.05268	0.04256	-1.04564	H	-3.04327	-5.63478	-1.03127
H	-2.70588	-0.91323	3.1438	H	-1.14133	-7.04479	-1.79686
H	1.55673	1.28198	-2.37779	C	0.47191	-2.20608	1.64539
H	4.11709	3.78657	0.01843	H	1.47336	-2.63404	1.54296
H	7.52714	0.36042	-1.47988	H	0.5715	-1.21509	2.09788
H	5.5342	-3.1159	0.08826	H	-0.11143	-2.84247	2.31868
H	7.55286	-2.06209	-0.91438	Thermal correction to Energy= 0.783022			
H	3.50208	-1.76257	0.49942	Thermal correction to Enthalpy= 0.783966			
H	5.51726	1.71873	-1.03155	Thermal correction to Gibbs Free Energy= 0.649454			
H	2.00281	4.26958	3.86602	Sum of electronic and zero-point Energies= -2678.165481			
H	5.69428	2.08336	4.19652	Sum of electronic and thermal Energies= -2678.118040			
H	4.10768	3.77292	5.10218	Sum of electronic and thermal Enthalpies= -2678.117095			
H	5.2001	0.9247	2.07575	Sum of electronic and thermal Free Energies= -2678.251607			
H	1.48791	3.08753	1.76853	SCF Done: E(RM06) = -2679.18710933			
H	-4.50952	4.34515	0.18703	TS6d''			
H	-0.50846	4.99615	-1.2611	Number of imaginary frequencies=1			
H	-2.85043	5.79759	-0.96449	Charge =0 Multiplicity = 1			
H	0.15629	2.7802	-0.40826	P	-1.55311	0.91493	0.7019
H	-3.8419	2.13301	1.04267	P	2.67239	0.956	-0.03548
H	-5.02705	-1.42175	-1.21212	C	-3.01144	0.37526	1.72165
H	-4.66804	-2.3955	2.96516	C	-3.40523	-0.97491	1.66967
H	-5.85034	-2.65764	0.7903	C	-3.68164	1.2314	2.60833
H	0.82995	-0.11342	3.01918	C	-4.44031	-1.45025	2.47594
H	-2.72162	2.30501	3.15577	C	-4.71456	0.75196	3.41976
H	1.15783	0.23273	5.45478	C	-5.09797	-0.5878	3.35748
H	-2.39033	2.66537	5.57049	C	-2.14141	0.54273	-1.01497
H	-0.45539	1.62695	6.7395	C	-1.1771	0.27627	-1.99873
Pd	0.75077	-0.28285	0.18917	C	-3.49885	0.52313	-1.37864
C	0.87906	-0.8392	-1.9458	C	-1.55494	0.01278	-3.31704
N	-0.02917	-0.83868	-3.0865	C	-3.87657	0.2537	-2.69512
H	-0.89043	-1.34656	-2.88537	C	-2.90577	0.00045	-3.66769
H	0.444	-1.29221	-3.86886				
O	2.11377	-0.86763	-2.20683				

C	-1.67099	2.76366	0.81682	H	-0.32342	2.80302	2.49911
C	-2.4424	3.55039	-0.05263	H	-3.0017	3.08326	-0.85665
C	-0.94864	3.40133	1.84024	H	-0.79018	-0.19183	-4.06142
C	-2.49336	4.93798	0.1016	H	-4.93071	0.23934	-2.96013
C	-1.01212	4.78562	2.00302	H	-3.203	-0.2131	-4.69118
C	-1.78372	5.55806	1.13201	H	-2.90457	-1.66525	0.99675
C	4.32589	0.46338	0.63506	H	-3.40408	2.27865	2.66764
C	4.45494	0.28116	2.02141	H	-4.72091	-2.4982	2.41593
C	5.45376	0.27953	-0.18401	H	-5.22134	1.4334	4.09848
C	5.69213	-0.05969	2.57499	H	-5.90079	-0.95812	3.98939
C	6.68563	-0.06483	0.37296	Pd	0.61361	0.24895	1.31571
C	6.80794	-0.23158	1.75505	C	0.51684	-1.12428	2.846
C	2.7132	0.187	-1.72414	C	0.80116	-2.70563	1.76861
C	2.64043	0.91962	-2.91732	H	1.07557	-2.28903	0.79553
C	2.739	-1.21787	-1.7991	C	2.0093	-3.37154	2.41718
C	2.59779	0.2647	-4.1528	H	1.77207	-3.78253	3.40385
C	2.70528	-1.86867	-3.03084	H	2.37761	-4.1969	1.79215
C	2.63088	-1.12846	-4.21482	H	2.81336	-2.64029	2.54205
C	2.86808	2.76514	-0.39023	C	-0.43314	-3.53648	1.63393
C	4.09258	3.4463	-0.31473	C	-1.09221	-3.62986	0.39479
C	1.71372	3.49263	-0.72628	C	-0.96387	-4.26468	2.71493
C	4.15977	4.81626	-0.57891	C	-2.23645	-4.41492	0.23868
C	1.78437	4.8576	-1.00504	H	-0.69374	-3.08466	-0.45783
C	3.00928	5.5244	-0.92924	C	-2.10906	-5.04615	2.56293
H	5.11615	5.32858	-0.5112	H	-0.48321	-4.20177	3.68609
H	0.87816	5.39981	-1.26048	C	-2.75246	-5.1265	1.32436
H	3.06479	6.59046	-1.13395	H	-2.72099	-4.47418	-0.73276
H	-0.12613	0.26577	-1.72534	H	-2.49926	-5.59786	3.41481
H	-4.26347	0.70944	-0.63056	H	-3.6399	-5.74282	1.20518
H	0.75185	2.98998	-0.75888	O	1.55461	-0.55699	3.26307
H	4.99674	2.91073	-0.04613	N	-0.59425	-1.27015	3.67313
H	2.54617	0.85097	-5.06692	H	-0.70858	-0.48677	4.31216
H	2.73312	-2.95467	-3.06658	H	-1.46012	-1.48168	3.19066
H	2.60119	-1.63559	-5.17551	Thermal correction to Energy= 0.781369			
H	2.79504	-1.80625	-0.88609	Thermal correction to Enthalpy= 0.782313			
H	2.61906	2.00427	-2.88849	Thermal correction to Gibbs Free Energy= 0.645678			
H	5.77608	-0.2024	3.64908	Sum of electronic and zero-point Energies= -2678.150814			
H	7.54915	-0.20412	-0.27261	Sum of electronic and thermal Energies= -2678.103295			
H	7.76759	-0.50337	2.18731	Sum of electronic and thermal Enthalpies= -2678.102351			
H	5.36894	0.40071	-1.26014	Sum of electronic and thermal Free Energies= -2678.238986			
H	3.58305	0.37081	2.66055	SCF Done: E(RM06) = -2679.16073244			
H	-3.09286	5.53308	-0.58264				
H	-0.44725	5.26123	2.80026				
H	-1.82618	6.63748	1.25237				

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