

Supporting Information For

Exploring the Reaction Mechanism of A Cationic Terminal Iridium Methylene Complex with Ethyl Diazoacetate, Lewis Base and Dihydrogen: A Quantum Chemistry Study

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Cartesian coordinates and electronic energies for all of the calculated structures

1				C	-3.747809	-2.098084	-1.339496
SCF done: -1185.94014				H	-4.457686	-2.259156	-0.521734
Ir	-0.000021	-0.553969	-0.057510	H	-2.866668	-2.727973	-1.170493
N	0.000011	1.580063	-0.146263	H	-4.228785	-2.430061	-2.266648
O	2.315699	1.584920	-0.167455	C	-3.131868	-0.343045	1.686342
O	-2.315689	1.584918	-0.167538	C	-4.613799	0.020482	1.664080
P	2.253236	-0.180535	0.005748	H	-4.992790	0.030659	2.692932
P	-2.253225	-0.180526	0.005734	H	-5.205294	-0.709324	1.103946
C	1.159641	2.265099	-0.186067	H	-4.776021	1.013452	1.234128
C	1.204854	3.655892	-0.249900	C	-2.921979	-1.786626	2.156079
H	2.166479	4.150404	-0.276301	H	-1.854561	-2.019908	2.212055
C	0.000004	4.345432	-0.280611	H	-3.395999	-2.514945	1.490230
H	0.000004	5.429283	-0.330983	H	-3.365241	-1.904472	3.151689
C	-1.204844	3.655886	-0.249937	C	-2.381890	0.604490	2.631235
H	-2.166473	4.150390	-0.276375	H	-2.738624	0.436889	3.653856
C	-1.159621	2.265095	-0.186104	H	-2.562598	1.651288	2.370876
C	3.361360	-0.622740	-1.476160	H	-1.303992	0.413412	2.596173
C	2.452982	-0.438017	-2.699495	C	-0.000050	-2.638644	-0.098326
H	3.010864	-0.715135	-3.601363	H	0.874931	-3.117150	0.363394
H	2.136294	0.605728	-2.798184	H	-0.000883	-2.970196	-1.152258
H	5.353728	0.076259	-0.873934	C	4.594031	0.269052	-1.632285
C	3.131710	-0.343169	1.686432	H	4.320891	1.326788	-1.593927
C	4.613633	0.020404	1.664356	H	5.047338	0.070088	-2.610668
H	4.992516	0.030495	2.693247	H	1.553517	-1.055610	-2.624020
H	4.775854	1.013423	1.234516	C	3.748145	-2.097934	-1.339490
H	5.205217	-0.709320	1.104210	H	4.457832	-2.259064	-0.521577
C	2.381601	0.604243	2.631338	H	2.867043	-2.727963	-1.170814
H	2.738332	0.436653	3.653960	H	4.229388	-2.429717	-2.266574
H	1.303728	0.413030	2.596234	H	-0.874233	-3.117230	0.364815
H	2.562185	1.651076	2.371027	TS₁₂			
C	2.921795	-1.786804	2.155997	SCF done: -4853.736400			
H	3.364926	-1.904737	3.151657	Ir	-3.820378	-0.784263	0.255842
H	3.395933	-2.515048	1.490149	N	-4.165313	-2.800101	-0.374741
H	1.854374	-2.020115	2.211804	O	-5.325557	-2.039190	-2.225884
C	-3.361158	-0.622860	-1.476273	O	-3.109096	-3.580564	1.529954
C	-4.593877	0.268831	-1.632551	P	-5.016640	-0.381128	-1.694868
H	-5.047078	0.069832	-2.610976	P	-2.728501	-1.910465	1.968381
H	-4.320814	1.326590	-1.594184	C	-4.854789	-3.062767	-1.503528
H	-5.353642	0.076004	-0.874275	C	-5.103948	-4.358664	-1.943357
C	-2.452687	-0.438132	-2.699531	H	-5.650158	-4.506605	-2.864844
H	-3.010495	-0.715304	-3.601428	C	-4.633373	-5.409068	-1.166075
H	-1.553197	-1.055677	-2.623967	H	-4.808475	-6.432245	-1.481722
H	-2.136050	0.605628	-2.798220				

C	-3.947820	-5.161072	0.014515	C	-3.183319	4.119799	0.914081
H	-3.571474	-5.946987	0.654822	C	-3.248759	5.028094	1.981694
C	-3.741652	-3.834153	0.382031	C	-4.208862	4.139401	-0.050855
C	-4.115404	0.203879	-3.259316	C	-4.309447	5.922525	2.082492
C	-2.849155	-0.662918	-3.325353	H	-2.449133	5.054303	2.713386
H	-2.214705	-0.299548	-4.141841	C	-5.270036	5.023133	0.060076
H	-3.091833	-1.711127	-3.523880	H	-4.165761	3.433635	-0.875994
H	-5.746519	0.765923	-4.599847	C	-5.323282	5.919050	1.130076
C	-6.834804	0.183533	-1.577656	H	-4.337840	6.628167	2.905863
C	-7.723740	-0.387578	-2.684085	H	-6.059263	5.014145	-0.685160
H	-8.763817	-0.122390	-2.461678	H	-6.151629	6.614835	1.215159
H	-7.651128	-1.476436	-2.728566	C	-1.185013	2.927413	1.936449
H	-7.482356	0.016721	-3.667901	C	0.205294	3.030243	1.781172
C	-7.321432	-0.344120	-0.219826	C	-1.704170	2.634336	3.212774
H	-8.370172	-0.056401	-0.084630	C	1.057218	2.811994	2.857745
H	-6.727082	0.059950	0.604813	H	0.620737	3.306850	0.821585
H	-7.260053	-1.436837	-0.173714	C	-0.848802	2.387951	4.276400
C	-6.883161	1.714007	-1.579219	H	-2.779685	2.578068	3.351343
H	-7.891631	2.035016	-1.295072	C	0.537360	2.465289	4.100305
H	-6.671779	2.127180	-2.570090	H	2.126640	2.918227	2.717466
H	-6.182797	2.147154	-0.855649	H	-1.260001	2.129614	5.247384
C	-0.839272	-2.023164	1.891205	H	1.211531	2.255430	4.925703
C	-0.276458	-3.147467	2.758612	B	4.383797	-0.175667	-0.330961
H	0.779085	-3.282839	2.508783	C	3.968337	1.172100	-1.181289
H	-0.801856	-4.089085	2.572646	C	2.977657	2.076606	-0.835265
H	-0.327517	-2.908804	3.824563	C	2.567218	3.127482	-1.644747
C	-0.535813	-2.322076	0.417535	C	3.122214	3.278074	-2.902386
H	0.547440	-2.441353	0.320228	C	4.110150	2.389909	-3.309813
H	-0.859251	-1.504528	-0.233047	C	4.503600	1.371349	-2.453041
H	-1.012742	-3.248707	0.081070	C	3.665280	-1.344432	-1.241678
C	-0.253155	-0.650995	2.259672	C	4.300889	-2.262448	-2.070157
H	-0.093375	-0.541676	3.336172	C	3.617956	-3.092042	-2.957966
H	-0.900797	0.171015	1.928392	C	2.240975	-3.003413	-3.066809
H	0.712532	-0.521054	1.759694	C	1.563100	-2.089794	-2.272333
C	-3.430258	-1.931473	3.733810	C	2.280752	-1.308555	-1.382560
C	-3.262656	-3.286796	4.425160	C	5.998399	-0.362468	-0.149540
H	-3.728235	-3.224727	5.415639	C	6.471847	-1.563079	0.373657
H	-2.215855	-3.560633	4.563804	C	7.803004	-1.809693	0.666659
H	-3.756620	-4.082663	3.864014	C	8.735920	-0.803699	0.451152
C	-2.734200	-0.826975	4.534475	C	8.314008	0.416500	-0.049444
H	-2.734660	0.131208	4.002649	C	6.965408	0.618097	-0.330449
H	-1.697224	-1.087096	4.765548	C	3.855781	-0.145217	1.228944
H	-3.266059	-0.687044	5.482323	C	3.231458	-1.178703	1.914917
C	-4.925503	-1.617991	3.592572	C	2.891254	-1.105197	3.264784
H	-5.387160	-1.637350	4.586450	C	3.148700	0.049393	3.978572
H	-5.428492	-2.363485	2.967169	C	3.795715	1.098585	3.344489
H	-5.091083	-0.636393	3.139791	C	4.146731	0.971996	2.011345
C	-4.939628	0.030375	-4.533406	F	2.315475	1.970263	0.332159
H	-5.365468	-0.974411	-4.605916	F	1.604060	3.963275	-1.226993
H	-4.284952	0.185114	-5.398546	F	2.700905	4.249440	-3.715973
H	-2.276042	-0.603778	-2.394087	F	4.652321	2.515828	-4.522446
C	-3.711042	1.664377	-3.059968	F	5.441350	0.530425	-2.908417
H	-4.573000	2.336734	-3.015366	F	5.630615	-2.390023	-2.078436
H	-3.117106	1.777679	-2.148336	F	4.283416	-3.958493	-3.721726
H	-3.088534	1.979637	-3.903598	F	1.574027	-3.771321	-3.928558
C	-3.837105	1.059317	1.074804	F	0.231996	-1.957758	-2.395364
H	-4.670720	1.719100	0.800589	F	1.562473	-0.434802	-0.638569
H	-3.751234	1.100373	2.168256	F	5.601346	-2.557731	0.614344
H	-2.914016	1.682550	0.732966	F	8.195299	-2.987111	1.158406
C	-2.050062	3.188375	0.773312	F	10.023068	-1.008775	0.730240
C	-1.468329	2.971411	-0.564488	F	9.202108	1.393058	-0.249331
C	-0.769242	1.781135	-0.848554	F	6.643973	1.835801	-0.789683
C	-1.556054	3.961112	-1.559881	F	2.866910	-2.313421	1.291085
C	-0.216637	1.572848	-2.105162	F	2.258327	-2.117808	3.869130
H	-0.689208	1.007705	-0.089108	F	2.758003	0.167557	5.251104
C	-0.959742	3.764654	-2.799517	F	4.001270	2.243916	4.007713
H	-2.053795	4.899910	-1.342284	F	4.752956	2.030573	1.455488
C	-0.304624	2.567846	-3.079969				
H	0.290023	0.636627	-2.311050				
H	-1.000960	4.551145	-3.545663				
H	0.154945	2.416363	-4.052145				
				2			
				SCF done:	-4853.77372		
				Ir	-3.971995	-0.644892	0.194103

N	-4.794606	-2.632918	0.083178	C	-0.469536	2.336063	-1.241081
O	-5.783637	-2.095848	-1.946896	C	-0.227777	4.662614	-1.780296
O	-3.843636	-3.131723	2.137976	C	0.095499	1.987288	-2.462479
P	-5.069550	-0.479558	-1.867800	H	-0.732992	1.549430	-0.537071
P	-3.144836	-1.502602	2.216618	C	0.337851	4.314973	-3.007270
C	-5.524687	-2.999672	-0.992714	H	-0.334369	5.710609	-1.521127
C	-6.025269	-4.288986	-1.128889	C	0.498606	2.979329	-3.355138
H	-6.599828	-4.547843	-2.007443	H	0.242303	0.939296	-2.708599
C	-5.752572	-5.196468	-0.110992	H	0.673792	5.094380	-3.683533
H	-6.126468	-6.211980	-0.191187	H	0.965717	2.713950	-4.298747
C	-5.011864	-4.830520	1.005506	C	-1.303727	5.508589	0.760376
H	-4.785087	-5.514981	1.811288	C	-0.166078	6.224262	1.145510
C	-4.544226	-3.521088	1.070125	C	-2.505370	6.195232	0.593027
C	-4.010230	-0.491976	-3.437436	C	-0.234594	7.596946	1.356006
C	-3.173070	-1.773893	-3.353431	H	0.775751	5.697729	1.277550
H	-2.437943	-1.762490	-4.164808	C	-2.578801	7.570121	0.807951
H	-3.790293	-2.669854	-3.465628	H	-3.393623	5.646342	0.288419
H	-5.327434	0.480771	-4.887733	C	-1.441874	8.274287	1.189811
C	-6.667339	0.539601	-1.965828	H	0.656725	8.140621	1.652545
C	-7.645425	0.022363	-3.022994	H	-3.523733	8.088040	0.676456
H	-8.592833	0.559790	-2.905485	H	-1.493847	9.345042	1.358634
H	-7.843114	-1.044662	-2.893875	C	-0.523837	3.299521	1.642322
H	-7.292424	0.193899	-4.039998	C	0.785753	2.836031	1.528754
C	-7.310587	0.418707	-0.577224	C	-1.172645	3.174830	2.876711
H	-8.241493	0.995463	-0.569112	C	1.428928	2.241921	2.612398
H	-6.649891	0.802050	0.205704	H	1.319707	2.942735	0.592243
H	-7.556999	-0.622728	-0.342632	C	-0.526406	2.595655	3.966988
C	-6.273356	1.994664	-2.235588	H	-2.182477	3.567962	2.987489
H	-7.167480	2.622160	-2.157842	C	0.778444	2.116364	3.835938
H	-5.860145	2.127042	-3.239398	H	2.445192	1.887278	2.482475
H	-5.544437	2.360843	-1.504139	H	-1.040478	2.524920	4.921821
C	-1.295495	-1.872023	2.300153	H	1.286733	1.650227	4.675954
C	-0.820588	-2.440193	3.635256	B	4.120588	-0.637430	-0.341609
H	0.238222	-2.694424	3.527202	C	4.074941	0.722413	-1.270703
H	-1.371631	-3.342631	3.916885	C	3.679012	1.992404	-0.877071
H	-0.889979	-1.703982	4.441431	C	3.437130	3.038818	-1.760658
C	-1.013838	-2.878193	1.177271	C	3.613409	2.837565	-3.117364
H	0.072230	-2.962996	1.065233	C	4.024372	1.590022	-3.567801
H	-1.427498	-2.539772	0.220474	C	4.242234	0.576500	-2.647093
H	-1.419776	-3.865765	1.415130	C	2.826233	-1.468443	-0.940843
C	-0.610466	-0.530907	2.000687	C	2.859506	-2.637289	-1.691797
H	-0.934697	0.276754	2.665818	C	1.722975	-3.226920	-2.244970
H	-0.780873	-0.227161	0.965786	C	0.492190	-2.616964	-2.088060
H	0.464091	-0.655596	2.141101	C	0.416895	-1.423166	-1.386350
C	-3.947384	-0.927971	3.834915	C	1.562764	-0.891718	-0.819993
C	-3.866889	-1.981652	4.941975	C	5.531522	-1.458514	-0.435073
H	-4.469438	-1.634820	5.788844	C	5.616336	-2.707953	0.172827
H	-2.848365	-2.133312	5.299865	C	6.779040	-3.456581	0.248289
H	-4.270479	-2.941384	4.609481	C	7.946870	-2.940342	-0.298071
C	-3.256960	0.373229	4.253813	C	7.919737	-1.695400	-0.903043
H	-3.269699	1.121772	3.453121	C	6.726662	-0.979084	-0.955275
H	-2.216294	0.210994	4.548831	C	3.961825	-0.342595	1.270111
H	-3.789994	0.793169	5.114129	C	3.084218	-0.968747	2.143807
C	-5.418234	-0.658761	3.491184	C	3.013006	-0.677177	3.501935
H	-5.934398	-0.316623	4.394584	C	3.892934	0.235605	4.055643
H	-5.918162	-1.569124	3.141731	C	4.837104	0.844154	3.237648
H	-5.513657	0.108847	2.717642	C	4.851623	0.539188	1.883441
C	-4.823302	-0.476618	-4.729365	F	3.460193	2.287572	0.417546
H	-5.564252	-1.281243	-4.752371	F	2.993983	4.215000	-1.307322
H	-4.136593	-0.627510	-5.569214	F	3.350167	3.814104	-3.989382
H	-2.616859	-1.830100	-2.413972	F	4.175357	1.377686	-4.878113
C	-3.075230	0.720906	-3.344066	F	4.606193	-0.618287	-3.138233
H	-3.609404	1.676005	-3.306503	F	4.005345	-3.274745	-1.941080
H	-2.422727	0.648230	-2.470249	F	1.811620	-4.367188	-2.930548
H	-2.435687	0.737983	-4.233070	F	-0.616424	-3.170996	-2.594728
C	-3.217550	1.040717	0.272736	F	-0.782425	-0.816363	-1.245493
H	-3.314282	1.812975	-0.502511	F	1.414800	0.248436	-0.120317
H	-2.578492	1.410748	1.086744	F	4.511512	-3.245775	0.720349
H	-2.269331	3.653758	0.485176	F	6.792655	-4.654979	0.837494
C	-1.230273	4.013837	0.490605	F	9.082013	-3.636964	-0.237813
C	-0.633291	3.679684	-0.877286	F	9.038121	-1.188046	-1.426521

F	6.796348	0.223637	-1.539989	C	2.942240	-1.899163	-2.034503
F	2.209950	-1.904445	1.716670	H	1.878861	-1.801917	-2.278026
F	2.083542	-1.257004	4.275904	H	3.066784	-2.702404	-1.302493
F	3.813773	0.541338	5.352223	H	3.482833	-2.184245	-2.942891
F	5.702784	1.713398	3.759099	H	-1.224063	1.550608	-1.900426
F	5.770865	1.161270	1.135871	C	0.027464	3.287554	-0.855870

TS₃₄

SCF done: 1600.910620

Ir	0.085274	-0.178218	-0.331596
N	0.405265	-2.000973	0.790203
O	-1.845756	-2.509327	0.615692
O	2.663258	-1.515700	0.943391
P	-2.101966	-1.002225	-0.254396
P	2.425056	-0.080623	-0.047249
C	-0.620490	-2.841518	1.038330
C	-0.451066	-4.044066	1.715328
H	-1.309226	-4.678554	1.890143
C	0.831380	-4.375992	2.132558
H	0.998848	-5.309196	2.659877
C	1.903170	-3.530505	1.875789
H	2.916608	-3.756344	2.178233
C	1.643968	-2.346140	1.195695
C	-3.326334	-0.207620	0.960987
C	-2.439609	0.300286	2.106629
H	-1.670218	0.988955	1.740606
H	-1.939622	-0.528895	2.619730
H	-3.069272	0.815713	2.841547
C	-4.016206	0.964438	0.259137
H	-4.706308	0.622254	-0.518300
H	-3.304890	1.670704	-0.181965
H	-4.608515	1.517428	0.997055
C	-4.354539	-1.192496	1.523958
H	-4.896841	-0.687960	2.331074
H	-3.874454	-2.079758	1.942403
H	-5.089531	-1.506437	0.782551
C	-2.873749	-1.704723	-1.836317
C	-4.231462	-2.361165	-1.589813
H	-5.004656	-1.623712	-1.357692
H	-4.184726	-3.097566	-0.782373
H	-4.538363	-2.881688	-2.503279
C	-1.873115	-2.746807	-2.353518
H	-2.209714	-3.095465	-3.335229
H	-1.815508	-3.610681	-1.686162
H	-0.872462	-2.314755	-2.464348
C	-2.994132	-0.566570	-2.856820
H	-3.480965	-0.958796	-3.755789
H	-2.008486	-0.191190	-3.146567
H	-3.598827	0.269884	-2.493037
C	3.231836	1.172258	1.143602
C	2.111682	1.583732	2.109087
H	2.519897	2.279736	2.850091
H	1.717968	0.713259	2.646541
H	1.272528	2.065835	1.599202
C	3.726068	2.380766	0.344231
H	2.969144	2.768932	-0.345911
H	4.619822	2.144117	-0.239153
H	3.984478	3.186119	1.039267
C	4.385550	0.563781	1.946324
H	5.221461	0.252894	1.318640
H	4.053788	-0.294930	2.532252
H	4.755492	1.327566	2.639058
C	3.521948	-0.574489	-1.518117
C	3.378724	0.496459	-2.604070
H	3.986109	0.202438	-3.466261
H	3.726941	1.479968	-2.276852
H	2.341615	0.577116	-2.942317
C	4.985692	-0.771689	-1.126928
H	5.523608	-1.186906	-1.986133
H	5.087784	-1.474439	-0.295180
H	5.473542	0.169355	-0.859735

C	2.942240	-1.899163	-2.034503
H	1.878861	-1.801917	-2.278026
H	3.066784	-2.702404	-1.302493
H	3.482833	-2.184245	-2.942891
H	-1.224063	1.550608	-1.900426
C	0.027464	3.287554	-0.855870
H	1.036713	3.295593	-0.468463
C	-0.225320	1.238212	-1.570285
C	-1.133188	3.531660	0.030477
O	-2.237217	3.805717	-0.376942
O	-0.783852	3.392713	1.306060
H	0.503822	1.473254	-2.356345
C	-1.819667	3.687677	2.271232
H	-2.707049	3.101305	2.018780
H	-2.077071	4.746474	2.177450
C	-1.262783	3.347887	3.633587
H	-0.373939	3.945141	3.848218
H	-2.011611	3.555464	4.401077
H	-0.992712	2.289878	3.688298
N	-0.106891	3.892173	-2.044521
N	-0.264361	4.277879	-3.081317

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SCF done: -1491.572302

Ir	-0.160132	-0.048837	0.379205
N	-0.493035	-1.827214	-0.679490
O	1.732834	-2.397691	-0.422328
O	-2.744918	-1.307281	-0.889750
P	2.099967	-0.749901	0.138122
P	-2.483352	0.145987	0.062344
C	0.524627	-2.700516	-0.879938
C	0.336272	-3.913599	-1.535598
H	1.183998	-4.570620	-1.674949
C	-0.942638	-4.226795	-1.972659
H	-1.119135	-5.167560	-2.483411
C	-2.002333	-3.352813	-1.759464
H	-3.013788	-3.564441	-2.078055
C	-1.736258	-2.159004	-1.103781
C	3.052280	-0.148190	-1.434292
C	2.059860	0.695705	-2.244682
H	1.736343	1.588613	-1.702620
H	1.167556	0.119188	-2.512954
H	2.547369	1.013112	-3.173068
C	4.288206	0.686533	-1.080582
H	5.069642	0.080052	-0.616048
H	4.051970	1.528804	-0.430427
H	4.699767	1.077971	-2.017669
C	3.484193	-1.354953	-2.278836
H	4.062921	-0.972011	-3.126049
H	2.631480	-1.908329	-2.678907
H	4.116423	-2.051690	-1.724632
C	3.228094	-1.315263	1.569726
C	4.291567	-2.288760	1.049361
H	5.016657	-1.797958	0.396030
H	3.847408	-3.134876	0.520393
H	4.841610	-2.679930	1.911787
C	2.301460	-2.049372	2.548983
H	2.902968	-2.410752	3.389369
H	1.823551	-2.912655	2.077821
H	1.521959	-1.392842	2.945969
C	3.899436	-0.127485	2.265385
H	4.509635	-0.526983	3.082433
H	3.182491	0.577786	2.686238
H	4.554275	0.431644	1.595315
C	-3.109238	1.432833	-1.194361
C	-1.899945	1.787467	-2.072013
H	-2.227869	2.484313	-2.850561
H	-1.491839	0.899818	-2.567990
H	-1.098232	2.261130	-1.496603
C	-3.604373	2.680954	-0.457070
H	-2.881708	3.062137	0.271807

H	-4.555631	2.503213	0.051392	H	3.703136	2.670645	-1.378523
H	-3.769084	3.472319	-1.195319	H	3.759268	2.195643	0.324668
C	-4.225372	0.858344	-2.072481	H	2.192947	2.327439	-0.502252
H	-5.096298	0.544986	-1.494504	C	4.768154	0.108341	-1.234313
H	-3.877438	0.006995	-2.659922	H	5.230912	0.649290	-2.066829
H	-4.547337	1.643704	-2.764526	H	4.829310	-0.961788	-1.451910
C	-3.672229	-0.220895	1.496373	H	5.354975	0.323126	-0.337162
C	-3.655090	0.956264	2.479178	C	-3.243658	-0.974944	1.712709
H	-4.162252	0.644872	3.398110	C	-4.411979	-1.920411	1.422134
H	-4.183125	1.829650	2.092985	H	-4.088433	-2.789656	0.845517
H	-2.640420	1.260280	2.752535	H	-5.228846	-1.431310	0.890559
C	-5.094531	-0.499363	1.009640	H	-4.807321	-2.276483	2.379554
H	-5.689683	-0.856491	1.856889	C	-2.204036	-1.704430	2.575194
H	-5.111927	-1.270819	0.234617	H	-1.366012	-1.051442	2.834321
H	-5.579228	0.402678	0.626733	H	-1.805465	-2.585845	2.060704
C	-3.091193	-1.472028	2.170406	H	-2.688508	-2.043395	3.496752
H	-2.061984	-1.309375	2.507361	C	-3.726076	0.288248	2.431334
H	-3.105995	-2.333589	1.495893	H	-4.113624	0.004563	3.415365
H	-3.707083	-1.718937	3.040952	H	-4.536575	0.783494	1.889033
H	1.131842	0.795198	2.600970	H	-2.915382	1.007575	2.591394
C	0.049901	1.935501	1.138701	C	-3.320289	0.567482	-1.092301
H	-0.841044	2.543677	1.017623	C	-4.766340	0.099846	-1.238174
C	0.149100	0.982268	2.180693	H	-5.229116	0.639084	-2.071786
C	1.291154	2.571954	0.638019	H	-5.355770	0.312894	-0.342318
O	2.413906	2.150896	0.845291	H	-4.823379	-0.970526	-1.455642
O	1.036933	3.655664	-0.092499	C	-3.245603	2.023809	-0.623327
H	-0.672093	0.834252	2.874252	H	-2.201246	2.327832	-0.497762
C	2.184523	4.357398	-0.614938	H	-3.770948	2.190758	0.321554
H	2.762173	3.665891	-1.237366	H	-3.708370	2.666072	-1.381283
H	2.815616	4.659046	0.225240	C	-2.582122	0.429723	-2.430823
C	1.667613	5.539097	-1.402129	H	-3.052650	1.097029	-3.160677
H	1.086495	6.204825	-0.761011	H	-2.641799	-0.591235	-2.817592
H	2.506802	6.102222	-1.815713	H	-1.526917	0.711574	-2.334862
H	1.033883	5.206780	-2.227334	C	0.000525	1.503040	1.304178

TS₃₅

SCF done: 1311.283106

Ir	0.000242	-0.072996	0.272672
N	0.000968	-1.989215	-0.725092
O	-2.316292	-2.003451	-0.693418
O	2.318236	-2.001780	-0.694487
P	-2.307802	-0.452264	0.143285
P	2.308404	-0.450984	0.142683
P	-0.002195	3.944049	-0.071764
C	-1.164107	-2.591997	-1.041302
C	-1.208041	-3.809901	-1.710123
H	-2.166318	-4.252870	-1.944612
C	0.001501	-4.407600	-2.042015
H	0.001713	-5.358484	-2.564583
C	1.210796	-3.809027	-1.710726
H	2.169274	-4.251320	-1.945673
C	1.166308	-2.591175	-1.041896
C	3.244426	-0.973414	1.712119
C	2.205904	-1.706225	2.573099
H	2.690512	-2.044854	3.494710
H	1.810046	-2.588186	2.057465
H	1.366100	-1.055513	2.832185
C	4.415043	-1.915946	1.421200
H	5.231421	-1.424240	0.891311
H	4.093934	-2.784948	0.842844
H	4.810131	-2.272783	2.378437
C	3.723487	0.290031	2.432562
H	2.910594	1.006468	2.594404
H	4.532135	0.788717	1.890640
H	4.112556	0.005812	3.415846
C	3.320203	0.570983	-1.091677
C	2.585732	0.430606	-2.431903
H	1.529367	0.708869	-2.338610
H	2.649843	-0.590129	-2.818496
H	3.055681	1.099577	-3.160608
C	3.238891	2.026918	-0.622700

H	3.703136	2.670645	-1.378523
H	3.759268	2.195643	0.324668
H	2.192947	2.327439	-0.502252
C	4.768154	0.108341	-1.234313
H	5.230912	0.649290	-2.066829
H	4.829310	-0.961788	-1.451910
H	5.354975	0.323126	-0.337162
C	-3.243658	-0.974944	1.712709
C	-4.411979	-1.920411	1.422134
H	-4.088433	-2.789656	0.845517
H	-5.228846	-1.431310	0.890559
H	-4.807321	-2.276483	2.379554
C	-2.204036	-1.704430	2.575194
H	-1.366012	-1.051442	2.834321
H	-1.805465	-2.585845	2.060704
H	-2.688508	-2.043395	3.496752
C	-3.726076	0.288248	2.431334
H	-4.113624	0.004563	3.415365
H	-4.536575	0.783494	1.889033
H	-2.915382	1.007575	2.591394
C	-3.320289	0.567482	-1.092301
C	-4.766340	0.099846	-1.238174
H	-5.229116	0.639084	-2.071786
H	-5.355770	0.312894	-0.342318
H	-4.823379	-0.970526	-1.455642
C	-3.245603	2.023809	-0.623327
H	-2.201246	2.327832	-0.497762
H	-3.770948	2.190758	0.321554
H	-3.708370	2.666072	-1.381283
C	-2.582122	0.429723	-2.430823
H	-3.052650	1.097029	-3.160677
H	-2.641799	-0.591235	-2.817592
H	-1.526917	0.711574	-2.334862
C	0.000525	1.503040	1.304178
H	-0.890281	1.956443	1.752800
H	0.892010	1.957677	1.750326
C	-1.438291	5.118967	0.236428
H	-2.382257	4.637399	-0.024822
H	-1.325858	6.029555	-0.358808
H	-1.465554	5.386768	1.294509
C	-0.004734	3.866176	-1.950099
H	0.879972	3.326925	-2.296258
H	-0.003064	4.871643	-2.380206
H	-0.892674	3.330799	-2.293968
C	1.434464	5.119371	0.232673
H	1.467851	5.382886	1.291645
H	1.317107	6.032231	-0.358129
H	2.377557	4.640393	-0.036565

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SCF done: -1311.315709

Ir	-0.045517	0.088393	0.150515
N	-0.141262	-1.977226	-0.380844
O	-2.442560	-1.837408	-0.606399
O	2.139754	-2.176513	-0.064981
P	-2.342325	-0.218036	0.057752
P	2.231110	-0.422938	0.105863
P	0.363886	3.466201	-0.113625
C	-1.321747	-2.573431	-0.652580
C	-1.431655	-3.921967	-0.970520
H	-2.409467	-4.333787	-1.180445
C	-0.270196	-4.682684	-0.989963
H	-0.319593	-5.738636	-1.233166
C	0.951981	-4.099662	-0.687670
H	1.881314	-4.652726	-0.675708
C	0.969630	-2.742904	-0.379267
C	3.216939	-0.408607	1.735834
C	2.190172	-0.800090	2.808918
H	2.683386	-0.792469	3.786911
H	1.800730	-1.807733	2.631562
H	1.342309	-0.108822	2.830249

C	4.377666	-1.405294	1.768051	C	1.162635	2.260443	-0.011714
H	5.217768	-1.092129	1.147528	C	1.206606	3.649393	0.012996
H	4.056822	-2.400742	1.452503	H	2.166958	4.146617	0.019670
H	4.740567	-1.477533	2.799143	C	0.000022	4.336456	0.025758
C	3.713345	1.015114	1.993688	H	0.000037	5.421068	0.044817
H	2.887724	1.736129	1.987133	C	-1.206581	3.649416	0.013618
H	4.469500	1.327482	1.265797	H	-2.166920	4.146658	0.020812
H	4.176694	1.057054	2.985152	C	-1.162649	2.260464	-0.011086
C	3.277399	-0.147964	-1.473540	C	3.309477	-0.481949	-1.596958
C	2.381162	-0.646946	-2.617801	C	2.310214	-0.282148	-2.745019
H	1.387183	-0.185938	-2.586120	H	2.830531	-0.435865	-3.696017
H	2.255634	-1.732750	-2.578707	H	1.901665	0.734091	-2.744725
H	2.856985	-0.399275	-3.572573	H	5.264134	0.345073	-1.029030
C	3.566662	1.338619	-1.675158	C	3.251890	-0.465204	1.608163
H	4.095539	1.468521	-2.625519	C	4.703054	0.008991	1.548118
H	4.207036	1.749788	-0.888695	H	5.133808	-0.049294	2.553445
H	2.644512	1.924042	-1.728442	H	4.771629	1.047303	1.211466
C	4.588433	-0.935582	-1.472211	H	5.313572	-0.618913	0.893739
H	4.997788	-0.934201	-2.488571	C	2.488417	0.326422	2.678668
H	4.438190	-1.975254	-1.170371	H	2.924053	0.101242	3.657589
H	5.336323	-0.478967	-0.819447	H	1.428258	0.050809	2.700144
C	-3.233713	-0.503257	1.716468	H	2.569406	1.403833	2.512081
C	-4.727218	-0.791038	1.583107	C	3.174915	-1.961120	1.930418
H	-4.925036	-1.584818	0.857360	H	3.687818	-2.142527	2.880402
H	-5.291488	0.100979	1.298315	H	3.655573	-2.584568	1.171419
H	-5.108428	-1.121554	2.555478	H	2.136357	-2.286210	2.048818
C	-2.528078	-1.710810	2.350458	C	-3.309018	-0.480839	-1.597351
H	-1.442833	-1.562964	2.387297	C	-4.473781	0.499347	-1.763672
H	-2.744461	-2.633002	1.804166	H	-4.909553	0.343144	-2.756314
H	-2.896162	-1.829607	3.374914	H	-4.136513	1.536226	-1.701929
C	-2.991607	0.729411	2.593560	H	-5.264648	0.343813	-1.029388
H	-3.499238	0.583488	3.552923	C	-2.309594	-0.279110	-2.744934
H	-3.388918	1.649095	2.149611	H	-2.829533	-0.432284	-3.696226
H	-1.923209	0.863229	2.787792	H	-1.473406	-0.981621	-2.681546
C	-3.385530	0.643255	-1.278282	H	-1.901860	0.737456	-2.743511
C	-4.720956	-0.044835	-1.574248	C	-3.813545	-1.926414	-1.586511
H	-5.123817	0.371985	-2.503941	H	-4.583755	-2.086502	-0.826677
H	-5.464014	0.116243	-0.793756	H	-3.004121	-2.647559	-1.426998
H	-4.587451	-1.119770	-1.721222	H	-4.259958	-2.149201	-2.561137
C	-3.597758	2.094961	-0.841747	C	-3.252343	-0.466291	1.607835
H	-2.643527	2.581316	-0.602403	C	-4.703562	0.007737	1.547756
H	-4.252696	2.169829	0.032277	H	-5.134261	-0.050447	2.553114
H	-4.069238	2.653767	-1.657580	H	-5.314032	-0.620346	0.893491
C	-2.518697	0.584887	-2.543479	H	-4.772297	1.045995	1.210982
H	-3.007431	1.160463	-3.337406	C	-3.175228	-1.962424	1.929047
H	-2.409068	-0.446920	-2.890106	H	-2.136711	-2.287101	2.048864
H	-1.518346	0.987095	-2.365659	H	-3.654380	-2.585552	1.168820
C	-0.112496	2.034314	0.942963	H	-3.689565	-2.144811	2.878069
H	-1.111574	2.314387	1.297845	C	-2.489233	0.324665	2.679096
H	0.543064	2.141423	1.820936	H	-2.924637	0.098200	3.657826
C	-0.633612	4.977146	0.270043	H	-2.570855	1.402193	2.513596
H	-1.688291	4.775394	0.071232	H	-1.428912	0.049628	2.700200
H	-0.304080	5.816763	-0.345577	C	-0.000091	-2.512329	-0.173675
H	-0.510913	5.226709	1.325769	H	0.897577	-3.075702	-0.447109
C	0.144906	3.169607	-1.919724	H	-0.897773	-3.075510	-0.447468
H	0.513966	2.167984	-2.148898	C	4.473607	0.498856	-1.764049
H	0.680388	3.929308	-2.493629	H	4.135514	1.535565	-1.704094
H	-0.919444	3.216034	-2.160395	H	4.910100	0.341470	-2.756192
C	2.112467	3.971968	0.192659	H	1.474562	-0.985248	-2.681173
H	2.173919	4.406359	1.193082	C	3.814923	-1.927190	-1.584415
H	2.425476	4.713100	-0.545783	H	4.585037	-2.086033	-0.824225
H	2.766932	3.103625	0.139213	H	3.005877	-2.648611	-1.424249
				H	4.261681	-2.150782	-2.558699
				H	-0.001012	-3.407196	1.136388
				H	-0.000116	-2.591740	1.244785
TS₃₆				6			
SCF done: -1186.258891				SCF done: -1186.36983			
Ir	0.000010	-0.550270	-0.012951	Ir	0.000125	-0.554401	-0.038249
N	-0.000017	1.571865	-0.018996	N	0.000140	1.602049	0.022087
O	2.318649	1.585037	-0.034994	O	-2.315181	1.585203	-0.016097
O	-2.318687	1.585081	-0.033650				
P	2.305883	-0.172114	-0.010642				
P	-2.305913	-0.172085	-0.010492				

O	2.315284	1.585559	-0.026416	Ir	-0.000360	-0.613273	-0.147775
P	-2.315261	-0.175070	-0.043713	N	-0.003475	1.567982	-0.179163
P	2.314981	-0.174615	-0.044481	O	-2.315019	1.538585	-0.264262
C	-1.163752	2.275990	0.022824	O	2.309793	1.553441	-0.154274
C	-1.209858	3.665159	0.056865	P	-2.333074	-0.197084	-0.008628
H	-2.167956	4.166941	0.062470	P	2.332762	-0.194447	0.001598
C	-0.000016	4.349156	0.074168	C	-1.167168	2.234257	-0.262576
H	-0.000067	5.433655	0.099862	C	-1.215343	3.620414	-0.354633
C	1.209904	3.665382	0.051640	H	-2.174588	4.116322	-0.415146
H	2.167914	4.167358	0.052974	C	-0.007254	4.307442	-0.370684
C	1.163900	2.276253	0.017663	H	-0.008767	5.389859	-0.441474
C	-3.162774	-0.515252	1.618956	C	1.202545	3.627481	-0.300690
C	-2.232464	0.118410	2.663685	H	2.160464	4.129297	-0.317595
H	-2.650459	-0.057247	3.659955	C	1.158593	2.240696	-0.209848
H	-2.131123	1.198629	2.524970	C	-3.173856	-0.206046	1.710292
H	-5.268664	-0.406103	1.058168	C	-2.084011	0.165631	2.724996
C	-3.388059	-0.461044	-1.583688	H	-2.556882	0.297964	3.703178
C	-4.494217	0.592878	-1.701521	H	-1.589430	1.107951	2.461297
H	-5.067083	0.376252	-2.609203	H	-5.132704	0.624094	1.139106
H	-4.080894	1.599212	-1.791068	C	-3.461945	-0.762535	-1.431632
H	-5.187526	0.575283	-0.859518	C	-4.913787	-0.315254	-1.251872
C	-2.450491	-0.350005	-2.792177	H	-5.472688	-0.600774	-2.148909
H	-3.051555	-0.410527	-3.704978	H	-4.993485	0.769677	-1.139733
H	-1.718767	-1.162549	-2.807758	H	-5.395863	-0.800414	-0.400259
H	-1.915929	0.606147	-2.803648	C	-2.911853	-0.154227	-2.726491
C	-3.982287	-1.871244	-1.512897	H	-3.546254	-0.488260	-3.553503
H	-4.438578	-2.101357	-2.481031	H	-1.892445	-0.483337	-2.936332
H	-4.765222	-1.945658	-0.753667	H	-2.935466	0.938311	-2.700717
H	-3.221882	-2.634926	-1.316741	C	-3.364570	-2.292768	-1.488754
C	3.161358	-0.506629	1.620403	H	-3.961021	-2.645288	-2.336183
C	4.556370	0.109465	1.705298	H	-3.758189	-2.769761	-0.586689
H	4.920750	0.017527	2.733950	H	-2.332861	-2.626357	-1.636374
H	4.544981	1.171177	1.442555	C	3.204925	-0.297550	1.700782
H	5.267759	-0.410806	1.058810	C	4.333958	0.734547	1.817995
C	2.234574	0.138250	2.661333	H	4.724095	0.683264	2.839793
H	2.651265	-0.034690	3.658614	H	3.969095	1.749219	1.646504
H	1.233700	-0.313496	2.642826	H	5.163763	0.540214	1.140341
H	2.140073	1.218290	2.516721	C	2.140085	0.032580	2.755668
C	3.202564	-2.020986	1.856808	H	2.634418	0.107295	3.729393
H	3.887822	-2.532666	1.178447	H	1.365263	-0.732662	2.814228
H	2.211628	-2.475288	1.757932	H	1.654574	0.994009	2.551926
H	3.555135	-2.199534	2.877984	C	3.746079	-1.715041	1.914550
C	3.388916	-0.469190	-1.581905	H	4.584994	-1.941130	1.251256
C	4.496128	0.583176	-1.703594	H	2.980132	-2.484239	1.780055
H	5.069540	0.362121	-2.609850	H	4.111657	-1.792755	2.943654
H	5.188706	0.568613	-0.860954	C	3.438146	-0.679486	-1.470201
H	4.083657	1.589436	-1.797816	C	4.898913	-0.264657	-1.285115
C	3.981614	-1.879684	-1.503465	H	5.439949	-0.501656	-2.206954
H	3.219977	-2.641598	-1.305316	H	5.387304	-0.807596	-0.473037
H	4.763179	-1.951765	-0.742557	H	4.996055	0.810147	-1.108393
H	4.439353	-2.114707	-2.469741	C	3.318283	-2.201217	-1.623132
C	2.452902	-0.363297	-2.792132	H	2.281038	-2.508538	-1.787185
H	3.055170	-0.428562	-3.703821	H	3.705284	-2.738283	-0.752058
H	1.919071	0.593180	-2.808918	H	3.907828	-2.510301	-2.491960
H	1.720682	-1.175443	-2.804870	C	2.881279	0.021054	-2.714389
C	0.000067	-2.620368	-0.022504	H	3.491289	-0.276455	-3.573044
H	-0.878755	-3.072139	-0.493268	H	2.935240	1.108967	-2.621114
H	-0.000604	-2.958688	1.027579	H	1.849305	-0.265907	-2.924678
C	-4.554973	0.106552	1.708195	C	-0.003882	-2.074123	1.030240
H	-4.538639	1.169918	1.452498	H	-0.897569	-2.608522	1.364669
H	-4.919823	0.009292	2.736174	H	0.887101	-2.609730	1.369249
H	-1.234643	-0.340013	2.642937	C	-4.291517	0.840988	1.795863
C	-3.210452	-2.030902	1.845859	H	-3.920757	1.843432	1.572810
H	-3.900762	-2.535009	1.167005	H	-4.667431	0.840825	2.824277
H	-2.222057	-2.489356	1.740864	H	-1.318105	-0.606630	2.806736
H	-3.560144	-2.213983	2.867235	C	-3.721664	-1.604771	2.010212
H	0.879413	-3.072358	-0.492040	H	-4.576183	-1.857965	1.377577
H	0.000447	-0.543275	-1.549101	H	-2.963730	-2.386001	1.901560
				H	-4.065321	-1.624712	3.049587
				H	-0.010086	-0.254914	-1.842132
				H	0.003763	-1.290247	-1.610670

TS₃₇
SCF done: -1186.28189

7
 SCF done: -1187.00756

Ir	-0.000825	-0.539841	0.050297
N	-0.000097	1.611471	-0.128709
O	2.316599	1.592819	-0.136757
O	-2.316815	1.596202	-0.112953
P	2.309088	-0.157775	0.032758
P	-2.309376	-0.156000	0.035394
C	1.164878	2.284914	-0.150913
C	1.211134	3.673539	-0.195126
H	2.169337	4.174829	-0.213143
C	0.001465	4.357989	-0.211693
H	0.002067	5.442292	-0.244957
C	-1.208945	3.675279	-0.183018
H	-2.166546	4.177968	-0.191288
C	-1.164219	2.286592	-0.139141
C	3.177844	-0.633207	-1.585277
C	2.067706	-0.562049	-2.645501
H	2.489920	-0.804220	-3.626232
H	1.632679	0.442264	-2.710542
H	5.146609	0.277765	-1.265510
C	3.326270	-0.362151	1.612612
C	4.796137	0.007854	1.409690
H	5.301567	-0.033118	2.380178
H	4.906477	1.022050	1.014833
H	5.308468	-0.691149	0.743593
C	2.699171	0.572702	2.654667
H	3.201665	0.406438	3.612659
H	1.632614	0.371583	2.794852
H	2.827987	1.622821	2.379995
C	3.169445	-1.821683	2.055758
H	3.703417	-1.957158	3.001632
H	3.590786	-2.525878	1.333066
H	2.117581	-2.077440	2.215658
C	-3.171815	-0.612028	-1.592136
C	-4.297648	0.356611	-1.959850
H	-4.665386	0.089773	-2.956425
H	-3.944347	1.389471	-1.992382
H	-5.141056	0.297132	-1.270415
C	-2.056346	-0.529494	-2.646056
H	-2.473542	-0.761016	-3.631500
H	-1.260751	-1.258829	-2.444190
H	-1.620553	0.475262	-2.698061
C	-3.689643	-2.050270	-1.493194
H	-4.530359	-2.135315	-0.799386
H	-2.908005	-2.752778	-1.186047
H	-4.044544	-2.361255	-2.481087
C	-3.330355	-0.381793	1.609545
C	-4.800251	-0.012179	1.406586
H	-5.309714	-0.070635	2.374043
H	-5.307658	-0.701017	0.726397
H	-4.911350	1.008332	1.028511
C	-3.171557	-1.846665	2.034440
H	-2.119594	-2.102975	2.193378
H	-3.590482	-2.542612	1.302379
H	-3.707382	-1.994757	2.977396
C	-2.708115	0.541027	2.665036
H	-3.214031	0.362769	3.619073
H	-2.836874	1.594156	2.402223
H	-1.641911	0.339272	2.806703
C	-0.005589	-2.611965	0.177537
H	0.853527	-3.060934	-0.334164
H	-0.903688	-3.056667	-0.265351
C	4.306890	0.329003	-1.960029
H	3.954957	1.361738	-2.008455
H	4.679342	0.048077	-2.950952
H	1.270921	-1.288731	-2.439764
C	3.692608	-2.071021	-1.465032
H	4.532456	-2.147223	-0.769153
H	2.909499	-2.767497	-1.147697

H	4.047800	-2.397495	-2.447773
H	-0.000092	-0.511616	1.564575
H	0.034067	-2.967768	1.213352

TS₇₆
 SCF done: -1187.005202

Ir	0.000009	-0.575853	0.011157
N	-0.000014	1.544245	-0.039827
O	2.334170	1.570809	0.011448
O	-2.334193	1.570743	0.011444
P	2.379737	-0.203417	0.025395
P	-2.379714	-0.203467	0.025385
C	1.169379	2.236383	-0.010201
C	1.207128	3.629081	-0.000325
H	2.166775	4.128784	0.014103
C	-0.000060	4.320729	-0.000813
H	-0.000078	5.405826	0.007344
C	-1.207224	3.629046	-0.000357
H	-2.166889	4.128715	0.014049
C	-1.169428	2.236347	-0.010216
C	3.449948	-0.444333	-1.595842
C	2.529213	-0.101743	-2.780863
H	3.099672	-0.234689	-3.706694
H	2.200442	0.941419	-2.743827
H	5.431938	0.246793	-0.906356
C	3.328999	-0.560089	1.693678
C	4.827803	-0.235305	1.613871
H	5.262385	-0.388378	2.607988
H	5.008855	0.805245	1.333494
H	5.365635	-0.889354	0.924098
C	2.682842	0.311179	2.784129
H	3.147056	0.056091	3.743041
H	1.608784	0.133307	2.871729
H	2.851242	1.375903	2.603309
C	3.112135	-2.052978	2.005366
H	3.610613	-2.284857	2.952852
H	3.542765	-2.709311	1.242723
H	2.051848	-2.295052	2.116646
C	-3.449853	-0.444477	-1.595888
C	-4.657703	0.510348	-1.626073
H	-5.105942	0.449247	-2.624040
H	-4.359604	1.547903	-1.460156
H	-5.431749	0.246991	-0.906492
C	-2.528998	-0.102088	-2.780873
H	-3.099413	-0.235015	-3.706734
H	-1.643778	-0.737416	-2.824377
H	-2.200088	0.941037	-2.743872
C	-3.909609	-1.910775	-1.668703
H	-4.606111	-2.169177	-0.866426
H	-3.075116	-2.617574	-1.643609
H	-4.436036	-2.063588	-2.617248
C	-3.329048	-0.559980	1.693649
C	-4.827864	-0.235297	1.613684
H	-5.262536	-0.388315	2.607770
H	-5.365594	-0.889415	0.923903
H	-5.008933	0.805224	1.333210
C	-3.112177	-2.052821	2.005573
H	-2.051947	-2.294828	2.117468
H	-3.542325	-2.709241	1.242731
H	-3.611183	-2.284680	2.952786
C	-2.683051	0.311556	2.783987
H	-3.146681	0.055987	3.743053
H	-2.852300	1.376184	2.603398
H	-1.608815	0.134499	2.871113
C	0.000081	-2.054531	-1.277243
H	0.886774	-2.655673	-1.496007
H	-0.886607	-2.655631	-1.496151
C	4.657863	0.510421	-1.625809
H	4.359847	1.547947	-1.459555
H	5.106042	0.449604	-2.623820
H	1.643921	-0.736965	-2.824480

C	3.909553	-1.910665	-1.668800
H	4.605843	-2.169297	-0.866417
H	3.074940	-2.617333	-1.644005
H	4.436149	-2.063408	-2.617262
H	-0.000113	-0.248799	1.599724
H	-0.000043	-2.116975	0.514307

H₂

SCF done: -1.1672114

H	0.000000	0.000000	0.368672
H	0.000000	0.000000	-0.368672

PMe₃

SCF done: -126.1317841

P	-0.000015	-0.000226	-0.628446
C	-1.200896	-1.132949	0.291504
H	-2.225800	-0.885153	0.007575
H	-1.097062	-1.032946	1.376413
H	-1.011069	-2.170739	0.009880
C	-0.381168	1.606221	0.291208
H	0.343961	2.371183	0.005831
H	-0.343974	1.466306	1.376029
H	-1.376096	1.959276	0.012045
C	1.582196	-0.472909	0.291358
H	1.879567	-1.485145	0.009632
H	1.443260	-0.430954	1.376111
H	2.386644	0.209380	0.008754

ethyl diazoacetate

SCF done: -415.7692032

C	1.290015	-0.821850	-0.000629
H	1.160707	-1.891367	-0.001262
C	0.219314	0.166040	-0.000957
O	0.375089	1.366643	0.000367
O	-0.977538	-0.446357	-0.001902
C	-2.105768	0.438818	-0.001154
H	-2.053097	1.082339	-0.884507
H	-2.049826	1.085042	0.879988
C	-3.348313	-0.424603	0.002216
H	-3.371025	-1.061003	0.889586
H	-4.240771	0.205258	0.002568
H	-3.373774	-1.063848	-0.883036
N	2.509535	-0.349707	0.000407
N	3.549879	0.082686	0.001320

[Ph₃C] [B(C₆F₅)₄]

SCF done: -3667.76865

C	-4.878362	0.192864	-0.004313
C	-4.222551	-1.083068	-0.150872
C	-3.049353	-1.352676	0.592294
C	-4.715362	-2.058981	-1.049328
C	-2.395782	-2.564733	0.444431
H	-2.687451	-0.627078	1.309908
C	-4.027513	-3.245941	-1.222266
H	-5.592025	-1.837267	-1.649399
C	-2.876313	-3.503137	-0.469312
H	-1.499401	-2.768862	1.022219
H	-4.368979	-3.971138	-1.952082
H	-2.341261	-4.436874	-0.614545
C	-6.324062	0.289794	-0.095386
C	-6.929640	1.451629	-0.617761
C	-7.139838	-0.779675	0.329249
C	-8.309539	1.532389	-0.720909
H	-6.303507	2.260716	-0.978873
C	-8.519627	-0.680659	0.243820
H	-6.678528	-1.661258	0.761727
C	-9.103507	0.470757	-0.285803
H	-8.768661	2.417754	-1.146327
H	-9.143102	-1.496508	0.592179
H	10.183952	0.540693	-0.361042
C	-4.076208	1.364458	0.223274

C	-2.793114	1.435886	-0.363625
C	-4.529601	2.438146	1.029848
C	-1.978756	2.533107	-0.140837
H	-2.469493	0.651089	-1.035934
C	-3.694741	3.512552	1.272432
H	-5.502021	2.374933	1.507879
C	-2.418883	3.559721	0.692075
H	-1.000897	2.569124	-0.606311
H	-4.019862	4.312943	1.927646
H	-1.759032	4.397437	0.901944
B	1.979430	-0.037560	-0.031307
C	1.073463	-0.983072	-1.040605
C	-0.056610	-0.608801	-1.751819
C	-0.898084	-1.502391	-2.405513
C	-0.599377	-2.851184	-2.397523
C	0.529955	-3.285188	-1.715279
C	1.326616	-2.355981	-1.061398
C	1.570336	-0.671433	1.434049
C	2.360253	-1.469140	2.254130
C	1.887454	-2.074851	3.417840
C	0.565755	-1.910020	3.796397
C	-0.263283	-1.128575	3.003108
C	0.254957	-0.541561	1.862706
C	3.581154	-0.100441	-0.341038
C	4.447356	0.526165	0.550788
C	5.815836	0.622429	0.360699
C	6.374790	0.074958	-0.786971
C	5.554493	-0.552082	-1.709846
C	4.183959	-0.622210	-1.477188
C	1.620592	1.565372	-0.139482
C	1.309750	2.418511	0.914126
C	1.043313	3.774273	0.740269
C	1.109562	4.335949	-0.523456
C	1.457088	3.533870	-1.603575
C	1.711009	2.186983	-1.383927
F	-0.446109	0.679371	-1.836130
F	-2.028533	-1.065252	-2.980029
F	-1.413487	-3.732199	-2.988903
F	0.808645	-4.589685	-1.671518
F	2.387393	-2.836787	-0.402316
F	3.637608	-1.719772	1.958556
F	2.696162	-2.829501	4.161243
F	0.091264	-2.493056	4.896470
F	-1.556419	-0.967735	3.331298
F	-0.609205	0.201303	1.132075
F	3.945943	1.070362	1.672381
F	6.595976	1.233400	1.254527
F	7.687940	0.157073	-0.998737
F	6.083466	-1.077424	-2.817120
F	3.459795	-1.228179	-2.429820
F	1.217037	1.974696	2.174039
F	0.671622	4.537403	1.776678
F	0.827045	5.627826	-0.698083
F	1.533698	4.061787	-2.825855
F	2.027439	1.451705	-2.458030

N₂

SCF done: -109.4853926

N	0.000000	0.000000	0.549047
N	0.000000	0.000000	-0.549047

CH₄

SCF done: -40.4861222

C	0.000000	0.000000	0.000000
H	0.629603	0.629603	0.629603
H	-0.629603	-0.629603	0.629603
H	-0.629603	0.629603	-0.629603
H	0.629603	-0.629603	-0.629603