

Supporting Information For

DFT Studies on the Mechanisms of Palladium-Catalyzed Intramolecular Arylation of a Silyl C(sp³)–H Bond

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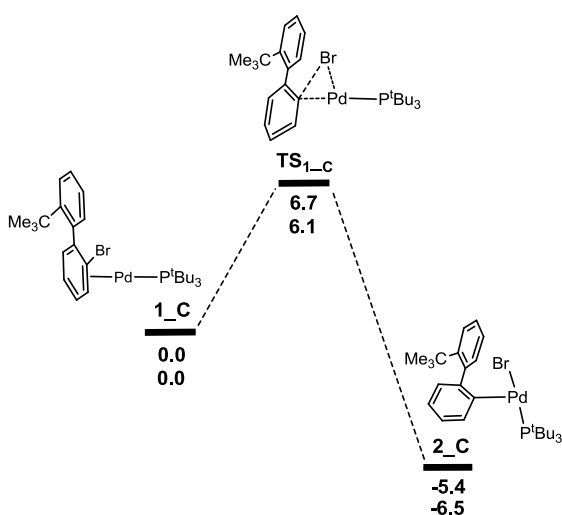


Fig. S1 Free energy profile calculated for the oxidative addition process for the CMe₃-containing substrate. The solvation-corrected relative free energies and electronic energies (in parentheses) are given in kcal/mol.

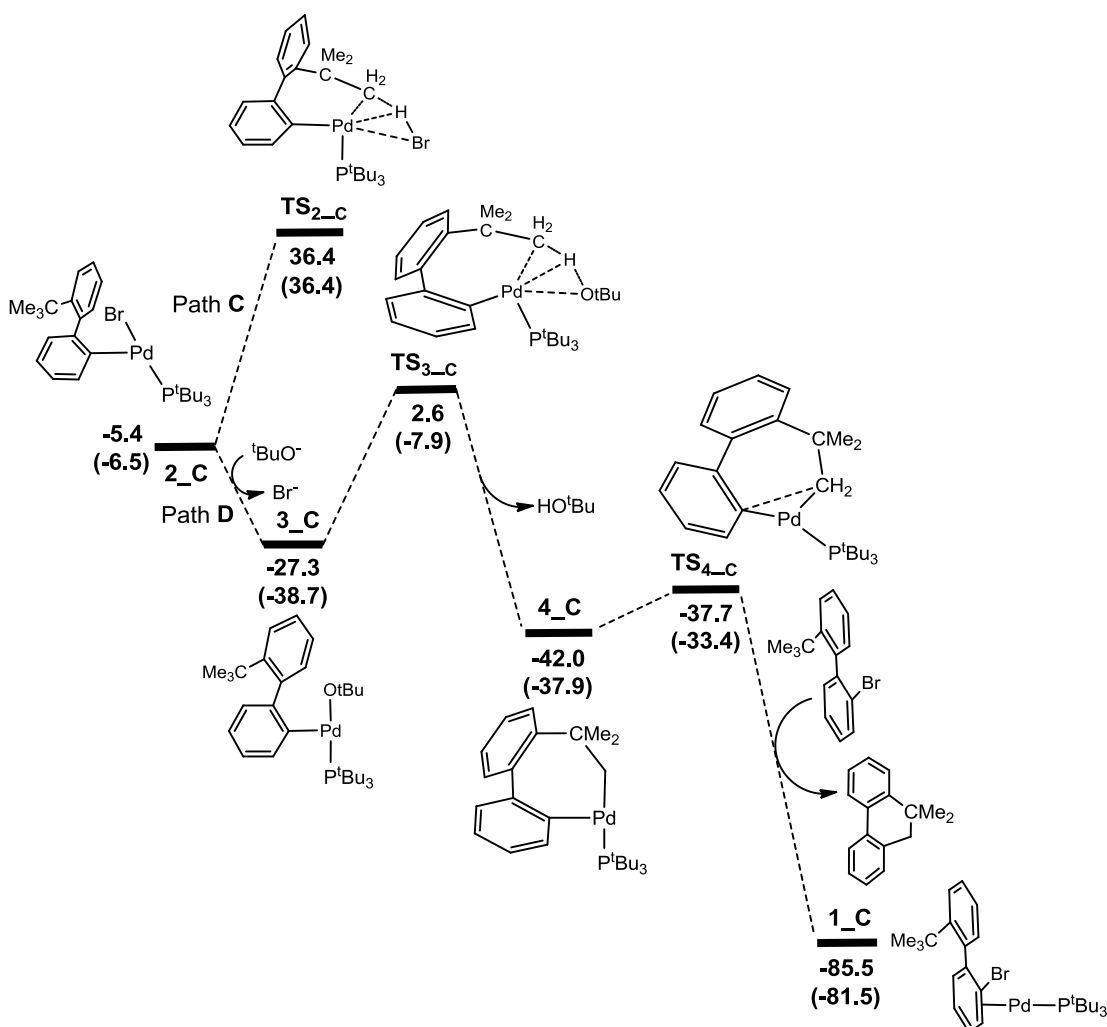


Fig. S2 Free energy profile calculated for the CMD and reductive elimination processes for the CMe₃-containing substrate. The solvation-corrected relative free energies and electronic energies (in parentheses) are given in kcal/mol.

Cartesian coordinates and electronic energies for all of the calculated structures

1				C	2.387555	3.352615	0.387159
SCF done:	-1205.749202			H	0.769836	1.926985	0.406517
Pd	-0.849571	-0.468432	-0.172016	C	3.771806	3.513027	0.401416
C	1.262068	-0.968256	-0.555371	H	5.669544	2.538575	0.414466
C	2.006846	-0.405454	0.528489	H	1.730323	4.218073	0.362841
C	2.108343	-1.160196	1.701488	H	4.211724	4.507087	0.387635
C	1.545013	-2.440195	1.820214	Si	5.359836	-0.345687	0.416956
C	0.824985	-2.981596	0.764052	C	6.966609	0.337648	-0.320028
C	0.670985	-2.255468	-0.435904	H	7.444760	1.086615	0.321661
H	2.646494	-0.728461	2.540083	H	7.685771	-0.480460	-0.450143
H	1.668627	-2.999074	2.743498	H	6.802681	0.792795	-1.303481
H	0.395166	-3.977011	0.835903	C	4.832048	-1.809808	-0.653872
H	0.259998	-2.741513	-1.313961	H	4.025233	-2.393455	-0.200976
C	2.670545	0.931748	0.447397	H	4.495886	-1.482067	-1.643757
C	4.081773	1.073604	0.445341	H	5.687854	-2.481590	-0.798439
C	1.847724	2.068876	0.408794	C	5.755383	-0.942906	2.171109
C	4.593859	2.386603	0.423677	H	6.615904	-1.623598	2.156331

H	6.008061	-0.103269	2.829327	H	7.254126	0.403157	-1.595188
H	4.915880	-1.482139	2.621738	H	5.946619	1.478701	-2.108569
Br	1.508948	-0.258958	-2.367480	C	4.765886	-1.456607	-1.060024
P	-3.111842	0.140798	0.170026	H	4.276810	-2.195697	-0.419266
C	-3.763124	-0.493119	1.911430	H	4.077439	-1.215339	-1.876784
C	-3.327790	2.092821	0.106486	H	5.655239	-1.928305	-1.497347
C	-4.241356	-0.643819	-1.234886	C	6.265647	-0.399585	1.432574
C	-2.754585	2.710713	1.400763	H	7.201779	-0.894636	1.144962
H	-1.742035	2.350115	1.609921	H	6.526638	0.477429	2.036558
H	-2.697874	3.799925	1.271614	H	5.709944	-1.093808	2.071463
H	-3.378616	2.525662	2.278220	P	-3.026482	0.166193	0.097105
C	-2.440522	2.625640	-1.043585	C	-3.815451	-0.485696	1.770505
H	-1.404402	2.288034	-0.934678	C	-3.234263	2.115613	0.026016
H	-2.785281	2.322554	-2.032180	C	-4.015196	-0.617903	-1.406252
H	-2.447632	3.724069	-1.015670	C	-2.793392	2.727478	1.373450
C	-4.767717	2.609222	-0.085180	H	-1.806666	2.367807	1.682935
H	-5.447079	2.266240	0.699668	H	-2.723251	3.816823	1.254407
H	-4.761444	3.707895	-0.053780	H	-3.502080	2.539370	2.183274
H	-5.191138	2.321864	-1.051117	C	-2.238190	2.653872	-1.028939
C	-2.641819	-0.243062	2.947760	H	-1.214307	2.332290	-0.813280
H	-2.451927	0.814617	3.133280	H	-2.475325	2.344000	-2.046715
H	-2.938778	-0.695310	3.904250	H	-2.263479	3.752048	-1.006906
H	-1.702000	-0.703724	2.625858	C	-4.650087	2.629720	-0.300280
C	-5.073077	0.142381	2.414725	H	-5.401946	2.275302	0.409620
H	-5.352360	-0.322100	3.370766	H	-4.650734	3.727798	-0.255828
H	-4.973419	1.215031	2.598828	H	-4.975979	2.352640	-1.306036
H	-5.907679	-0.007570	1.724974	C	-2.787570	-0.232042	2.898867
C	-3.945341	-2.025012	1.853283	H	-2.624547	0.825331	3.109111
H	-4.809812	-2.331134	1.259462	H	-3.154370	-0.697167	3.823995
H	-3.052344	-2.520565	1.458422	H	-1.818618	-0.683083	2.656303
H	-4.107950	-2.396881	2.873761	C	-5.171337	0.129908	2.166700
C	-5.756829	-0.658855	-0.956484	H	-5.526124	-0.348550	3.090302
H	-6.275759	-1.082265	-1.827918	H	-5.102930	1.201629	2.370467
H	-6.019042	-1.281702	-0.097361	H	-5.941300	-0.022576	1.405882
H	-6.167277	0.340566	-0.790327	C	-3.974953	-2.019143	1.688262
C	-3.755003	-2.092417	-1.474164	H	-4.782295	-2.329884	1.021495
H	-3.936066	-2.755354	-0.627538	H	-3.047313	-2.505753	1.368739
H	-4.293110	-2.506733	-2.338010	H	-4.219328	-2.399851	2.688837
H	-2.682908	-2.109680	-1.694929	C	-5.549181	-0.642843	-1.261022
C	-3.990379	0.104354	-2.561906	H	-5.988428	-1.054980	-2.180117
H	-2.922089	0.170671	-2.793254	H	-5.882221	-1.278760	-0.436668
H	-4.470365	-0.457218	-3.374666	H	-5.976476	0.352875	-1.115517
H	-4.416330	1.109990	-2.573308	C	-3.496351	-2.061359	-1.607455
TS₁				H	-3.746714	-2.731496	-0.784391
SCF done: -1205.741262				H	-3.951947	-2.475046	-2.517513
Pd	-0.696307	-0.487484	-0.042850	H	-2.409158	-2.071457	-1.738273
C	1.199463	-1.269653	0.056317	C	-3.650769	0.141508	-2.700502
C	2.150357	-0.600408	0.870620	H	-2.567236	0.214571	-2.837637
C	2.737265	-1.350074	1.902338	H	-4.054233	-0.416968	-3.555598
C	2.464241	-2.708356	2.087493	H	-4.080609	1.144657	-2.742091
C	1.584053	-3.363437	1.226030	2			
C	0.967919	-2.654117	0.191806	SCF done: -1205.757064			
H	3.419866	-0.841176	2.577197	Pd	-0.382959	-0.633697	0.305574
H	2.947843	-3.250915	2.894933	C	1.327731	-1.415024	0.950885
H	1.383817	-4.425479	1.342029	C	2.403059	-0.588070	1.325352
H	0.330854	-3.164764	-0.522208	C	3.448511	-1.154745	2.074486
Br	1.006160	-0.545655	-2.073887	C	3.452176	-2.511490	2.400103
C	2.516717	0.839601	0.710108	C	2.404687	-3.331167	1.974820
C	3.826902	1.242514	0.342555	C	1.354123	-2.787157	1.230014
C	1.533246	1.807776	0.969503	H	4.260830	-0.512745	2.406974
C	4.074797	2.627822	0.267151	H	4.273951	-2.927760	2.976858
C	1.811829	3.170126	0.885284	H	2.408426	-4.393198	2.207735
H	0.538474	1.471644	1.254131	H	0.560855	-3.432080	0.863663
C	3.095372	3.583912	0.535824	Br	0.217113	-1.597606	-1.907021
H	5.062473	2.976146	-0.021666	C	2.412094	0.878085	1.021674
H	1.032786	3.898334	1.096025	C	3.319412	1.472832	0.108905
H	3.334182	4.642186	0.466133	C	1.496778	1.681262	1.725691
Si	5.283869	0.092288	-0.113393	C	3.246229	2.871299	-0.047384
C	6.461860	1.069437	-1.232066	C	1.456621	3.065284	1.552539
H	6.953450	1.899806	-0.712294	H	0.844882	1.210986	2.457382

	C	2.338474	3.664462	0.656331	H	-0.079821	-0.837865	-3.275097
	H	3.919214	3.363972	-0.743985	C	2.324742	-1.568786	0.720372
	H	0.754004	3.666448	2.124296	C	2.909502	-0.340098	1.116092
	H	2.326289	4.741132	0.506876	C	2.148421	-2.591853	1.667852
	Si	4.656035	0.568987	-0.919983	C	3.257823	-0.188260	2.470405
	C	4.918533	1.559544	-2.514392	C	2.507709	-2.414629	3.004228
	H	5.324809	2.562250	-2.338929	H	1.710308	-3.534297	1.349997
	H	5.632408	1.031724	-3.158771	C	3.057901	-1.200732	3.411252
	H	3.984280	1.667855	-3.077299	H	3.708262	0.743122	2.803233
	C	4.220112	-1.195806	-1.410815	H	2.354275	-3.219438	3.718943
	H	4.263480	-1.889429	-0.566489	H	3.338876	-1.043741	4.449712
	H	3.215229	-1.260537	-1.841205	Si	3.385852	1.027206	-0.117030
	H	4.936203	-1.542251	-2.167462	C	3.732111	2.616079	0.851148
	C	6.284303	0.585457	0.050961	H	4.578579	2.509834	1.539444
	H	7.102586	0.188417	-0.562718	H	3.981269	3.427285	0.156318
	H	6.560037	1.601417	0.357303	H	2.859996	2.939171	1.430904
	H	6.221974	-0.030776	0.954780	H	0.706861	2.469921	-0.888125
	P	-2.748360	0.254534	-0.007927	C	4.985518	0.481610	-0.977506
	C	-3.430470	0.415751	1.822404	H	5.332101	1.245352	-1.684517
	C	-2.786412	2.014723	-0.861216	H	5.788646	0.304437	-0.251964
	C	-3.917049	-0.961155	-1.003188	H	4.830170	-0.447151	-1.538432
	C	-2.167082	3.060592	0.089740	C	2.045349	1.372840	-1.389789
	H	-1.169720	2.765187	0.429492	H	2.140460	2.422831	-1.706958
	H	-2.054097	4.003325	-0.461689	H	2.180294	0.797357	-2.307733
	H	-2.792592	3.272037	0.960125	Br	-0.145402	3.672142	-0.325621
	C	-1.849667	1.952529	-2.091523	P	-2.106464	-0.371289	0.225016
	C	-0.842546	1.628331	-1.813857	C	-2.220569	0.015702	2.145483
	H	-2.207351	1.285382	-2.875347	C	-3.527618	0.627734	-0.708410
	H	-1.776292	2.960160	-2.522742	C	-2.494151	-2.287161	-0.031442
	C	-4.178411	2.513306	-1.296186	C	-2.743751	-2.570026	-1.529839
	H	-4.879643	2.589110	-0.460365	H	-2.796260	-3.658147	-1.667234
	H	-4.075686	3.518561	-1.727709	H	-3.684158	-2.156316	-1.898055
	H	-4.630457	1.881495	-2.064538	H	-1.926234	-2.204721	-2.156660
	C	-2.271486	0.959364	2.691376	C	-3.694380	-2.817352	0.780605
	H	-1.938823	1.957375	2.406579	H	-4.623064	-2.276682	0.591314
	H	-2.597090	1.002926	3.739595	H	-3.864146	-3.865749	0.499013
	H	-1.401349	0.288859	2.653404	H	-3.502887	-2.805920	1.856459
	C	-4.672523	1.308010	2.009216	C	-3.118494	0.708452	-2.198764
	H	-4.979986	1.279896	3.064049	H	-2.146861	1.199843	-2.316657
	H	-4.480580	2.354540	1.760226	H	-3.065689	-0.266142	-2.686343
	H	-5.522973	0.967190	1.413203	H	-3.865026	1.307529	-2.737555
	C	-3.746560	-0.986801	2.387659	C	-3.593109	2.082013	-0.198201
	H	-4.637155	-1.436683	1.945093	H	-2.624423	2.581432	-0.240479
	H	-2.908141	-1.680174	2.261520	H	-4.276085	2.641523	-0.851443
	H	-3.934014	-0.892382	3.465560	H	-3.987057	2.160634	0.817233
	C	-5.426905	-0.754283	-0.767972	C	-4.948761	0.037503	-0.598027
	H	-5.981183	-1.446633	-1.416379	H	-5.642689	0.709790	-1.120843
	H	-5.731147	-0.970017	0.259489	H	-5.047187	-0.944486	-1.064319
	H	-5.759020	0.257445	-1.015287	H	-5.291906	-0.037725	0.437640
	C	-3.528492	-2.409413	-0.621821	C	-1.544474	1.383010	2.389344
	H	-3.731663	-2.652071	0.421956	H	-1.549151	1.586936	3.468643
	H	-4.120054	-3.100315	-1.237702	H	-0.500612	1.377242	2.059095
	H	-2.471052	-2.601200	-0.825551	H	-2.047789	2.213818	1.895646
	C	-3.635597	-0.829134	-2.516631	C	-1.253714	-3.120622	0.356568
	H	-2.573931	-0.951176	-2.748118	H	-0.390585	-2.866641	-0.257125
	H	-4.180103	-1.630444	-3.033686	H	-0.972242	-3.017615	1.403630
	H	-3.987863	0.116752	-2.934491	H	-1.488459	-4.179890	0.183167
					C	-3.646743	0.046108	2.730765
					H	-3.577149	0.231566	3.811428
TS ₂					H	-4.260289	0.845598	2.309650
SCF done:	-1205.695521				H	-4.179914	-0.897637	2.597955
Pd	0.128884	0.567956			C	-1.389234	-1.018897	2.934737
C	0.969295	-1.089321	-1.404413		H	-1.868254	-1.999690	2.985679
C	1.914058	-1.854312	-0.691037		H	-0.379320	-1.139266	2.531630
C	2.455253	-2.994451	-1.321165		H	-1.287124	-0.659246	3.967145
C	2.095262	-3.360538	-2.616296					
C	1.174766	-2.581575	-3.317615	3				
C	0.623550	-1.446827	-2.714304	SCF done:	-1425.604554			
H	3.184078	-3.588960	-0.775693	Pd	-0.465276	0.705113	0.057145	
H	2.539418	-4.239033	-3.076547	P	-2.710960	-0.262983	0.091011	
H	0.888646	-2.844982	-4.333099	C	-3.204232	-0.150176	1.991182	

C	-3.874231	0.972085	-0.906071	H	-1.422758	1.047467	2.482997
C	-3.080304	-2.085158	-0.545557	H	-2.846719	2.041543	2.118729
C	0.524857	-0.476823	-1.215598	C	-1.915409	-2.999583	-0.106447
C	1.599338	-1.275721	-0.767821	H	-0.959283	-2.642811	-0.495273
C	2.212111	-2.132581	-1.704039	H	-1.834502	-3.106285	0.976189
C	1.836956	-2.157005	-3.045975	H	-2.089360	-4.002681	-0.518343
C	0.826232	-1.304275	-3.486517	C	-4.714456	-0.085240	2.291162
C	0.175470	-0.470318	-2.570762	H	-4.857816	-0.090693	3.380378
H	3.004381	-2.789724	-1.354222	H	-5.180775	0.827722	1.913829
H	2.335801	-2.829165	-3.739179	H	-5.263162	-0.939233	1.887467
H	0.533898	-1.286159	-4.533839	C	-2.602119	-1.348193	2.755687
H	-0.610251	0.186947	-2.926108	H	-3.096638	-2.295174	2.529880
C	2.104609	-1.318176	0.643283	H	-1.530830	-1.452027	2.564727
C	3.443397	-0.996773	0.983116	H	-2.725817	-1.168004	3.831630
C	1.231326	-1.782031	1.639254	TS₃			
C	3.828702	-1.176160	2.326850	SCF done: -1425.562453			
C	1.641321	-1.945280	2.960714	Pd	0.057364	0.455204	-0.543400
H	0.221237	-2.049931	1.355861	P	-2.118765	-0.390801	0.216828
C	2.955603	-1.642891	3.308710	C	-2.221733	-0.046704	2.152263
H	4.845758	-0.933955	2.624908	C	-3.407003	0.756399	-0.717460
H	0.942942	-2.318976	3.706077	C	-2.682733	-2.256627	-0.091644
H	3.300786	-1.767500	4.332142	C	0.687940	-1.257458	-1.362626
Si	4.793507	-0.276983	-0.158935	C	1.663611	-2.066495	-0.740772
C	5.800463	0.958033	0.867867	C	2.194514	-3.154178	-1.462234
H	6.356430	0.487331	1.686523	C	1.803993	-3.427417	-2.772329
H	6.534793	1.462586	0.227454	C	0.863477	-2.604380	-3.391079
H	5.151523	1.727126	1.301439	C	0.312428	-1.529108	-2.686271
H	3.254472	1.229798	-1.375062	H	2.939930	-3.781114	-0.978454
C	5.966110	-1.665042	-0.704557	H	2.238907	-4.268087	-3.306291
H	6.823590	-1.254603	-1.252760	H	0.556332	-2.792007	-4.417323
H	6.356745	-2.221312	0.155807	H	-0.414766	-0.891787	-3.182523
H	5.466383	-2.382826	-1.365205	C	2.132339	-1.862624	0.669282
O	1.199435	1.795406	0.341577	C	2.867277	-0.720249	1.077272
C	1.186762	3.163733	-0.016392	C	1.861007	-2.883990	1.594919
C	2.548182	3.735831	0.432146	C	3.245145	-0.641243	2.430676
H	2.616414	4.812387	0.229154	C	2.258508	-2.781955	2.928570
H	2.683510	3.574934	1.507212	H	1.323901	-3.767390	1.260088
H	3.365644	3.232528	-0.092749	C	2.942844	-1.645006	3.353093
C	0.063707	3.922230	0.727014	H	3.804177	0.223559	2.776694
H	-0.921480	3.557892	0.404850	H	2.032022	-3.584443	3.626352
H	0.153320	3.759439	1.807256	H	3.253452	-1.543632	4.390049
H	0.094014	5.002653	0.534318	Si	3.533749	0.593220	-0.131821
C	1.017658	3.361567	-1.536959	C	4.315249	1.990680	0.875741
H	0.049522	2.965373	-1.868030	H	5.159711	1.644771	1.483130
H	1.065288	4.422880	-1.813713	H	4.697967	2.765560	0.200537
H	1.801582	2.827119	-2.082474	H	3.585600	2.467229	1.539679
C	4.136019	0.650102	-1.662629	H	1.285849	1.996084	-0.531403
H	4.903306	1.339369	-2.037602	C	4.895050	-0.220939	-1.170213
H	3.847593	-0.015323	-2.480575	H	5.342477	0.504312	-1.861311
C	-3.087100	-2.116909	-2.089823	H	5.696876	-0.618719	-0.536417
H	-3.155442	-3.166072	-2.406223	H	4.496430	-1.048822	-1.767049
H	-3.941212	-1.596125	-2.526899	O	0.337661	2.652993	0.198458
H	-2.165010	-1.710700	-2.512631	C	0.253196	4.013168	-0.212619
C	-4.407494	-2.689809	-0.042277	C	1.640246	4.679738	-0.060260
H	-5.283515	-2.112120	-0.346534	H	1.591647	5.754276	-0.277675
H	-4.515247	-3.694477	-0.473421	H	2.003734	4.551861	0.965101
H	-4.434722	-2.806859	1.043377	H	2.377003	4.236260	-0.737612
C	-3.223030	1.230639	-2.284455	C	-0.720911	4.754719	0.726449
H	-2.218703	1.650344	-2.171155	H	-1.739795	4.366438	0.642624
H	-3.153106	0.338060	-2.906938	H	-0.396002	4.635552	1.765846
H	-3.833768	1.963565	-2.828661	H	-0.752571	5.827557	0.496356
C	-3.919444	2.344700	-0.200152	C	-0.217517	4.146014	-1.675869
H	-2.919151	2.748081	-0.017505	H	-1.214978	3.713367	-1.807283
H	-4.438115	3.053121	-0.859348	H	-0.261713	5.196840	-1.989369
H	-4.467008	2.326849	0.744089	H	0.468246	3.621891	-2.351478
C	-5.325782	0.492426	-1.111222	C	2.187965	1.315044	-1.227120
H	-5.885486	1.282123	-1.630788	H	2.525779	2.269597	-1.659278
H	-5.392318	-0.404330	-1.731216	H	1.996436	0.689520	-2.103931
H	-5.843009	0.295184	-0.168990	C	-2.981053	-2.486214	-1.589946
C	-2.514991	1.108339	2.573781	H	-3.881824	-1.974917	-1.935211
H	-2.742603	1.169483	3.646715				

H	-2.140302	-2.199495	-2.224837	C	-1.699263	0.020570	-2.254682
H	-3.147143	-3.561336	-1.739312	H	-1.277536	-0.651089	-3.022536
C	-3.934007	-2.666543	0.716498	H	-1.912399	0.985235	-2.727118
H	-4.793634	-2.015003	0.550871	C	3.611854	1.659015	-1.671994
H	-4.226137	-3.677143	0.400325	H	2.661410	1.709176	-2.213900
H	-3.740068	-2.714914	1.790226	H	4.113336	2.627893	-1.795820
C	-1.542795	-3.231871	0.272766	H	4.247674	0.907479	-2.145818
H	-1.915652	-4.255541	0.130839	C	2.640687	2.651956	0.366397
H	-0.678477	-3.099427	-0.376064	H	1.648158	2.746173	-0.079980
H	-1.210376	-3.146074	1.306094	H	2.521221	2.655887	1.449880
C	-4.890030	0.351103	-0.608500	H	3.218526	3.547943	0.101313
H	-5.493151	1.121246	-1.108453	C	4.768633	1.327850	0.530100
H	-5.115174	-0.597421	-1.100626	H	5.359452	0.468344	0.204215
H	-5.236104	0.293235	0.426483	H	5.343949	2.232333	0.287824
C	-2.999368	0.807018	-2.209242	H	4.681339	1.288943	1.619138
H	-1.971271	1.166066	-2.325184	C	2.444915	-1.370587	-2.491251
H	-3.083623	-0.154717	-2.717295	H	2.828449	-0.453971	-2.938907
H	-3.662749	1.511874	-2.728173	H	2.765626	-2.209540	-3.124061
C	-3.257392	2.189959	-0.177299	H	1.347021	-1.334740	-2.544596
H	-2.212000	2.498874	-0.158644	C	4.465702	-1.789425	-1.046458
H	-3.803293	2.874084	-0.840761	H	4.725533	-2.664215	-1.658974
H	-3.676100	2.309926	0.824438	H	4.987149	-0.931433	-1.477811
C	-1.425370	1.237242	2.473131	H	4.867768	-1.962706	-0.044482
H	-1.422266	1.365538	3.564398	C	2.295253	-2.951367	-0.608913
H	-0.388519	1.181135	2.135145	H	2.666951	-3.310799	0.352861
H	-1.854398	2.138014	2.037688	H	1.203106	-2.889052	-0.558620
C	-3.653001	0.109666	2.705495	H	2.546551	-3.714825	-1.357407
H	-3.587086	0.243449	3.793867	C	3.563942	-1.407673	2.393103
H	-4.161577	0.991562	2.308728	H	3.479446	-1.635255	3.464877
H	-4.284949	-0.761709	2.524417	H	3.733090	-2.358065	1.880070
C	-1.515375	-1.188738	2.914965	H	4.454774	-0.787990	2.262472
H	-2.079173	-2.124321	2.910565	C	1.065802	-1.641523	2.175179
H	-0.507646	-1.380097	2.535396	H	1.146914	-2.596528	1.655761
H	-1.414003	-0.881998	3.964028	H	1.007180	-1.861754	3.249703
4				H	0.123403	-1.172746	1.880925
SCF done: -1191.932532				C	2.037792	0.532383	2.826136
Pd	-0.056401	0.154752	-1.006291	H	1.165218	1.110659	2.505752
P	2.227472	-0.148712	0.057821	H	1.846187	0.187319	3.850627
C	2.935333	-1.614675	-1.042999	H	2.904547	1.196679	2.869564
C	3.394855	1.409453	-0.163567	TS₄			
C	2.271696	-0.705095	1.931795	SCF done: -1191.923685			
C	-1.196785	1.584176	-0.178676	Pd	0.031399	0.380599	-0.842992
C	-2.136665	1.324391	0.840793	P	2.269176	-0.130332	-0.013733
C	-2.769090	2.420419	1.464755	C	3.344634	-0.835646	-1.499637
C	-2.516240	3.733680	1.076237	C	3.160960	1.466757	0.693377
C	-1.623074	3.977647	0.032305	C	2.201755	-1.488911	1.399938
C	-0.981973	2.907124	-0.596585	C	-1.526178	1.545653	-0.200521
H	-3.494595	2.221652	2.249914	C	-2.296069	1.127236	0.912516
H	-3.029044	4.555612	1.568954	C	-2.854903	2.111111	1.751667
H	-1.428439	4.994611	-0.300712	C	-2.686334	3.471479	1.504423
H	-0.300681	3.108613	-1.418088	C	-1.957307	3.878168	0.384993
C	-2.500778	-0.049557	1.306823	C	-1.402726	2.922613	-0.466717
C	-2.956188	-1.054872	0.415257	H	-3.452569	1.789797	2.601103
C	-2.435079	-0.320345	2.683651	H	-3.139728	4.205213	2.165505
C	-3.300014	-2.304311	0.959447	H	-1.826335	4.935674	0.167625
C	-2.785468	-1.569980	3.196195	H	-0.851459	3.246416	-1.344840
H	-2.086105	0.458835	3.356940	C	-2.541961	-0.308653	1.239651
C	-3.214817	-2.571778	2.328242	C	-2.989747	-1.219531	0.251322
H	-3.654907	-3.092937	0.300808	C	-2.374285	-0.751230	2.561768
H	-2.717261	-1.757130	4.265128	C	-3.242825	-2.545965	0.632252
H	-3.488914	-3.552038	2.710781	C	-2.632133	-2.076189	2.916308
Si	-3.219130	-0.725842	-1.442343	H	-2.022675	-0.050757	3.315069
C	-3.619864	-2.378614	-2.283788	C	-3.067335	-2.980825	1.948689
H	-4.530116	-2.847005	-1.891248	H	-3.590296	-3.259571	-0.111378
H	-3.774716	-2.216644	-3.357651	H	-2.487764	-2.398845	3.944552
H	-2.798276	-3.097717	-2.175731	H	-3.269616	-4.015482	2.214206
C	-4.720341	0.415696	-1.626920	Si	-3.273705	-0.608967	-1.513725
H	-4.941904	0.599014	-2.685774	C	-3.404097	-2.092047	-2.682377
H	-5.614128	-0.022822	-1.167175	H	-4.269285	-2.725705	-2.453159
H	-4.539720	1.385137	-1.149696	H	-3.515758	-1.752715	-3.719342

H	-2.505818	-2.718952	-2.633127	H	-6.527464	0.613583	1.302522
C	-4.875931	0.392341	-1.601211	C	-4.905293	-1.469641	0.367373
H	-5.051761	0.763277	-2.618601	H	-4.064509	-1.968139	-0.115997
H	-5.740963	-0.216415	-1.312956	H	-4.619739	-1.236633	1.398165
H	-4.835460	1.256976	-0.930200	H	-5.732155	-2.189169	0.401313
C	-1.800509	0.457131	-1.991744	C	-5.698781	-0.570427	-1.853546
H	-1.130244	-0.110700	-2.672872	H	-6.499368	-1.320550	-1.883051
H	-2.068680	1.381314	-2.505524	H	-6.037800	0.309234	-2.413049
C	3.528594	2.399376	-0.480252	H	-4.831829	-0.989835	-2.370288
H	2.668920	2.579148	-1.134417	Br	-1.722212	-0.575603	2.251999
H	3.841422	3.368605	-0.069859	P	2.943197	0.197824	-0.109285
H	4.358486	2.023037	-1.083192	C	3.733464	-0.585600	-1.730287
C	2.134897	2.248923	1.547114	C	3.089414	2.154047	-0.243842
H	1.242282	2.499978	0.967295	C	4.004549	-0.384782	1.437031
H	1.814916	1.711521	2.439904	C	2.573571	2.602757	-1.628216
H	2.601869	3.186704	1.878817	H	1.589902	2.177208	-1.852543
C	4.425924	1.205007	1.534033	H	2.469534	3.696101	-1.625434
H	5.193654	0.655629	0.983160	H	3.256876	2.348185	-2.441351
H	4.863063	2.168872	1.829971	C	2.115342	2.769443	0.789284
H	4.210653	0.657061	2.455173	H	1.105254	2.362360	0.673117
C	3.034718	0.014597	-2.755300	H	2.421412	2.608129	1.823176
H	3.367895	1.049302	-2.672123	H	2.067861	3.855189	0.627186
H	3.551440	-0.429460	-3.617313	C	4.494817	2.748726	-0.027176
H	1.960877	0.025476	-2.972008	H	5.232904	2.358638	-0.732914
C	4.869274	-0.864193	-1.276198	H	4.448380	3.837292	-0.171665
H	5.349555	-1.333259	-2.146428	H	4.869374	2.577597	0.985114
H	5.296961	0.137267	-1.178923	C	2.679998	-0.487643	-2.859076
H	5.156836	-1.443423	-0.395129	H	2.484468	0.535970	-3.180366
C	2.868140	-2.265872	-1.834391	H	3.049259	-1.040505	-3.734125
H	3.160203	-3.002228	-1.082482	H	1.729140	-0.931543	-2.546272
H	1.781637	-2.311795	-1.964756	C	5.054560	0.044091	-2.211276
H	3.328204	-2.573397	-2.782953	H	5.413411	-0.505838	-3.092594
C	3.529606	-2.207069	1.708917	H	4.934178	1.087192	-2.514204
H	3.370348	-2.906773	2.541151	H	5.843814	-0.001627	-1.456615
H	3.894275	-2.796547	0.863747	C	3.959941	-2.095105	-1.498922
H	4.323661	-1.518991	2.011484	H	4.785286	-2.304911	-0.814392
C	1.135780	-2.533544	0.993989	H	3.055371	-2.583299	-1.121419
H	1.422665	-3.127701	0.125878	H	4.212791	-2.561641	-2.460568
H	0.988115	-3.228703	1.831552	C	5.534614	-0.364474	1.254626
H	0.174555	-2.057166	0.778859	H	6.011929	-0.650198	2.202482
C	1.679382	-0.837354	2.698448	H	5.875569	-1.077432	0.499433
H	0.749272	-0.286128	2.528988	H	5.914515	0.623890	0.983992
H	1.460687	-1.633714	3.422122	C	3.555131	-1.818885	1.805171
H	2.407875	-0.170083	3.164874	H	3.797110	-2.558542	1.041454
1_C				H	4.065360	-2.121203	2.730206
SCF done: -1239.920202				H	2.475030	-1.853896	1.980617
Pd	0.690605	-0.479473	0.128094	C	3.639372	0.489990	2.656045
C	-1.424586	-1.116134	0.392375	H	2.555496	0.546885	2.801088
C	-2.182563	-0.504272	-0.655192	H	4.070356	0.031728	3.556171
C	-2.169495	-1.131418	-1.905043	H	4.039636	1.504439	2.591418
C	-1.513749	-2.352561	-2.125723	C	-5.368433	-0.201218	-0.385836
C	-0.806195	-2.956268	-1.095891	TS1_c			
C	-0.743541	-2.344995	0.174542	SCF done: -1239.912262			
H	-2.694433	-0.650014	-2.724311	Pd	0.499658	-0.529404	0.009343
H	-1.557910	-2.816487	-3.106989	C	-1.354899	-1.398515	-0.181329
H	-0.309263	-3.910863	-1.245940	C	-2.308425	-0.735708	-0.994640
H	-0.328772	-2.887116	1.017131	C	-2.797149	-1.447251	-2.100582
C	-2.910393	0.794809	-0.469363	C	-2.436548	-2.773320	-2.353839
C	-4.321159	0.949982	-0.363800	C	-1.558658	-3.431565	-1.492506
C	-2.081113	1.931449	-0.441191	C	-1.033188	-2.756407	-0.388152
C	-4.798172	2.271357	-0.261265	H	-3.486597	-0.938693	-2.770145
C	-2.587988	3.221000	-0.329279	H	-2.852226	-3.290646	-3.213972
H	-1.008366	1.773574	-0.517148	H	-1.290082	-4.470781	-1.663982
C	-3.966298	3.388312	-0.245173	H	-0.395467	-3.271908	0.321731
H	-5.863874	2.444965	-0.184759	Br	-1.265137	-0.783678	1.979287
H	-1.916067	4.074822	-0.312222	C	-2.703073	0.701043	-0.811056
H	-4.401469	4.381022	-0.162120	C	-3.924110	1.166576	-0.261514
C	-6.694672	0.231983	0.289090	C	-1.765507	1.633946	-1.301986
H	-7.234459	0.994678	-0.281590	C	-4.121239	2.564261	-0.258243
H	-7.359157	-0.635900	0.361690	C	-1.989422	3.004689	-1.275181

H	-0.843292	1.246447	-1.726510	H	0.798824	-3.447089	0.942888
C	-3.191028	3.473097	-0.748102	Br	0.208856	-1.894304	-1.843981
H	-5.044416	2.960185	0.152001	C	2.613158	0.882851	0.839338
H	-1.242545	3.690642	-1.665726	C	3.354242	1.525402	-0.192253
H	-3.406350	4.538053	-0.715288	C	1.787763	1.652955	1.683084
C	-5.264840	0.791567	1.839514	C	3.203521	2.921942	-0.293486
H	-5.495199	1.858060	1.921816	C	1.666803	3.034952	1.555598
H	-6.091842	0.236984	2.299532	H	1.266589	1.141837	2.488067
H	-4.357864	0.597218	2.422014	C	2.386132	3.672202	0.550716
C	-4.875418	-1.195500	0.412945	H	3.747466	3.457106	-1.061325
H	-4.856728	-1.646387	-0.581424	H	1.034652	3.597342	2.237770
H	-3.961017	-1.479647	0.939225	H	2.322867	4.749404	0.419661
H	-5.719637	-1.636353	0.957264	C	4.560029	1.655742	-2.450609
C	-6.380940	0.595286	-0.423608	H	5.084296	2.600657	-2.271943
H	-7.208054	0.024859	0.016679	H	5.178398	1.079536	-3.147140
H	-6.668812	1.651365	-0.421590	H	3.609956	1.875893	-2.950526
H	-6.273829	0.280564	-1.468440	C	3.884129	-0.574693	-1.619112
P	2.798638	0.223696	-0.034141	H	3.863402	-1.302862	-0.808506
C	3.689341	-0.418457	-1.659688	H	2.884962	-0.545367	-2.063810
C	2.929617	2.180874	0.014568	H	4.581676	-0.950155	-2.377715
C	3.750407	-0.500591	1.523170	C	5.726351	0.702514	-0.459219
C	2.523343	2.755745	-1.359858	H	6.463210	0.277256	-1.152319
H	1.564858	2.353222	-1.703530	H	6.093382	1.683199	-0.133609
H	2.406089	3.843059	-1.260884	H	5.677683	0.048355	-0.415501
H	3.272658	2.584168	-2.136063	P	-2.529728	0.277089	0.036925
C	1.869328	2.695917	1.017106	C	-3.137853	0.560953	1.878275
H	0.866808	2.343090	0.754815	C	-2.532967	1.991094	-0.905331
H	2.068015	2.400513	2.047333	C	-3.788367	-0.933635	-0.850067
H	1.862753	3.794229	0.986827	C	-1.839049	3.061646	-0.036973
C	4.310292	2.752182	0.391741	H	-0.846350	2.743971	0.295575
H	5.103152	2.415826	-0.281379	H	-1.700224	3.962681	-0.649013
H	4.272310	3.848816	0.330380	H	-2.427644	3.356816	0.835268
H	4.603684	2.501556	1.414369	C	-1.644282	1.821901	-2.161305
C	2.706794	-0.223102	-2.838857	H	-0.642315	1.469821	-1.898193
H	2.509614	0.823958	-3.070722	H	-2.055653	1.127653	-2.893884
H	3.137432	-0.682797	-3.739023	H	-1.543964	2.799671	-2.652030
H	1.747422	-0.712478	-2.636536	C	-3.918988	2.522076	-1.319685
C	5.036283	0.246631	-2.004826	H	-4.587823	2.662908	-0.466118
H	5.457342	-0.237438	-2.897171	H	-3.793368	3.501211	-1.802196
H	4.932755	1.309162	-2.239894	H	-4.419718	1.872807	-2.041695
H	5.772648	0.146946	-1.203099	C	-1.927487	1.098096	2.677953
C	3.909038	-1.942478	-1.547071	H	-1.560527	2.062771	2.327411
H	4.695928	-2.209662	-0.838218	H	-2.216348	1.214340	3.731487
H	2.989045	-2.464993	-1.264785	H	-1.090382	0.386870	2.651422
H	4.217047	-2.324714	-2.529394	C	-4.332046	1.517537	2.057305
C	5.289176	-0.465792	1.447775	H	-4.602199	1.560132	3.121775
H	5.701671	-0.855288	2.388903	H	-4.101531	2.538688	1.744284
H	5.683840	-1.092556	0.643854	H	-5.217604	1.186734	1.509224
H	5.683699	0.545166	1.315159	C	-3.489484	-0.796034	2.526735
C	3.281728	-1.961305	1.723011	H	-4.416826	-1.228410	2.145718
H	3.598704	-2.632487	0.924035	H	-2.686214	-1.529550	2.399540
H	3.709894	-2.342325	2.660279	H	-3.625025	-0.641029	3.605451
H	2.191010	-2.014938	1.802343	C	-5.277343	-0.647003	-0.569881
C	3.298339	0.260911	2.788223	H	-5.885065	-1.354402	-1.150605
H	2.207652	0.292493	2.875303	H	-5.545654	-0.786128	0.480498
H	3.684565	-0.268904	3.669176	H	-5.580356	0.360232	-0.867692
H	3.685682	1.281252	2.833069	C	-3.453320	-2.377957	-0.405431
C	-5.075300	0.332441	0.369478	H	-3.628287	-2.557112	0.655954
2_c				H	-4.100624	-3.069087	-0.962226
SCF done: -1239.928946				H	-2.415423	-2.633011	-0.636578
Pd	-0.167152	-0.663207	0.285294	C	-3.561469	-0.895574	-2.377717
C	1.564667	-1.429381	0.891673	H	-2.515593	-1.075194	-2.640503
C	2.647569	-0.580224	1.187663	H	-4.157230	-1.700305	-2.828680
C	3.702120	-1.097566	1.959353	H	-3.892446	0.039887	-2.834787
C	3.720256	-2.434500	2.358104	C	4.349284	0.825022	-1.159501
C	2.671990	-3.282243	1.996341	TS2_c			
C	1.601792	-2.783268	1.247955	SCF done: -1239.865363			
H	4.510516	-0.433625	2.254546	Pd	0.226188	0.527065	-0.621748
H	4.552746	-2.811808	2.946161	C	1.049563	-1.151775	-1.348339
H	2.685804	-4.329668	2.287675	C	2.087014	-1.785283	-0.640532

C	2.664998	-2.943737	-1.191841	C	3.316382	1.032725	-0.122124
C	2.252900	-3.442552	-2.428021	3_c			
C	1.248920	-2.782740	-3.136925	SCF done: -1459.776539			
C	0.656017	-1.633023	-2.600883	Pd	0.185398	0.749612	-0.198006
H	3.461486	-3.442561	-0.644626	P	2.382591	-0.298144	-0.149560
H	2.723817	-4.331416	-2.839219	C	2.582426	-1.226018	-1.871620
H	0.927506	-3.152383	-4.107823	C	3.542749	1.293618	-0.175178
H	-0.113227	-1.114836	-3.166378	C	3.030805	-1.478427	1.282085
C	2.514773	-1.311282	0.710714	C	-0.671225	0.019066	1.454304
C	2.977153	0.003741	0.987232	C	-1.679760	-0.966996	1.419044
C	2.413735	-2.245647	1.755673	C	-2.223287	-1.391397	2.648556
C	3.259106	0.310477	2.329497	C	-1.837163	-0.836128	3.866018
C	2.717463	-1.916999	3.075262	C	-0.871600	0.169678	3.880289
H	2.065004	-3.247012	1.518323	C	-0.294709	0.589344	2.678766
C	3.127590	-0.619282	3.362526	H	-2.977982	-2.174196	2.629564
H	3.604170	1.302769	2.590718	H	-2.287890	-1.184962	4.791343
H	2.622569	-2.661151	3.861721	H	-0.561583	0.627733	4.816540
H	3.358850	-0.324303	4.382950	H	0.452669	1.375957	2.700705
C	3.578064	2.438985	0.465599	C	-2.131692	-1.716024	0.186915
H	4.441812	2.453338	1.138409	C	-3.273527	-1.451713	-0.612853
H	3.800064	3.135559	-0.349778	C	-1.364165	-2.867556	-0.086151
H	2.709616	2.828858	1.007151	C	-3.514979	-2.338635	-1.685339
H	0.884441	2.313854	-0.913575	C	-1.643220	-3.733866	-1.136438
C	4.639801	0.560173	-0.788754	H	-0.535533	-3.088910	0.576468
H	4.940657	1.263290	-1.575384	C	-2.730463	-3.451562	-1.959931
H	5.451422	0.504003	-0.052813	H	-4.369577	-2.154219	-2.327467
H	4.522385	-0.428276	-1.244019	H	-1.027502	-4.614648	-1.300681
C	2.245424	1.179058	-1.243664	H	-2.979935	-4.098704	-2.797077
H	2.367732	2.172815	-1.697870	C	-4.338946	0.536228	-1.737725
H	2.433420	0.496558	-2.070852	H	-4.564861	-0.053451	-2.632418
Br	-0.012888	3.593045	-0.570383	H	-5.106085	1.316714	-1.656097
P	-2.017823	-0.372635	0.244535	H	-3.367489	1.021514	-1.869720
C	-2.170077	0.185729	2.121165	H	-3.132923	1.143395	0.644658
C	-3.433975	0.511449	-0.796803	C	-5.720477	-0.970843	-0.239125
C	-2.356078	-2.311387	0.169398	H	-6.479129	-0.186859	-0.125002
C	-2.596052	-2.748883	-1.292630	H	-6.024710	-1.604652	-1.078132
H	-2.642766	-3.845741	-1.314847	H	-5.735133	-1.587498	0.667758
H	-3.537022	-2.381433	-1.706169	O	-1.290839	1.977980	-0.780656
H	-1.776777	-2.449146	-1.950354	C	-1.360694	3.366765	-0.502043
C	-3.550494	-2.785103	1.023849	C	-2.676407	3.879230	-1.125341
H	-4.485328	-2.275775	0.782976	H	-2.780324	4.964467	-0.998305
H	-3.705132	-3.856829	0.837913	H	-2.698438	3.652509	-2.196882
H	-3.364883	-2.673134	2.094465	H	-3.536665	3.391955	-0.657230
C	-3.000893	0.452994	-2.281392	C	-0.179409	4.114300	-1.156630
H	-2.036508	0.950168	-2.430577	H	0.769906	3.799979	-0.707182
H	-2.922497	-0.563948	-2.669377	H	-0.144197	3.893346	-2.230099
H	-3.748217	0.981249	-2.888822	H	-0.263598	5.201814	-1.032303
C	-3.515632	2.009033	-0.432080	C	-1.369748	3.656017	1.011003
H	-2.549695	2.510678	-0.515539	H	-0.429714	3.332626	1.471738
H	-4.196925	2.495321	-1.143218	H	-1.492297	4.728945	1.206852
H	-3.919294	2.185817	0.567430	H	-2.187730	3.119944	1.501886
C	-4.850559	-0.081492	-0.651952	C	-4.095765	0.639323	0.730860
H	-5.543485	0.527147	-1.248862	H	-4.883137	1.403699	0.710169
H	-4.929985	-1.105828	-1.021584	H	-4.152410	0.136762	1.700015
H	-5.210755	-0.060225	0.380255	C	3.246424	-0.668042	2.578943
C	-1.513892	1.577977	2.252740	H	3.455580	-1.376992	3.390870
H	-1.563715	1.888548	3.305193	H	4.098647	0.011814	2.522751
H	-0.456841	1.546749	1.969036	H	2.355047	-0.103767	2.864294
H	-1.997908	2.351592	1.657620	C	4.340808	-2.223924	0.952724
C	-1.094720	-3.070702	0.638325	H	5.165958	-1.550946	0.710007
H	-0.232490	-2.842155	0.012400	H	4.641093	-2.803237	1.836422
H	-0.826523	-2.870852	1.675093	H	4.226004	-2.934092	0.130972
H	-1.294767	-4.147844	0.553963	C	3.089985	2.236884	0.965117
C	-3.606866	0.251022	2.677434	H	2.024427	2.474486	0.884617
H	-3.559607	0.550466	3.733582	H	3.271178	1.829869	1.960008
H	-4.224900	0.991187	2.163945	H	3.653750	3.176253	0.887493
H	-4.123226	-0.710510	2.636551	C	3.312611	2.067394	-1.492387
C	-1.336805	-0.757201	3.015893	H	2.253161	2.271595	-1.676806
H	-1.793295	-1.741589	3.139923	H	3.818511	3.038985	-1.416728
H	-0.314625	-0.885235	2.646397	H	3.725567	1.557932	-2.365143
H	-1.267930	-0.307458	4.015263				

C	5.053771	1.026858	-0.030989	H	0.815740	3.271199	-2.464582
H	5.587757	1.981901	-0.130416	C	2.407179	1.077515	-1.031125
H	5.318036	0.616798	0.946476	H	2.789451	1.981508	-1.531340
H	5.442296	0.356081	-0.800496	H	2.258272	0.391833	-1.866645
C	1.687595	-0.501567	-2.906903	C	-2.796599	-2.689252	-1.312208
H	1.731890	-1.056406	-3.853811	H	-3.711651	-2.260263	-1.723791
H	0.639779	-0.481656	-2.586717	H	-1.961177	-2.452791	-1.973248
H	2.001342	0.521800	-3.118278	H	-2.920148	-3.780339	-1.324947
C	1.934897	-2.516015	1.606618	C	-3.750310	-2.643947	0.998798
H	1.007748	-2.032903	1.922035	H	-4.637136	-2.046364	0.779428
H	1.715271	-3.182984	0.772625	H	-4.000951	-3.691392	0.783370
H	2.286970	-3.141085	2.438498	H	-3.548067	-2.581667	2.070330
C	4.021344	-1.313778	-2.419629	C	-1.327535	-3.121703	0.620272
H	4.005585	-1.901504	-3.347615	H	-1.651888	-4.171499	0.636903
H	4.441258	-0.337136	-2.670765	H	-0.484730	-3.044911	-0.065509
H	4.707146	-1.813555	-1.731112	H	-0.975284	-2.871607	1.620085
C	2.019554	-2.658789	-1.758069	C	-4.829278	0.143377	-0.734167
H	2.644075	-3.317858	-1.150592	H	-5.460463	0.813315	-1.334038
H	0.999883	-2.669197	-1.365512	H	-4.990371	-0.868125	-1.112391
H	1.983273	-3.092218	-2.766385	H	-5.198185	0.187604	0.293573
C	-4.326635	-0.323264	-0.448037	C	-2.917983	0.513958	-2.336093
TS_{3_c}				H	-1.919926	0.943368	-2.472674
SCF done: -1459.732158				H	-2.904998	-0.508470	-2.716360
Pd	0.178700	0.418390	-0.522522	H	-3.619146	1.087958	-2.956936
P	-2.050468	-0.344501	0.230486	C	-3.316912	2.110900	-0.492415
C	-2.230406	0.228230	2.109965	H	-2.291899	2.483208	-0.461547
C	-3.366854	0.615989	-0.859978	H	-3.859687	2.679105	-1.259634
C	-2.520229	-2.262799	0.145993	C	-3.794879	2.325004	0.466376
C	0.770262	-1.306157	-1.342061	C	-1.598047	1.626058	2.292750
C	1.823212	-2.017918	-0.731691	H	-1.531552	1.822091	3.371672
C	2.371799	-3.125356	-1.402942	H	-0.597647	1.718456	1.865592
C	1.929364	-3.498990	-2.672637	H	-2.205598	2.422226	1.861782
C	0.923517	-2.759130	-3.292747	C	-3.677883	0.296659	2.639348
C	0.349965	-1.668084	-2.627954	H	-3.640362	0.599520	3.694768
H	3.171300	-3.683805	-0.921220	H	-4.275302	1.048597	2.116675
H	2.377754	-4.351256	-3.176279	H	-4.208573	-0.654933	2.594408
H	0.580773	-3.023868	-4.290388	C	-1.413832	-0.742679	2.990320
H	-0.426954	-1.095778	-3.127340	H	-1.873651	-1.729544	3.076497
C	2.314232	-1.677676	0.644051	H	-0.386295	-0.862257	2.632456
C	2.982317	-0.471610	0.992901	H	-1.360501	-0.324433	4.003643
C	2.070540	-2.645946	1.633272	C	3.498082	0.552624	-0.052602
C	3.288303	-0.287967	2.353251	4_c			
C	2.408785	-2.444873	2.969730	SCF done: -1226.105529			
H	1.588059	-3.572845	1.336250	Pd	-0.166620	-0.061694	-0.962574
C	3.003130	-1.240842	3.332048	P	2.139054	-0.170528	0.061232
H	3.777485	0.623258	2.671879	C	3.454236	0.392075	-1.279999
H	2.201831	-3.213281	3.710119	C	2.447456	0.846523	1.706277
H	3.264538	-1.040923	4.368139	C	2.409186	-2.075401	0.439928
C	4.126790	1.789051	0.629009	C	-1.201668	1.511304	-0.293276
H	4.987775	1.524778	1.252567	C	-2.242453	1.317161	0.634519
H	4.489729	2.476897	-0.142395	C	-2.824991	2.444871	1.244789
H	3.399180	2.331510	1.241045	C	-2.422229	3.738063	0.913727
H	1.502806	1.863671	-0.417185	C	-1.423804	3.923046	-0.043920
C	4.624996	-0.134234	-0.871227	C	-0.822428	2.813281	-0.647505
H	5.041956	0.572037	-1.600077	H	-3.629005	2.296423	1.961811
H	5.440415	-0.467996	-0.217252	H	-2.897243	4.593487	1.387074
H	4.250939	-1.002673	-1.420635	H	-1.110103	4.926378	-0.323576
O	0.562868	2.606553	0.179221	H	-0.042966	2.969144	-1.388009
C	0.463156	3.904329	-0.401449	C	-2.727478	-0.045501	1.007680
C	1.819358	4.631374	-0.261640	C	-3.178844	-1.002724	0.057520
H	1.752990	5.667945	-0.615451	C	-2.741443	-0.367971	2.373690
H	2.129917	4.645805	0.788711	C	-3.601821	-2.246626	0.549583
H	2.602754	4.130853	-0.839636	C	-3.163864	-1.614372	2.834765
C	-0.587400	4.712613	0.384925	H	-2.392104	0.377747	3.083173
H	-1.583232	4.269601	0.297456	C	-3.592047	-2.561583	1.910922
H	-0.319879	4.736438	1.446863	H	-3.962500	-3.000501	-0.139808
H	-0.645775	5.746054	0.019969	H	-3.153045	-1.837142	3.898661
C	0.073032	3.839205	-1.892356	H	-3.927619	-3.542531	2.238451
H	-0.897476	3.347702	-2.019735	C	-3.871537	-1.853733	-2.260041
H	0.005087	4.842312	-2.332413	H	-4.896589	-2.086736	-1.946228

H	-3.905474	-1.578095	-3.319969	H	-3.327123	4.185742	1.957101
H	-3.269558	-2.766029	-2.177995	H	-1.876494	4.897071	0.056306
C	-4.225396	0.520928	-1.672731	H	-0.797305	3.196742	-1.379109
H	-4.351230	0.699402	-2.747783	C	-2.702292	-0.338465	0.993370
H	-5.213820	0.304277	-1.249414	C	-3.002511	-1.205663	-0.088808
H	-3.857627	1.442945	-1.221944	C	-2.663820	-0.846961	2.299753
C	-1.867912	-0.390721	-2.069319	C	-3.232247	-2.556829	0.200312
H	-1.474051	-1.316627	-2.531133	C	-2.898743	-2.196478	2.563976
H	-1.946068	0.367363	-2.857098	H	-2.423164	-0.170188	3.115612
C	2.586993	2.346481	1.365917	C	-3.178350	-3.055720	1.505306
H	1.747718	2.709376	0.765250	H	-3.468922	-3.246660	-0.601674
H	2.583342	2.912444	2.306841	H	-2.854985	-2.568707	3.584273
H	3.522009	2.584119	0.853613	H	-3.360966	-4.112107	1.685489
C	1.176997	0.728367	2.580612	C	-3.352266	-1.764787	-2.564401
H	0.291323	1.078491	2.044507	H	-4.273490	-2.335277	-2.397223
H	0.983399	-0.285444	2.930878	H	-3.420753	-1.320483	-3.563764
H	1.308661	1.362397	3.468124	H	-2.507992	-2.463947	-2.565984
C	3.677112	0.410984	2.526666	C	-4.450179	0.226922	-1.559458
H	4.609979	0.482919	1.961247	H	-4.615469	0.601907	-2.577224
H	3.771835	1.070870	3.400147	H	-5.324529	-0.368406	-1.271573
H	3.586708	-0.609726	2.906017	H	-4.388210	1.085762	-0.887652
C	2.947379	1.721496	-1.888882	C	-1.932016	0.188985	-1.966102
H	2.935867	2.547785	-1.177884	H	-1.292112	-0.424417	-2.632628
H	3.612105	2.008605	-2.715273	H	-2.229460	1.070751	-2.535565
H	1.935441	1.604833	-2.291325	C	2.929416	2.581356	0.575298
C	4.900060	0.574794	-0.778993	H	2.102762	2.839313	-0.094434
H	5.543004	0.841150	-1.629536	H	3.017896	3.387722	1.315271
H	4.990286	1.380972	-0.046972	H	3.859797	2.569595	0.002112
H	5.309695	-0.336124	-0.334383	C	1.448377	1.530776	2.243485
C	3.464854	-0.619807	-2.446741	H	0.563037	1.804208	1.663728
H	3.910761	-1.580769	-2.180759	H	1.188374	0.684420	2.879570
H	2.458571	-0.795884	-2.843290	H	1.697026	2.372274	2.904626
H	4.066654	-0.200698	-3.264010	C	3.891587	0.926499	2.194396
C	3.871167	-2.541860	0.574673	H	4.790293	0.733546	1.602899
H	3.885898	-3.612328	0.823119	H	4.107553	1.785151	2.845369
H	4.438404	-2.421343	-0.352048	C	3.722762	0.066584	2.847840
H	4.406046	-2.015809	1.370051	C	3.069239	1.084761	-2.384708
C	1.719006	-2.863727	-0.700303	H	3.239286	2.061984	-1.932202
H	2.176308	-2.713258	-1.678520	H	3.691080	1.029057	-3.288884
H	1.772012	-3.937667	-0.475476	H	2.017873	1.033888	-2.687992
H	0.654177	-2.602239	-0.770987	C	4.925902	0.021810	-1.060802
C	1.645056	-2.457104	1.726742	H	5.541776	-0.024694	-1.969872
H	0.603308	-2.122116	1.697534	H	5.153024	0.971499	-0.569711
H	1.636315	-3.551932	1.812655	H	5.253589	-0.788007	-0.403991
H	2.113423	-2.069573	2.634233	C	3.252047	-1.373030	-2.298586
C	-3.265840	-0.678696	-1.452973	H	3.609199	-2.274754	-1.796322
TS_{4c}				H	2.204307	-1.522722	-2.582206
SCF done: -1226.099998				H	3.831511	-1.268585	-3.225518
Pd	-0.099751	0.244715	-0.868392	C	3.650774	-2.439560	1.123101
P	2.149282	-0.117606	0.024732	H	3.573797	-3.383050	1.681191
C	3.440489	-0.094752	-1.453588	H	4.163196	-2.667208	0.184407
C	2.662921	1.257960	1.325062	H	4.289044	-1.768676	1.703617
C	2.236138	-1.869987	0.902450	C	1.410845	-2.864445	0.050814
C	-1.577608	1.510718	-0.274761	H	1.833079	-3.043708	-0.938729
C	-2.437695	1.105310	0.764884	H	1.378376	-3.830457	0.573286
C	-3.045950	2.085027	1.569842	H	0.379813	-2.515849	-0.073151
C	-2.839425	3.443300	1.330942	C	1.515214	-1.791665	2.265529
C	-2.030875	3.840398	0.262743	H	0.512551	-1.362670	2.171829
C	-1.419162	2.879544	-0.546450	H	1.399511	-2.812125	2.654423
H	-3.714218	1.772005	2.368523	H	2.075605	-1.225192	3.012905
				C	-3.165076	-0.642379	-1.516915