Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information for

P-Heterocyclic Carbenes as Effective Catalysts for the Activation of Single and Multiple Bonds. A Theoretical Study

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Table S1. Coordinates and energies of the calculated molecules at B3LYP/def-TZVP

H2	B3LYP/TZVP		
2			
E(SCF)=	-1,179649		
H	0,000000	0,000000	0,371893
H	0,000000	0,000000	-0,371893

1N	B3LYP/TZVP			**1N H2 TS**	B3LYP/TZVP			**1N H2 Product**	B3LYP/TZVP		
12				14				14			
E(SCF)=	-211,393483			E(SCF)=	-212,537268			E(SCF)=	-212,658715		
C	0,085575	0,118916	-1,238463	C	1,481465	-0,040993	0,796639	C	1,441863	0,182547	0,886217
C	-0,879063	0,375513	-0,074658	C	1,366723	0,643817	-0,584898	C	1,464214	0,456488	-0,644011
N	-0,199926	-0,348680	1,039375	C	0,091496	0,026810	-1,195138	C	0,021250	0,181127	-1,106369
C	0,794614	-1,153576	0,773091	N	-0,598074	-0,508089	-0,006548	N	-0,468343	-0,764462	-0,100689
C	0,957057	-1,064995	-0,730486	C	0,061454	-0,399059	1,149881	C	-0,012521	-0,227262	1,183212
H	-0,550712	-0,244589	1,982352	H	-1,560656	-0,802401	-0,050770	H	-1,472907	-0,890279	-0,137904
H	-1,000785	1,430455	0,175538	H	-0,530148	0,766040	-1,708054	H	-0,552891	1,122924	-1,115868
H	-1,870633	-0,055459	-0,238501	H	0,312518	-0,780857	-1,899118	H	-0,030053	-0,252769	-2,106574
H	0,707104	0,998125	-1,414702	H	1,226869	1,716366	-0,443059	H	1,772892	1,474920	-0,882420
H	-0,440998	-0,104241	-2,165726	H	2,239719	0,491784	-1,219644	H	2,158148	-0,221426	-1,141676
H	2,009742	-0,974637	-1,002654	H	1,954639	0,581907	1,552146	H	1,739217	1,053315	1,471618
H	0,626702	-2,028198	-1,137206	H	2,048676	-0,975480	0,715417	H	2,124115	-0,630001	1,137308
				H	-0,405640	1,204820	2,049620	H	-0,590760	0,656778	1,500886
				H	-0,425898	0,094031	2,107894	H	-0,091021	-0,979525	1,970155

1P	B3LYP/TZVP			**1P H2 TS**	B3LYP/TZVP			**1P H2 Product**	B3LYP/TZVP		
12				14				14			
E(SCF)=	-497,937017			E(SCF)=	-499,111796			E(SCF)=	-499,272993		
C	0,986923	-1,109263	-0,846778	C	0,185494	0,075870	-1,424397	C	0,003133	-1,387609	-0,009989
C	0,099152	0,101947	-1,264092	P	-1,178039	0,363137	-0,132522	P	1,372803	-0,062285	0,004221
C	-0,921058	0,419195	-0,144114	C	-0,055032	0,272625	1,303770	C	0,101183	1,325148	0,170233
P	-0,213100	-0,506704	1,341480	C	1,338003	0,206123	0,761123	C	-1,233899	0,757583	-0,322299
C	1,233663	-1,173611	0,632619	C	1,438933	0,620208	-0,721670	C	-1,339763	-0,668254	0,230906
H	0,217261	0,407639	2,328617	H	-1,714713	-0,941242	0,045995	H	1,508315	0,041314	-1,414286
H	-1,034140	1,487548	0,036581	H	-0,035978	0,605443	-2,350277	H	0,204523	-2,134672	0,757549
H	-1,909017	0,013006	-0,363176	H	0,288129	-0,986613	-1,652171	H	0,016441	-1,898720	-0,972944
H	0,754137	0,965638	-1,400187	H	1,453827	1,713113	-0,782062	H	-1,536927	-0,617664	1,306165
H	-0,400779	-0,073933	-2,219298	H	2,356472	0,255893	-1,190851	H	-2,172006	-1,216985	-0,217103
H	1,931455	-1,119694	-1,397791	H	2,079454	0,682665	1,407055	H	-2,081600	1,373662	-0,007979
H	0,514081	-2,072606	-1,103786	H	1,532832	-0,878201	0,838901	H	-1,239871	0,732568	-1,416647
				H	-0,011788	2,277387	1,799319	H	0,038442	1,598784	1,226464
				H	-0,163976	1,549039	2,119280	H	0,426138	2,210821	-0,376988

2N	B3LYP/TZVP			**2N H2 TS**	B3LYP/TZVP			**2N H2 Product**	B3LYP/TZVP		
10				12				12			
E(SCF)=	-210,163156			E(SCF)=	-211,304894			E(SCF)=	-211,433988		

C	0,048451	0,079805	-1,211806
C	-0,921072	0,151554	-0,059304
C	-0,25836	-0,240715	1,026254
N	1,08379	-0,560466	0,633945
C	1,371151	-0,408522	-0,65009
H	1,768064	-0,882623	1,304152
H	-0,571348	-0,337955	2,055
H	-1,953665	0,460834	-0,10125
H	0,205143	1,044864	-1,707716
H	-0,274563	-0,60072	-2,008324

C	1,442011	-0,213318	-0,494873
C	0,149477	0,197716	-1,172129
C	-0,856233	0,242622	-0,039491
C	-0,275015	-0,285392	1,039699
N	1,063142	-0,626605	0,741081
H	1,713266	-0,958213	1,434521
H	-0,679920	-0,493361	2,018392
H	-1,883331	0,559417	-0,121169
H	0,239432	1,113483	-1,749677
H	-0,130143	-0,603168	-1,873843
H	2,407174	0,462735	-0,622075
H	2,218107	1,479892	-0,275517

C	1,202172	-0,051698	0,056176
C	0,319518	1,205401	-0,124199
C	-1,069648	0,646728	0,107440
C	-1,015106	-0,685116	0,028803
N	0,276291	-1,169524	-0,233331
H	0,512725	-2,048306	0,205912
H	-1,836865	-1,386230	0,081842
H	-1,967242	1,238830	0,193475
H	0,600002	2,004038	0,565227
H	0,413527	1,607792	-1,140512
H	2,062909	-0,072913	-0,612218
H	1,562882	-0,108640	1,091406

2P	B3LYP/TZVP		
10			
E(SCF)=	-496,70968		
C	-1,165143	-0,808671	0,003445
C	-1,240541	0,706846	-0,017012
C	-0,060509	1,334495	0,007485
P	1,199852	0,043287	0,307614
C	0,233011	-1,365635	-0,002351
H	2,311241	0,103678	-0,559601
H	0,086051	2,405362	0,025007
H	-2,19435	1,223072	-0,046965
H	-1,665661	-1,230124	-0,881658
H	-1,731584	-1,252472	0,835125

2P H2 TS	B3LYP/TZVP		
12			
E(SCF)=	-497,877962		
C	-0,112350	1,346381	0,184948
C	-1,247337	0,714164	-0,111219
C	-1,169868	-0,796943	-0,101578
C	0,233442	-1,312405	0,065695
P	1,305039	0,161684	0,283831
H	1,433866	-0,037528	1,690857
H	-0,009800	2,422314	0,243168
H	-2,188716	1,220887	-0,300513
H	-1,708157	-1,282994	-0,919398
H	-1,672944	-1,171718	0,808332
H	0,636701	-1,989297	-1,264118
H	0,642266	-1,584744	-1,958004

2P H2 Product	B3LYP/TZVP		
12			
E(SCF)=	-498,040004		
C	-0,060289	1,330990	0,082546
P	-1,337774	0,008721	-0,046261
C	0,020136	-1,293708	0,223265
C	1,369073	-0,616429	-0,121831
C	1,187682	0,875274	-0,005926
H	-1,846444	0,073582	1,288993
H	-0,314033	2,383337	0,115899
H	2,052935	1,530337	-0,040987
H	2,173986	-0,974195	0,527349
H	1,673931	-0,867809	-1,144535
H	-0,165474	-2,168580	-0,398022
H	0,006301	-1,614829	1,264177

3N	B3LYP/TZVP		
11			
E(SCF)=	-227,4595572		
C	-0,766564	0,932843	-0,071340
C	0,765625	0,933489	0,071441
N	1,062425	-0,509338	-0,072868
C	0,000639	-1,330312	0,000114
N	-1,061864	-0,510362	0,072240
H	2,000331	-0,864688	-0,022231
H	1,259776	1,525757	-0,699194
H	1,083487	1,301930	1,051470
H	-1,084832	1,301381	-1,051177
H	-1,261397	1,524130	0,699614
H	-1,999495	-0,866732	0,024625

3N H2 TS	B3LYP/TZVP		
13			
E(SCF)=	-228,583358		
N	-0,239623	-1,145226	-0,172267
C	1,123018	-0,632587	0,046577
C	0,882985	0,892107	0,168548
N	-0,506613	1,027680	-0,307238
C	-1,152053	-0,155842	-0,159184
H	-1,017791	1,854071	-0,039669
H	0,959705	1,217811	1,211662
H	1,572020	1,473053	-0,442814
H	1,563678	-1,045859	0,956708
H	1,765851	-0,881899	-0,799776
H	-0,501696	-2,070922	0,119748
H	-2,078689	-0,101653	1,686651
H	-2,163132	-0,243843	0,328381

3N H2 Product	B3LYP/TZVP		
13			
E(SCF)=			
N	-0,426338	1,187082	-0,134264
C	0,979827	0,787863	0,061827
C	0,984259	-0,782728	0,061520
N	-0,419667	-1,189231	-0,133880
C	-1,187864	-0,003176	0,264444
H	-0,582341	-1,369084	-1,119018
H	1,615233	-1,207719	-0,719806
H	1,346360	-1,159977	1,020400
H	1,608983	1,216961	-0,718596
H	1,338566	1,166912	1,021312
H	-0,589962	1,365778	-1,119358
H	-2,187529	-0,006338	-0,168966
H	-1,284604	-0,003240	1,354295

3P	B3LYP/TZVP
11	

3P H2 TS	B3LYP/TZVP
13	

3P H2 Product	B3LYP/TZVP
13	

E(SCF)=	-800,60366			E(SCF)=	-801,761120			E(SCF)=	-801,9207703			
C	-0,000747	-1,468789	-0,000773	C	-0,009402	-1,383176	-0,047963	C	-0,000036	-1,386796	0,000008	
P	1,367419	-0,416711	0,181840	P	1,491669	-0,337676	0,026353	P	1,570175	-0,330902	0,006450	
C	0,717888	1,314286	-0,271852	C	0,681989	1,395370	-0,101463	C	0,689652	1,298847	0,329805	
C	-0,715931	1,314893	0,271876	C	-0,759455	1,289694	0,420074	C	-0,689833	1,298803	-0,329644	
P	-1,368632	-0,415405	-0,181916	P	-1,398644	-0,311750	-0,344513	P	-1,570069	-0,330993	-0,006542	
H	2,351293	-0,777955	-0,775279	H	-2,409200	-0,768487	0,543011	H	-1,643289	-0,162606	1,410594	
H	1,334755	2,085546	0,187493	H	-0,783116	1,219213	1,510194	H	-0,597481	1,412972	-1,412459	
H	-2,345319	-0,776984	0,781859	H	1,864853	-0,538365	-1,331772	H	1,643039	-0,162030	-1,410634	
H	-0,725956	1,451563	1,355440	H	-0,076361	-2,179387	1,106048	H	-0,009274	-2,034258	0,876518	
H	-1,331284	2,086878	-0,188396	H	-0,063020	-1,787289	1,851674	H	0,009645	-2,034885	-0,875974	
H	0,727449	1,450345	-1,355485	H	1,262671	2,100343	0,494147	H	1,323586	2,115497	-0,026728	
				H	-1,361659	2,145851	0,112170	H	-1,323822	2,115621	0,026469	
				H	0,691669	1,738191	-1,136955	H	0,597298	1,412979	1,412571	

4N	B3LYP/TZVP			**4N H2 TS**	B3LYP/TZVP			**4N H2 Product**	B3LYP/TZVP		
9				11				11			
E(SCF)=	-226,254329			E(SCF)=	-227,367548			E(SCF)=	-227,4653488		
N	1,049511	-0,401215	0,000100	C	-1,099665	0,000030	-0,176724	C	1,179450	-0,000024	0,099224
C	0,673571	0,938061	-0,000026	N	-0,273781	-1,079435	-0,148350	N	0,299541	1,146495	-0,188052
C	-0,677361	0,935709	0,000193	C	1,035852	-0,674473	0,095710	C	-1,018497	0,666822	0,053183
N	-1,047782	-0,405318	0,000137	C	1,035925	0,674390	0,095717	C	-1,018528	-0,666780	0,053172
C	0,002516	-1,274405	-0,000622	N	-0,273673	1,079457	-0,148415	N	0,299493	-1,146510	-0,188046
H	-1,999783	-0,728837	0,000139	H	-0,617660	2,016632	-0,030701	H	0,547685	-1,979423	0,328272
H	-1,382864	1,747745	0,000313	H	1,843650	1,374405	0,207447	H	-1,856696	-1,343635	0,066197
H	1,375729	1,752988	-0,000065	H	1,843527	-1,374559	0,207375	H	-1,856636	1,343715	0,066216
H	2,002456	-0,722357	0,000685	H	-0,617786	-2,016490	-0,030818	H	0,547771	1,979400	0,328259
				H	-2,170358	0,000008	0,049720	H	2,059021	-0,000045	-0,546792
				H	-2,281861	0,000169	1,586115	H	1,511071	-0,000025	1,157061

4P	B3LYP/TZVP			**4P H2 TS**	B3LYP/TZVP			**4P H2 Product**	B3LYP/TZVP		
9				11				11			
E(SCF)=	-799,3747693			E(SCF)=	-800,527743			E(SCF)=	-800,6859433		
C	-0,000459	-1,444408	-0,000495	C	-0,007976	-1,343151	-0,040474	C	-0,002096	-1,300602	0,234193
P	1,333667	-0,354808	0,114873	P	1,489049	-0,271164	-0,045165	P	-1,519907	-0,274132	-0,209542
C	0,669415	1,337040	-0,061794	C	0,637639	1,376683	0,120788	C	-0,668702	1,330581	0,084732
C	-0,668751	1,337529	0,061849	C	-0,694851	1,354011	0,205999	C	0,664181	1,342578	0,081454
P	-1,333880	-0,354340	-0,114675	P	-1,416247	-0,270853	-0,262568	P	1,562961	-0,273256	-0,003647
H	2,370712	-0,596716	-0,813114	H	-2,343983	-0,613274	0,753426	H	1,619967	-0,363757	-1,432155
H	1,288758	2,224370	-0,093499	H	-1,304063	2,240663	0,346427	H	1,234770	2,262347	0,157954
H	-2,369940	-0,596632	0,813994	H	1,641286	-0,327116	-1,462569	H	-2,216975	-0,355555	1,034360
H	-1,287571	2,225224	0,092294	H	0,004148	-2,100077	1,153537	H	0,053218	-2,194893	-0,385399
				H	0,082827	-1,680705	1,874399	H	-0,041956	-1,615452	1,276398
				H	1,218887	2,285511	0,232912	H	-1,255135	2,242790	0,144408

5N	B3LYP/TZVP	**5N H2 TS**	B3LYP/TZVP	**5N H2 Product**	B3LYP/TZVP
8		10		10	
E(SCF)=	-242,292333	E(SCF)=	-243,400675	E(SCF)=	-243,505494

C	-0,337758	-1,211463	-0,000124	N	-0,117309	1,088248	-0,167185	N	0,187615	1,136285	-0,176695
N	0,906692	-0,634321	0,000068	C	-1,089586	0,120813	-0,170624	C	-1,083726	0,457268	0,102718
C	0,819863	0,739745	-0,000130	N	-0,373816	-1,027402	-0,150228	N	-0,687251	-0,930906	-0,194360
N	-0,419343	1,113817	0,000090	N	0,968617	-0,816703	0,118348	N	0,711758	-1,042066	0,059938
N	-1,089842	-0,098825	0,000024	C	1,084375	0,469154	0,096268	C	1,156140	0,152915	0,043170
H	-2,095362	-0,076135	0,000013	H	-0,311373	2,069069	-0,056924	H	0,333500	2,033977	0,260635
H	1,661487	1,411583	-0,000166	H	2,012810	0,998307	0,226668	H	2,206445	0,394848	0,109907
H	1,758692	-1,169835	0,000403	H	-0,749631	-1,947931	-0,005683	H	-1,177090	-1,628163	0,349339
				H	-2,144331	0,264934	0,115379	H	-1,876414	0,788469	-0,568715
				H	-2,118658	0,366822	1,560155	H	-1,405780	0,606580	1,151332

5P	B3LYP/TZVP			**5P H2 TS**	B3LYP/TZVP			**5P H2 Product**	B3LYP/TZVP		
8				10				10			
E(SCF)=	-815,427150			E(SCF)=	-816,580724			E(SCF)=	-816,738594		
P	0,230345	0,116891	-1,196718	C	1,734137	-0,598845	-0,671060	C	-0,107498	-1,304661	0,183827
N	-1,018518	0,046884	0,072412	P	1,231352	-1,130479	0,951749	P	-1,673441	-0,263574	0,208372
C	-0,477767	-0,204743	1,197601	C	-0,320296	-0,080069	1,105636	C	-0,700319	1,328617	-0,101032
P	1,266242	-0,849961	1,059087	N	-0,818343	0,358753	0,028000	N	0,563430	1,347052	-0,113551
C	1,695138	-0,567866	-0,572024	P	0,254456	0,202866	-1,406935	P	1,373871	-0,138941	0,374073
H	2,167219	-0,405138	2,053338	H	2,182005	-0,628405	1,875519	H	-1,753521	-0,071565	1,623709
H	-1,050534	-0,206787	2,121213	H	-0,870208	-0,005038	2,044565	H	-1,254574	2,244208	-0,315601
H	-0,303078	-0,663335	-2,248779	H	-0,282231	-1,020844	-1,904744	H	2,002099	-0,378422	-0,882591
				H	2,812214	0,321124	-0,715256	H	-0,072319	-1,856701	-0,754599
				H	2,672778	1,071784	-0,381238	H	-0,131388	-2,023015	1,002135

6N	B3LYP/TZVP			**6N H2 TS**	B3LYP/TZVP			**6N H2 Product**	B3LYP/TZVP		
59				61				61			
E(SCF)=	-952,544336			E(SCF)=	-953,687349			E(SCF)=	-953,804286		
C	4,595189	0,044664	-1,420442	C	-2,260145	-1,076210	-0,200850	C	-2,223871	-0,954235	-0,433677
C	3,769996	-1,244614	-1,390929	C	-1,388314	-0,009281	0,106661	C	-1,371841	0,123016	-0,078205
C	3,126154	-1,469353	-0,019782	C	-1,778652	1,328831	-0,128467	C	-1,821279	1,452231	-0,287888
C	2,265258	-0,282118	0,473944	C	-3,084370	1,574441	-0,554691	C	-3,123452	1,672557	-0,739824
C	3,102756	1,022423	0,373892	C	-3,978738	0,539355	-0,774973	C	-3,975086	0,618209	-1,024729
C	3,744371	1,245791	-0,999639	C	-3,556996	-0,769927	-0,620599	C	-3,514560	-0,681273	-0,890863
C	1,017444	-0,139070	-0,385111	N	-0,068637	-0,280132	0,644040	N	-0,051801	-0,097690	0,429074
N	-0,004788	-0,073169	0,426244	C	1,010916	-0,363830	-0,132070	C	1,016464	-0,518590	-0,467544
C	0,270137	-0,133675	1,947042	C	2,260770	-0,399797	0,723571	C	2,300691	-0,484257	0,389652
C	1,755301	-0,531304	1,923806	C	1,707726	-0,773189	2,122411	C	1,737357	-0,820149	1,788975
C	-1,360573	0,060284	-0,080739	C	0,201967	-0,425894	2,135107	C	0,278635	-0,300040	1,866868
C	-1,895895	1,340417	-0,321455	C	2,905765	1,019692	0,723836	C	2,974319	0,907834	0,361937
C	-3,227192	1,429430	-0,734004	C	3,522425	1,404539	-0,625047	C	3,661707	1,237213	-0,969870
C	-3,995730	0,295398	-0,940507	C	4,553669	0,371961	-1,088109	C	4,658265	0,150660	-1,382608
C	-3,424040	-0,957372	-0,783514	C	3,960963	-1,039713	-1,092333	C	3,990269	-1,227256	-1,399663
C	-2,099736	-1,104562	-0,367920	C	3,341559	-1,397305	0,260177	C	3,330750	-1,541524	-0,052473
C	-1,052075	2,608781	-0,285121	C	-0,815877	2,506083	-0,036549	C	-0,900269	2,654537	-0,128207
C	-0,663824	3,014599	-1,719649	C	-1,359325	3,678780	0,793445	C	-1,479614	3,751166	0,777339
C	-1,476981	-2,495737	-0,371514	C	-1,833239	-2,540653	-0,205692	C	-1,772031	-2,410843	-0,410715
C	-2,341257	-3,559571	0,320357	C	-1,789918	-3,077774	-1,648777	C	-1,596988	-2,949727	-1,843127
C	-1,142820	-2,910606	-1,816701	C	-0,419775	2,978705	-1,447834	C	-0,527039	3,235865	-1,504774
C	-1,724917	3,776612	0,450640	C	-2,735490	-3,437236	0,658251	C	-2,716514	-3,324666	0,386920

C	-0,609810	-1,167059	2,651929
C	0,036772	1,232506	2,602320
H	1,856573	-1,590820	2,170983
H	2,327434	0,027848	2,666029
H	-3,661722	2,403810	-0,916933
H	-4,012471	-1,838420	-1,005783
H	-5,028335	0,387014	-1,255667
H	-0,529878	-2,443937	0,161324
H	-2,600130	-3,270027	1,340518
H	-3,272346	-3,744054	-0,219467
H	-1,801676	-4,508702	0,364375
H	-2,048949	-2,987418	-2,422757
H	-0,645970	-3,884436	-1,828190
H	-0,479849	-2,180534	-2,282682
H	-0,125347	2,382535	0,234841
H	-0,132228	2,203338	-2,218336
H	-1,549000	3,259985	-2,311665
H	-0,014616	3,894150	-1,703963
H	-2,613156	4,132271	-0,075537
H	-1,034320	4,620106	0,523687
H	-2,026690	3,499671	1,462636
H	3,911644	-1,645054	0,726234
H	2,511187	-2,374746	-0,039229
H	2,984371	-1,186756	-2,148092
H	4,399249	-2,103665	-1,642935
H	3,892087	0,963621	1,132972
H	2,483574	1,884154	0,639725
H	4,356280	2,152611	-0,969963
H	2,960420	1,410504	-1,742577
H	5,008533	0,206349	-2,420072
H	5,450813	-0,052460	-0,740357
H	-1,669022	-0,918675	2,567652
H	-0,454579	-2,170629	2,259463
H	-0,355885	-1,184362	3,714219
H	-0,998634	1,556241	2,490888
H	0,245721	1,155236	3,671580
H	0,689271	2,002240	2,191948

C	-0,624164	-1,544006	2,773492
C	-0,097797	0,880645	2,881901
H	1,831769	-1,847775	2,273083
H	2,238504	-0,265408	2,929645
H	-3,401955	2,594616	-0,729585
H	-4,240585	-1,577377	-0,850609
H	-4,991003	0,752525	-1,097363
H	-0,813199	-2,598548	0,172009
H	-2,813210	-3,079036	1,684946
H	-3,747399	-3,497462	0,251275
H	-2,336388	-4,454039	0,684509
H	-2,782255	-3,070033	-2,106717
H	-1,423223	-4,106858	-1,652398
H	-1,115368	-2,485737	-2,266580
H	0,092939	2,157009	0,445396
H	0,008299	2,160980	-2,029196
H	-1,285890	3,362727	-1,992037
H	0,321459	3,779776	-1,387636
H	-2,224455	4,147149	0,319257
H	-0,592547	4,450162	0,899205
H	-1,659321	3,362710	1,793801
H	4,129578	-1,403146	1,023952
H	2,911277	-2,398959	0,220978
H	3,193685	-1,125126	-1,869008
H	4,732578	-1,773092	-1,343472
H	3,686800	1,019711	1,493026
H	2,175015	1,772355	1,026849
H	3,984538	2,393012	-0,545048
H	2,728257	1,486989	-1,373007
H	4,927407	0,631107	-2,082720
H	5,418222	0,400027	-0,413385
H	0,973119	-0,982969	-1,140027
H	1,083542	-2,115592	-1,111702
H	-0,345456	-1,636195	3,825822
H	-1,692026	-1,325804	2,731526
H	-0,440232	-2,503937	2,294417
H	0,092820	0,737183	3,947245
H	0,525697	1,705140	2,540217
H	-1,144569	1,165773	2,767839

C	-0,619594	-1,325791	2,581630
C	0,185270	1,012081	2,670754
H	1,736292	-1,906428	1,915728
H	2,356110	-0,406880	2,588331
H	-3,470968	2,687893	-0,888297
H	-4,170034	-1,502770	-1,153413
H	-4,984167	0,807672	-1,371615
H	-0,797901	-2,446252	0,071152
H	-2,874407	-2,954834	1,400629
H	-3,694329	-3,410423	-0,091722
H	-2,298803	-4,332503	0,454941
H	-2,550782	-2,966531	-2,375692
H	-1,206584	-3,970726	-1,823829
H	-0,906691	-2,332577	-2,420690
H	0,016502	2,289565	0,327708
H	-0,078945	2,476065	-2,148038
H	-1,405715	3,630171	-2,021255
H	0,190970	4,052889	-1,394299
H	-2,365908	4,215042	0,337766
H	-0,742210	4,542921	0,932721
H	-1,761973	3,357946	1,755122
H	4,111416	-1,606536	0,715316
H	2,848683	-2,523441	-0,087454
H	3,237001	-1,257096	-2,195218
H	4,723196	-2,002127	-1,641917
H	3,724549	0,937281	1,161019
H	2,240969	1,681184	0,597275
H	4,166674	2,204080	-0,888179
H	2,909590	1,354135	-1,757477
H	5,086674	0,379767	-2,362459
H	5,493544	0,135861	-0,672034
H	1,067764	0,150742	-1,330913
H	0,872011	-1,534483	-0,868973
H	-0,322836	-1,411305	3,629833
H	-1,666096	-1,015673	2,557778
H	-0,542361	-2,315755	2,134574
H	0,444202	0,830797	3,716820
H	0,859110	1,776474	2,286268
H	-0,831480	1,407564	2,647534

6P	B3LYP/TZVP		
59			
E(SCF)=	-1239,103484		
C	-3,359198	0,520456	0,607986
C	-2,510084	-0,684067	0,093149
C	-3,433000	-1,586583	-0,767453
C	-4,179153	-0,839755	-1,875145
C	-4,997894	0,325716	-1,313487
C	-4,114065	1,269934	-0,494490
C	-1,383287	-0,100545	-0,755533
P	0,020609	-0,536584	0,042587

6P H2 TS	B3LYP/TZVP		
61			
E(SCF)=	-1240,254925		
C	-3,765023	0,645861	0,474203
C	-2,612535	-0,369813	0,262120
C	-3,214935	-1,575411	-0,528179
C	-3,909330	-1,174257	-1,830880
C	-5,011128	-0,140102	-1,584154
C	-4,474273	1,069843	-0,814153
C	-1,458311	0,196680	-0,577382
P	-0,029491	-0,455137	0,159147

6P H2 Product	B3LYP/TZVP		
61			
E(SCF)=	-1240,405390		
C	-2,920678	-0,217816	-0,443302
C	-1,627970	0,335648	-0,210516
C	-1,517729	1,739535	-0,028795
C	-2,656705	2,539702	-0,152478
C	-3,902565	1,999084	-0,413404
C	-4,027099	0,627288	-0,540769
P	-0,234438	-0,938990	-0,322747
C	1,416707	-0,207660	-0,877748

C	-0,531464	-1,178060	1,748869
C	0,246681	-2,408350	2,226840
C	-1,975195	-1,538668	1,314482
C	1,641128	0,302607	-0,178469
C	2,765208	-0,494340	-0,499207
C	3,996938	0,132684	-0,686797
C	4,124130	1,507350	-0,567645
C	3,016885	2,281165	-0,258799
C	1,760318	1,707945	-0,054919
C	2,677741	-2,001616	-0,706616
C	2,751925	-2,352358	-2,202272
C	0,587025	2,630739	0,245024
C	0,877655	3,612207	1,390701
C	-0,468576	-0,086300	2,825677
C	0,137788	3,371674	-1,025990
C	3,724964	-2,781171	0,101718
H	-2,832145	-2,393506	-1,196858
H	-4,722114	2,058596	-0,039949
H	-2,652890	-1,454672	2,169263
H	-1,979611	-2,587711	1,007586
H	4,866616	-0,460915	-0,938541
H	3,129721	3,354673	-0,176843
H	5,088178	1,978042	-0,720605
H	-0,250826	2,007490	0,554909
H	1,209522	3,091095	2,291084
H	1,645598	4,341613	1,124073
H	-0,027314	4,171856	1,638239
H	0,936982	4,007359	-1,416011
H	-0,722872	4,008906	-0,807997
H	-0,154184	2,663451	-1,801916
H	1,694640	-2,327504	-0,357985
H	1,963323	-1,848054	-2,763159
H	3,712636	-2,054395	-2,629090
H	2,638409	-3,429388	-2,347991
H	4,740654	-2,579624	-0,245352
H	3,553647	-3,855204	-0,000227
H	3,679289	-2,530238	1,163166
H	-4,082028	0,118855	1,328703
H	-2,725026	1,217386	1,161363
H	-3,394564	1,756992	-1,156195
H	-4,161692	-2,060562	-0,096609
H	-4,831214	-1,538107	-2,408798
H	-3,453002	-0,458209	-2,596577
H	-5,483906	0,873892	-2,125757
H	-5,801538	-0,065582	-0,676665
H	-0,865980	-0,475743	3,768799
H	0,560584	0,230861	3,010044
H	-1,050508	0,794775	2,558633
H	-0,204384	-2,805342	3,141848
H	0,242757	-3,205632	1,481741
H	1,285268	-2,160691	2,459123

C	-0,619092	-0,491821	1,969269
C	-2,086240	-0,896453	1,659973
C	1,686431	0,149966	-0,217559
C	2,649179	-0,866790	-0,461699
C	3,950220	-0,494126	-0,801854
C	4,316623	0,837446	-0,901775
C	3,378723	1,824903	-0,653969
C	2,064079	1,510615	-0,305274
C	2,340856	-2,361612	-0,409023
C	2,305965	-2,966243	-1,822054
C	1,102887	2,662806	-0,065398
C	1,610013	3,641083	1,006029
C	0,784842	3,403100	-1,375730
C	3,302323	-3,134822	0,506419
H	-2,420949	-2,299156	-0,726163
C	-0,537103	0,864105	2,673027
H	-5,292274	1,752257	-0,564107
C	0,103938	-1,556352	2,797952
H	-1,725172	2,100546	-0,259270
H	-2,149441	-1,986942	1,665760
H	-2,735262	-0,539748	2,464605
H	-4,496976	0,161827	1,131094
H	-3,391743	1,522051	1,008994
H	-3,938795	-2,068982	0,132063
H	-3,786092	1,636566	-1,448532
H	-4,328416	-2,065072	-2,308423
H	-3,166453	-0,761641	-2,518495
H	-5,818815	-0,605449	-1,005760
H	-5,452280	0,179743	-2,532481
H	4,688836	-1,261155	-0,997289
H	5,331691	1,104440	-1,171534
H	3,671044	2,864693	-0,730836
H	0,167831	2,245054	0,299482
H	0,040656	4,183122	-1,200344
H	1,678363	3,877264	-1,789621
H	0,387924	2,720260	-2,128781
H	0,844410	4,390990	1,218633
H	1,846602	3,126397	1,939089
H	2,507713	4,172061	0,682052
H	1,339461	-2,481959	0,006000
H	2,041691	-4,025752	-1,777600
H	1,569039	-2,458659	-2,447083
H	3,278007	-2,883025	-2,314343
H	2,982547	-4,176388	0,588289
H	4,324599	-3,137707	0,122066
H	3,325056	-2,708453	1,511223
H	-1,625603	1,437104	-0,890626
H	-1,019133	0,800077	3,654621
H	0,499050	1,168880	2,833394
H	-1,042851	1,650930	2,110345
H	-0,363340	-1,654451	3,782780
	0,071419	-2,534057	2,313377

C	2,532216	-0,802039	0,048348
C	3,536600	-1,644789	-0,777493
C	4,417804	-0,825286	-1,725803
C	5,171483	0,278048	-0,978683
C	4,202262	1,158578	-0,186322
C	3,327312	0,324447	0,756916
C	1,852850	-1,746275	1,086500
C	0,394892	-1,369830	1,432882
C	-0,221468	2,471791	0,302782
C	-0,341579	3,336528	1,569979
C	-3,193756	-1,714700	-0,611100
C	-3,550267	-2,053879	-2,066915
C	0,266933	3,324551	-0,881914
C	-4,269463	-2,227607	0,359976
C	-0,356576	-2,607685	1,948670
C	0,290463	-0,273826	2,498663
H	1,838976	-2,754596	0,661500
H	2,455401	-1,807736	1,998750
H	-2,564774	3,611920	-0,031442
H	-5,005239	0,201384	-0,726553
H	-4,771068	2,640797	-0,504538
H	-2,277578	-2,255289	-0,382494
H	-4,021513	-1,981164	1,394528
H	-5,255426	-1,808937	0,146827
H	-4,353307	-3,314516	0,282863
H	-4,460125	-1,539109	-2,385338
H	-3,714581	-3,128502	-2,181403
H	-2,744650	-1,761089	-2,742932
H	0,536802	1,726555	0,512669
H	0,381760	2,726964	-1,788168
H	-0,442054	4,124755	-1,105671
H	1,230255	3,788177	-0,653529
H	-1,022560	4,177764	1,427786
H	0,635117	3,749704	1,835263
H	-0,704364	2,753621	2,417831
H	4,184817	-2,186009	-0,077468
H	2,984372	-2,405217	-1,338264
H	3,800843	-0,374483	-2,510865
H	5,122060	-1,489252	-2,235193
H	3,974673	-0,141298	1,509030
H	2,650784	0,982722	1,304860
H	4,752716	1,904726	0,393938
H	3,571055	1,718611	-0,884543
H	5,752991	0,884379	-1,678902
H	5,890703	-0,179024	-0,288529
H	1,552494	-0,544391	-1,906136
H	1,454394	0,875864	-0,908609
H	-1,399450	-2,374364	2,175831
H	-0,343234	-3,418951	1,218633
H	0,102683	-2,974179	2,872715
H	-0,749011	0,020930	2,655472
H	0,675042	-0,650391	3,453133

				1,151362	-1,290256	2,960760	H	0,855567	0,621622	2,253310

For your convenience now all reactant molecules

H2			
2			
E(SCF)=	-1,179649		
H	0,000000	0,000000	-0,001893
H	0,000000	0,000000	0,741893

CH4			
5			
E(SCF)=	-40,537041		
C	-0,034061	-0,058802	0,194058
H	0,200323	-0,339701	1,220237
H	0,887648	0,169986	-0,340194
H	-0,543620	-0,885472	-0,300364
H	-0,681410	0,817602	0,194263

NH3			
4			
E(SCF)=	-56,583709		
N	-0,009781	0,016942	-0,006917
H	0,004269	-0,007394	1,005765
H	0,949667	-0,007395	-0,331230
H	-0,468430	-0,826133	-0,331230

OH2			
3			
E(SCF)=	-76,460622		
O	-0,020420	0,000000	-0,014439
H	0,017135	0,000000	0,947426
H	0,898954	0,000000	-0,299652

SiH4			
5			
E(SCF)=	-291,908643		
H	-0,000003	0,000000	-0,397497
Si	-0,000002	0,000000	1,088999
H	1,401488	0,000000	1,584502
H	-0,700742	1,213736	1,584498
H	-0,700742	-1,213736	1,584498

C6H6			
12			
E(SCF)=	-232,328392		
H	0,000000	0,000000	0,013534
C	0,000000	0,000000	1,096916

C	1,205580	0,000000	1,792958
C	1,205580	0,000000	3,185042
C	0,000000	0,000000	3,881084
C	-1,205580	0,000000	3,185042
C	-1,205580	0,000000	1,792958
H	2,143817	0,000000	1,251267
H	2,143817	0,000000	3,726733
H	0,000000	0,000000	4,964466
H	-2,143817	0,000000	3,726733
H	-2,143817	0,000000	1,251267

C2H6

8

E(SCF)= -79,862335

C	0,027362	-0,011889	-0,038606
C	-0,027362	0,011889	1,488606
H	1,056186	0,047267	-0,400803
H	-0,409693	-0,929820	-0,438142
H	0,409693	0,929820	1,888142
H	-1,056186	-0,047267	1,850803
H	0,521746	-0,828395	1,919524
H	-0,521746	0,828395	-0,469524

C2H4

6

E(SCF)= -78,621545

H	-0,029073	0,000000	0,008170
C	0,003948	0,000000	1,091279
C	1,152196	0,000000	1,754221
H	-0,950563	0,000000	1,604238
H	1,185217	0,000000	2,837330
H	2,106707	0,000000	1,241262

C2H2

4

E(SCF)= -77,362334

C	0,001933	0,000000	0,003019
C	0,000801	0,000000	1,201002
H	0,017358	0,000000	-1,059663
H	0,008894	0,000000	2,263763

CH3F

5

E(SCF)= -139,802536

C	0,034266	-0,155202	0,101100
H	-0,099637	0,539570	0,931994
H	1,038938	-0,053571	-0,312718
H	-0,710053	0,038793	-0,672752
F	-0,130262	-1,455531	0,570266

CH3Cl

5			
E(SCF)=	-500,150822		
C	0,026585	-0,046047	0,002019
H	0,016215	-0,028085	1,087623
H	1,045612	-0,024667	-0,371829
H	-0,501445	-0,917860	-0,371829
Cl	-0,827856	1,433889	-0,597317

****

Now reaction scheme molecules
1N without hydrogen (see above)

1N	B3LYP/TZVP		
12			
E(SCF)=	-211,393483		
C	0,085575	0,118916	-1,238463
C	-0,879063	0,375513	-0,074658
N	-0,199926	-0,348680	1,039375
C	0,794614	-1,153576	0,773091
C	0,957057	-1,064995	-0,730486
H	-0,550712	-0,244589	1,982352
H	-1,000785	1,430455	0,175538
H	-1,870633	-0,055459	-0,238501
H	0,707104	0,998125	-1,414702
H	-0,440998	-0,104241	-2,165726
H	2,009742	-0,974637	-1,002654
H	0,626702	-2,028198	-1,137206

1N CH4 TS				**1N CH4 Product**			
17				17			
E(SCF)=	-251,874273			E(SCF)=	-251,989739		
C	1,579607	-0,300239	0,651595	C	1,440679	0,295897	0,815786
C	1,291280	0,736194	-0,462077	C	1,395989	0,461213	-0,721286
C	0,010292	0,205301	-1,133910	C	-0,075195	0,112556	-1,102761
N	-0,540957	-0,687276	-0,101495	N	-0,844945	0,015900	0,146317
C	0,229266	-0,879089	0,979165	C	0,122056	-0,432458	1,160458
C	-0,480786	0,590068	2,757518	C	-0,383564	-0,213103	2,576419
H	-1,474693	-1,057346	-0,172309	H	-1,184029	0,938032	0,406992
H	-0,694764	1,001894	-1,386043	H	-0,530316	0,842949	-1,772497
H	0,225184	-0,358300	-2,047288	H	-0,110627	-0,855502	-1,609917
H	1,099091	1,712343	-0,015475	H	1,659093	1,477654	-1,018489
H	2,111614	0,844985	-1,171184	H	2,098262	-0,209333	-1,220034
H	2,077904	0,122557	1,520630	H	1,448814	1,273017	1,308606
H	2,210865	-1,108451	0,263200	H	2,323339	-0,247962	1,158568
H	-0,186562	-0,853107	2,049574	H	0,268809	-1,508512	1,002709
H	0,118700	0,520193	3,665442	H	0,341850	-0,573364	3,308769
H	-0,293897	1,516211	2,217995	H	-0,548201	0,851915	2,769594
H	-1,544234	0,450018	2,954020	H	-1,325231	-0,739638	2,740728

1N NH3 TS				**1N NH3 Product**			
16				16			

E(SCF)=	-267,938613			E(SCF)=	-268,033233		
C	-0,018770	0,584951	1,236812	C	0,753093	-0,093759	-0,592769
C	1,104028	1,334666	0,577950	C	-0,137924	1,161426	-0,476137
C	0,924487	1,032439	-0,927814	C	-1,172495	0,755499	0,581267
C	0,217940	-0,335242	-0,939945	C	-1,424358	-0,725820	0,251894
N	-0,387382	-0,380327	0,402611	N	-0,206102	-1,183721	-0,442655
N	-1,738388	2,117979	1,747143	N	1,843352	-0,204715	0,386059
H	-1,092013	-1,059487	0,644610	H	0,227580	-1,996685	-0,029073
H	-0,547232	-0,414854	-1,715008	H	-1,630223	-1,319148	1,146908
H	0,918799	-1,166030	-1,065481	H	-2,293259	-0,826721	-0,408061
H	0,276745	1,786739	-1,376880	H	-0,751205	0,860369	1,585434
H	1,863197	1,016765	-1,480198	H	-2,081033	1,357716	0,546701
H	1,094227	2,394413	0,819161	H	0,440824	2,047404	-0,212741
H	2,050958	0,920224	0,946300	H	-0,631758	1,351643	-1,433291
H	-0,718927	1,030315	2,036901	H	1,232411	-0,140230	-1,575397
H	-1,338158	3,027161	1,513369	H	2,618167	0,402739	0,140975
H	-2,377633	1,899886	0,982009	H	1,533719	0,046246	1,319897

1N OH2 TS				**1N OH2 Product**			
15				15			
E(SCF)=	-287,838444			E(SCF)=	-287,914256		
N	0,115454	-0,034716	-0,041587	N	-0,159579	-1,098450	-0,559431
C	0,045535	-0,027412	1,431757	C	-1,344764	-0,786155	0,266168
C	1,533297	0,030079	1,824610	C	-1,249968	0,733402	0,528230
C	2,235921	0,549865	0,547456	C	-0,167073	1,212819	-0,453015
C	1,295291	0,190842	-0,562503	C	0,757505	-0,003461	-0,544094
O	1,922161	-1,664036	-1,711031	O	1,624442	-0,102646	0,615634
H	-0,663957	-0,329706	-0,611520	H	0,278431	-1,984457	-0,348505
H	-0,517290	0,845798	1,772712	H	-2,253922	-1,046032	-0,283498
H	-0,459715	-0,924692	1,790986	H	-1,354127	-1,346572	1,205503
H	1,705092	0,661801	2,694747	H	-2,203240	1,241468	0,382257
H	1,891561	-0,973282	2,054556	H	-0,924664	0,916680	1,552295
H	2,350143	1,640232	0,562550	H	-0,588049	1,419812	-1,439957
H	3,222155	0,121085	0,385171	H	0,358650	2,105682	-0,112682
H	1,592102	-0,245703	-1,589604	H	1,383508	-0,004708	-1,443221
H	2,879355	-1,762200	-1,801259	H	2,326967	0,553656	0,531513

1N SiH4 TS				**1N SiH4 Product**			
17				17			
E(SCF)=	-503,275336			E(SCF)=	-503,368318		
C	0,348040	-0,982913	0,807641	C	0,119508	-0,399721	1,099149
C	1,658559	-0,319656	0,452916	C	1,487555	0,230955	0,731379
C	1,309154	0,708665	-0,649209	C	1,435055	0,364552	-0,813673
C	0,046806	0,116729	-1,297446	C	-0,038613	0,033872	-1,186227
N	-0,456164	-0,768958	-0,226932	N	-0,822413	0,053599	0,060592
Si	-0,584766	0,616453	3,157849	Si	-0,511359	-0,050182	2,860640
H	-1,386528	-1,158559	-0,271282	H	-1,110211	1,008094	0,255277
H	-0,700320	0,868980	-1,560291	H	-0,465957	0,726401	-1,912374
H	0,272022	-0,469840	-2,193151	H	-0,102551	-0,969419	-1,615727
H	1,076340	1,672143	-0,193240	H	1,708685	1,372888	-1,128470
H	2,111344	0,859003	-1,370923	H	2,128065	-0,323684	-1,300580
H	2,152641	0,117792	1,318447	H	1,592713	1,217800	1,191369

H	2,317760	-1,102060	0,058503	H	2,328086	-0,374749	1,074499
H	-0,081721	-0,783143	1,978124	H	0,204525	-1,489662	0,999642
H	-0,163315	0,373552	4,577303	H	0,552301	-0,376135	3,851309
H	-0,097903	1,995739	2,813291	H	-0,839638	1,401302	2,975711
H	-2,084040	0,712028	3,167759	H	-1,725396	-0,848761	3,176337

1N C6H6 CC TS				**1N C6H6 CC Product**			
24				24			
E(SCF)=	-443,686173			E(SCF)=	-443,720937		
N	0,731566	0,050236	-0,835847	N	0,651435	-0,314765	-0,729378
C	-0,065767	-0,216114	0,380333	C	0,093828	-0,514210	0,612150
C	1,025909	-0,312609	1,459339	C	1,030275	0,328138	1,496462
C	2,215902	0,450397	0,827185	C	2,382032	0,328947	0,731859
C	1,996741	0,363912	-0,668524	C	2,076236	-0,419616	-0,564345
C	3,173143	-0,496127	-1,863623	C	3,012131	-0,381649	-1,720209
C	3,338436	-1,699404	-1,078998	C	2,852897	-1,706912	-0,854473
C	2,496578	-2,783267	-1,284896	C	2,222489	-2,833056	-1,531528
C	1,599243	-2,805255	-2,349372	C	1,636769	-2,716404	-2,743676
C	1,673421	-1,773194	-3,312677	C	1,801977	-1,520176	-3,545068
C	2,492311	-0,687514	-3,130081	C	2,520304	-0,470656	-3,100136
H	0,355312	-0,096418	-1,764693	H	0,282459	-0,957791	-1,419704
H	-0,755479	0,614017	0,558895	H	-0,943529	-0,178152	0,650941
H	-0,648510	-1,130543	0,266266	H	0,123154	-1,568656	0,927582
H	0,701186	0,102103	2,413530	H	0,647973	1,345079	1,588802
H	1,300948	-1,356316	1,615952	H	1,118897	-0,084361	2,501907
H	2,180663	1,514467	1,089409	H	2,703780	1,349548	0,513651
H	3,189215	0,076795	1,137153	H	3,180802	-0,155033	1,295253
H	3,996488	0,205868	-1,864620	H	3,915920	0,200721	-1,570619
H	4,080906	-1,725298	-0,291508	H	3,646732	-1,940525	-0,153032
H	2,571610	-3,645106	-0,629818	H	2,255378	-3,797928	-1,037358
H	0,954545	-3,659353	-2,511693	H	1,149037	-3,573897	-3,192123
H	1,114416	-1,871208	-4,237980	H	1,434444	-1,528920	-4,564395
H	2,584756	0,070134	-3,899119	H	2,788331	0,331400	-3,778314

1N C6H6 CH TS				**1N C6H6 CH Product**			
24				24			
E(SCF)=	-443,670574			done:	-443,781658		
N	0,444174	-0,725471	0,998916	N	0,638299	-0,539569	1,275516
H	0,199336	-1,398384	1,707421	H	0,097151	-0,811920	2,082599
C	-0,179421	-0,749369	-0,337714	C	-0,037297	-0,788748	-0,013532
H	0,169037	-1,622040	-0,898810	H	0,444458	-1,624987	-0,531275
H	-1,267204	-0,804289	-0,261880	H	-1,090567	-1,057347	0,117902
C	0,313613	0,574207	-0,948633	C	0,120783	0,515960	-0,814063
H	-0,434385	1,353255	-0,798029	H	-0,771397	1,137686	-0,714299
H	0,506421	0,485921	-2,017419	H	0,280860	0,337662	-1,878057
C	1,579196	0,907561	-0,123623	C	1,316710	1,201589	-0,141384
H	1,767040	1,973838	-0,026943	H	1,345977	2,278751	-0,302525
H	2,465998	0,449325	-0,577884	H	2,253584	0,775817	-0,508822
C	1,344072	0,237519	1,204337	C	1,149499	0,831767	1,351144
C	0,293550	2,004950	2,457759	C	0,281434	1,829363	2,112187
C	0,749689	3,301146	2,674382	C	0,883817	2,940076	2,711149

C	-0,100140	4,268728	3,214332	C	0,129491	3,888800	3,390961
C	-1,414737	3,937812	3,535701	C	-1,251485	3,742167	3,490414
C	-1,876471	2,642059	3,318510	C	-1,863883	2,639075	2,906708
C	-1,016939	1,683916	2,776980	C	-1,103054	1,692268	2,225242
H	1,774576	3,575456	2,434177	H	1,960787	3,056936	2,648907
H	0,260892	5,277661	3,385343	H	0,619529	4,739086	3,850415
H	-2,076328	4,687235	3,954134	H	-1,842071	4,476666	4,024171
H	-2,900438	2,383112	3,567662	H	-2,937295	2,511501	2,982754
H	-1,390703	0,674754	2,603979	H	-1,596431	0,834746	1,784022
H	1,372941	0,838703	2,196246	H	2,131061	0,828127	1,836013

1N C2H6 CC TS				**1N C2H6 CC Product**			
20				20			
E(SCF)=	-291,111422			E(SCF)=	-291,317040		
N	0,038961	0,191772	0,006329	N	-0,218911	-0,922375	-0,750016
C	0,056998	-0,233147	1,423014	C	-1,588466	-0,787687	-0,237747
C	1,527122	-0,000988	1,831878	C	-1,699495	0,704438	0,163107
C	2,150081	0,765598	0,625322	C	-0,263441	1,260775	0,033212
C	1,190585	0,593404	-0,529779	C	0,647914	0,016867	-0,012104
C	1,742853	0,103257	-2,326844	C	1,936942	0,257381	-0,797796
C	2,106754	-1,552912	-1,084108	C	0,984591	-0,471396	1,411990
H	-0,814135	0,139983	-0,529596	H	0,121313	-1,876358	-0,707524
H	-0,638179	0,381613	2,000617	H	-2,306558	-1,063867	-1,013039
H	-0,248995	-1,277565	1,529675	H	-1,789421	-1,427374	0,633107
H	1,600242	0,570287	2,756830	H	-2,390094	1,244558	-0,484768
H	2,033107	-0,950872	1,999506	H	-2,076706	0,801616	1,182036
H	2,186044	1,838282	0,844617	H	-0,155356	1,811355	-0,902720
H	3,164856	0,451931	0,391480	H	0,004731	1,934939	0,848037
H	2,514230	0,865578	-2,373379	H	2,550836	1,025649	-0,321064
H	2,048092	-0,707626	-3,012058	H	2,536406	-0,655607	-0,855761
H	0,824632	0,506065	-2,752601	H	1,704540	0,573895	-1,815427
H	3,115740	-1,701763	-1,459544	H	1,609285	0,252822	1,941195
H	1,377901	-2,173825	-1,596366	H	1,531977	-1,417543	1,373937
H	2,056809	-1,701039	-0,008536	H	0,083163	-0,629727	2,008133

1N C2H6 CH TS				**1N C2H6 CH Product**			
20				20			
E(SCF)=	-291,202399			E(SCF)=	-291,316716		
C	0,318939	0,698412	1,160888	C	0,173571	0,738029	0,331278
C	1,791389	0,752928	0,843640	C	1,708634	0,903852	0,328286
C	2,014329	-0,416996	-0,145309	C	2,276892	-0,538954	0,285047
C	0,915845	-1,422527	0,239656	C	1,029847	-1,439471	0,307506
N	-0,084406	-0,558848	0,887842	N	-0,001726	-0,584803	-0,282948
C	-0,589343	2,118582	-0,556799	C	-0,576118	1,839786	-0,412362
H	-0,967646	-0,924499	1,200983	H	-0,933647	-0,956087	-0,142847
H	0,494831	-1,942768	-0,624055	H	1,155309	-2,355785	-0,272397
H	1,282664	-2,177116	0,944078	H	0,795955	-1,727136	1,346067
H	1,859830	-0,071990	-1,168858	H	2,842071	-0,698360	-0,633775
H	3,011360	-0,852681	-0,081965	H	2,943594	-0,753755	1,121002
H	2,108333	1,718846	0,456205	H	2,018514	1,465308	-0,555319
H	2,348335	0,569668	1,770643	H	2,045491	1,461473	1,203208

C	-1,889942	1,472875	-0,943385	C	-2,097432	1,683201	-0,392832
H	0,226072	1,956303	-1,258515	H	-0,218576	1,857518	-1,446451
H	-0,654942	3,169472	-0,271398	H	-0,304671	2,801557	0,035713
H	-2,707286	1,783589	-0,285748	H	-2,479382	1,639222	0,631273
H	-2,204196	1,695472	-1,971178	H	-2,586272	2,523272	-0,890804
H	-1,816141	0,377791	-0,877156	H	-2,411559	0,773809	-0,910533
H	-0,353085	1,608226	0,961646	H	-0,173062	0,732133	1,381646

1N C2H4 CC TS				**1N C2H4 CC Product**			
18				18			
E(SCF)=	-289,993344			E(SCF)=	-290,066604		
N	-0,136552	0,408360	0,006977	C	1,468229	0,553007	-0,757626
C	-0,027914	0,042035	1,436732	C	0,120076	0,129508	-1,366773
C	1,484331	-0,201035	1,586532	N	-0,820345	0,392556	-0,271431
C	2,086468	0,528978	0,362802	C	-0,162780	-0,111395	0,921250
C	0,988635	0,563804	-0,679204	C	1,296362	0,314157	0,768226
C	1,237111	-0,543039	-2,273859	H	-1,729968	-0,027982	-0,422930
C	1,573699	-1,752461	-1,708738	H	-0,146165	0,708697	-2,252519
H	-1,042894	0,483292	-0,431501	H	0,154241	-0,934073	-1,650317
H	-0,387000	0,863588	2,063731	H	1,653309	1,609224	-0,955449
H	-0,629350	-0,844240	1,656647	H	2,298578	-0,012959	-1,180852
H	1,864632	0,159960	2,542493	H	1,487054	1,232950	1,325831
H	1,699780	-1,268051	1,512048	H	1,974162	-0,450682	1,148567
H	2,308315	1,574522	0,610139	C	-0,875832	-0,151091	2,228055
H	3,005885	0,077099	-0,002348	C	-0,525493	-1,452762	1,523410
H	0,249102	-0,406533	-2,697990	H	-0,325501	0,109503	3,124279
H	1,997009	0,039770	-2,777900	H	-1,917512	0,147485	2,245556
H	0,815421	-2,437532	-1,351009	H	0,257905	-2,069177	1,948586
H	2,602996	-2,008809	-1,494440	H	-1,339490	-2,010642	1,074096

1N C2H4 CH TS				**1N C2H4 CH Product**			
18				18			
E(SCF)=	-289,964844			E(SCF)=	-290,078249		
N	0,411352	0,644760	1,269296	N	0,479470	0,676157	1,357675
C	1,695509	0,687054	0,910917	C	1,740390	0,987589	0,686701
C	1,887293	-0,359194	-0,155113	C	1,920775	-0,234253	-0,239818
C	0,467099	-0,589232	-0,722859	C	0,490979	-0,507862	-0,728500
C	-0,454221	-0,230775	0,455701	C	-0,388578	-0,137583	0,482232
C	2,019885	2,718598	-0,331600	C	1,798520	2,288545	-0,083923
C	0,875395	3,375053	-0,394655	C	0,796758	3,132147	-0,303213
H	0,048925	1,170266	2,048261	H	0,020849	1,485713	1,749845
H	-1,360827	0,292013	0,145222	H	-1,288292	0,400888	0,166360
H	-0,748265	-1,111189	1,035922	H	-0,719226	-1,032457	1,019053
H	0,291247	0,097772	-1,550941	H	0,259355	0,137777	-1,577565
H	0,303592	-1,606604	-1,077353	H	0,347318	-1,540245	-1,048939
H	2,613734	-0,061151	-0,907331	H	2,623836	-0,047291	-1,052115
H	2,258825	-1,270191	0,329531	H	2,294948	-1,075433	0,347588
H	2,892030	3,012303	-0,918840	H	2,783867	2,530281	-0,479382
H	0,010349	3,052223	0,191818	H	-0,204432	2,946007	0,069574
H	0,702049	4,258484	-1,010794	H	0,939886	4,046022	-0,866145
H	2,280376	1,688876	0,877563	H	2,551726	1,013498	1,424410

1N C2H2 CC TS	***first and highest TS, multistep reaction!***			**1N C2H2 CC Product**	***last and lowest lying product of multistep reaction***		
16				16			
E(SCF)=	-288,735528			E(SCF)=	-288,799447		
N	0,484602	1,167820	-0,115358	N	-0,194796	-1,105429	-0,367955
C	1,705144	0,604149	0,509820	C	-1,528776	-0,917299	0,201496
C	1,476411	-0,905076	0,334296	C	-1,754631	0,587301	0,014839
C	0,419202	-0,977306	-0,795385	C	-0,373327	1,179957	0,333067
C	-0,310265	0,349591	-0,778050	C	0,620520	0,076816	-0,067302
C	-2,225927	0,276704	-0,174710	C	1,898031	0,300398	-0,795716
C	-2,311127	-0,413457	0,850109	C	2,011256	-0,037748	0,455656
H	0,260832	2,145897	0,000852	H	0,255503	-1,969939	-0,096784
H	2,593101	0,960731	-0,020327	H	-2,268710	-1,523724	-0,325641
H	1,781815	0,915295	1,554061	H	-1,584650	-1,172361	1,272005
H	2,399200	-1,436313	0,101851	H	-2,025362	0,787695	-1,024078
H	1,065421	-1,330193	1,251889	H	-2,549274	0,975803	0,652994
H	0,901148	-1,052092	-1,777569	H	-0,175119	2,112667	-0,196419
H	-0,260358	-1,821750	-0,707018	H	-0,282600	1,385827	1,403593
H	-2,756243	0,872043	-0,886360	H	2,381171	0,506495	-1,737673
H	-1,903484	-1,035837	1,614906	H	2,661985	-0,308278	1,273524

1N C2H2 CH TS				**1N C2H2 CH Product**			
16				16			
E(SCF)=	-288,726394			E(SCF)=	-288,825509		
C	0,278831	0,306800	0,900203	C	-0,368945	0,213154	0,780791
C	1,698575	0,227757	0,440495	C	0,584315	1,286045	0,173558
C	1,610784	-0,304644	-1,010720	C	1,694834	0,479596	-0,547936
C	0,152428	-0,035221	-1,423066	C	1,205288	-0,973009	-0,502264
N	-0,511743	0,108929	-0,112386	N	0,452472	-1,010499	0,755581
C	-0,323299	2,566283	2,114191	C	-1,626725	0,090332	0,027275
C	-0,445623	3,781014	2,017812	C	-2,656983	-0,049810	-0,577353
H	-1,510260	0,256505	-0,030487	H	-0,113324	-1,845457	0,852262
H	0,035654	0,898094	-1,980330	H	0,579790	-1,192466	-1,380392
H	-0,300689	-0,844087	-1,995143	H	2,021625	-1,696566	-0,477010
H	2,317279	0,180561	-1,681376	H	1,862123	0,822895	-1,569053
H	1,811634	-1,376264	-1,031671	H	2,637211	0,570147	-0,006843
H	2,107361	1,240091	0,502617	H	0,040604	1,941305	-0,504616
H	2,301686	-0,395412	1,102492	H	1,000265	1,903784	0,968717
H	-0,087013	0,890932	1,824717	H	-0,619049	0,456370	1,816373
H	-0,564614	4,839548	1,999477	H	-3,567255	-0,164370	-1,112932

1N CH3F CF TS				**1N CH3F CF Product**			
17				17			
E(SCF)=	-351,121460			E(SCF)=	-351,286513		
C	1,388026	0,905280	-0,185607	C	0,304144	-1,061184	-0,596231
C	0,114892	0,134969	0,035059	C	-0,615154	0,022212	-0,040497
N	0,114556	-0,237619	1,288353	N	0,215413	1,163179	-0,001280
C	1,354595	0,007381	2,067779	C	1,603401	0,791758	0,322237
C	2,325069	0,473036	0,970856	C	1,662811	-0,731616	0,049147

C	-1,004230	-0,846991	-1,496665	C	-1,940042	0,243258	-0,738330
F	0,635235	-1,568827	-1,085778	F	-0,963212	-0,402399	1,316190
H	-0,647197	-0,763536	1,692644	H	-0,163683	1,946110	0,512873
H	1,170097	0,772517	2,827251	H	2,292770	1,351154	-0,315081
H	1,673763	-0,907434	2,568999	H	1,858422	1,011391	1,363186
H	2,981689	1,272242	1,312987	H	2,501544	-1,003160	-0,591324
H	2,942380	-0,362718	0,642703	H	1,770913	-1,276851	0,986316
H	1,140326	1,972195	-0,125890	H	0,345223	-0,967270	-1,683341
H	1,801150	0,714998	-1,172549	H	-0,063787	-2,055653	-0,348806
H	-0,993261	0,075790	-2,058115	H	-2,545763	-0,661952	-0,695665
H	-0,988193	-1,718227	-2,145068	H	-2,494338	1,047064	-0,250361
H	-1,831575	-0,889027	-0,800291	H	-1,773940	0,516216	-1,780516

1N CH3F CH TS				**1N CH3F CH Product**			
17				17			
E(SCF)=	-351,147180			E(SCF)=	-351,261850		
C	1,560980	-0,458994	0,652059	C	0,302607	1,117166	0,555454
C	1,367013	0,652466	-0,408793	C	1,416988	0,973925	-0,492084
C	0,051520	0,268017	-1,108874	C	1,936213	-0,454020	-0,258795
N	-0,592733	-0,598789	-0,107210	N	0,820431	-1,179678	0,384061
C	0,169669	-0,955799	0,932331	C	-0,322906	-0,284166	0,606920
C	-0,302684	0,413604	2,922932	C	-1,409656	-0,485072	-0,445322
F	0,937290	0,625834	3,539606	F	-2,537289	0,291689	-0,140294
H	-1,544827	-0,909837	-0,214648	H	0,578232	-2,045130	-0,077032
H	-0,574942	1,132016	-1,342808	H	2,250689	-0,935492	-1,188537
H	0,222035	-0,288842	-2,035832	H	2,803745	-0,443881	0,409420
H	1,255988	1,616832	0,088963	H	1,006359	1,073588	-1,499926
H	2,197722	0,728736	-1,109593	H	2,197640	1,727600	-0,383711
H	2,064355	-0,118238	1,554082	H	-0,432084	1,884440	0,311082
H	2,144102	-1,291035	0,240128	H	0,728002	1,360761	1,531430
H	-0,229160	-0,968035	2,013592	H	-0,775254	-0,475038	1,585066
H	-0,622675	1,336412	2,434678	H	-1,068564	-0,192340	-1,441726
H	-1,015525	0,079018	3,682376	H	-1,735648	-1,528964	-0,468873

1N CH3Cl CCl TS				**1N CH3Cl CCl Product**			
17				17			
E(SCF)=	-711,478770			E(SCF)=	-711,626592		
C	0,104914	0,204090	0,083609	C	0,277136	0,463854	0,107961
N	0,118934	-0,191553	1,322500	N	-0,590091	0,799758	-0,913272
C	1,373709	0,020042	2,093422	C	-1,818494	-0,004666	-0,876573
C	2,334862	0,513268	0,999436	C	-1,849440	-0,565104	0,567617
C	1,393944	0,943508	-0,154936	C	-0,637559	0,082523	1,263757
C	-1,130393	-0,841541	-1,572618	C	1,400530	1,438622	0,364559
Cl	0,904105	-2,065833	-1,235350	Cl	1,260314	-1,262197	-0,348989
H	-0,643820	-0,716122	1,729227	H	-0,186712	0,991688	-1,818729
H	1,198689	0,758982	2,879709	H	-2,679513	0,627802	-1,101937
H	1,686426	-0,916170	2,557034	H	-1,786237	-0,814009	-1,611392
H	2,976006	1,320999	1,350176	H	-2,784528	-0,333480	1,076359
H	2,965183	-0,308131	0,662193	H	-1,734780	-1,647413	0,550614
H	1,157660	2,014113	-0,112152	H	-0,923780	1,007353	1,774634
H	1,798947	0,734576	-1,141846	H	-0,147464	-0,568802	1,982189

H	-0,982805	0,084009	-2,104110	H	2,062467	1,066480	1,143721
H	-1,181246	-1,713159	-2,203140	H	1,992263	1,600206	-0,536514
H	-1,897792	-0,807048	-0,816486	H	0,973953	2,394671	0,680624

1N CH3Cl CH TS				**1N CH3Cl CH Product**			
17				17			
done:	-711,500170			E(SCF)=	-711,607338		
C	0,202210	-0,899046	0,917918	C	0,273754	-0,727283	1,283464
C	1,581138	-0,392684	0,607379	C	1,647905	-0,362737	0,707337
C	1,366245	0,655405	-0,512550	C	1,319178	0,671211	-0,381773
C	0,044323	0,224596	-1,171603	C	-0,046207	0,212685	-0,929493
N	-0,578061	-0,591061	-0,113195	N	-0,582039	-0,707988	0,093992
C	-0,349694	0,401303	3,013738	C	-0,228009	0,257597	2,342519
Cl	1,100190	0,396770	4,103990	Cl	0,716245	0,140685	3,908150
H	-1,539528	-0,888792	-0,173334	H	-1,567069	-0,592576	0,285521
H	-0,596530	1,067137	-1,439568	H	-0,710267	1,062737	-1,114856
H	0,202310	-0,382763	-2,067949	H	0,068570	-0,320160	-1,878547
H	1,256396	1,646861	-0,071119	H	1,242206	1,669952	0,053687
H	2,187196	0,694391	-1,227299	H	2,083750	0,718304	-1,157436
H	2,076348	-0,000593	1,493594	H	2,330909	0,011246	1,468999
H	2,179814	-1,236874	0,245899	H	2,094658	-1,254665	0,263864
H	-0,189298	-0,917136	2,002558	H	0,282881	-1,726035	1,727758
H	-0,462671	1,402590	2,603469	H	-0,146992	1,291951	2,015257
H	-1,216153	0,113403	3,608641	H	-1,260301	0,043773	2,612638

****

Now reaction scheme molecules
1P without hydrogen (see above)

1P	B3LYP/TZVP		
12			
E(SCF)=	-497,937017		
C	0,986923	-1,109263	-0,846778
C	0,099152	0,101947	-1,264092
C	-0,921058	0,419195	-0,144114
P	-0,213100	-0,506704	1,341480
C	1,233663	-1,173611	0,632619
H	0,217261	0,407639	2,328617
H	-1,034140	1,487548	0,036581
H	-1,909017	0,013006	-0,363176
H	0,754137	0,965638	-1,400187
H	-0,400779	-0,073933	-2,219298
H	1,931455	-1,119694	-1,397791
H	0,514081	-2,072606	-1,103786

1P CH4 TS				**1P CH4 Product**			
17				17			
E(SCF)=	-538,457822			done:	-538,598259		
P	-1,240543	0,257468	-0,070176	P	0,370370	-1,369055	0,058878
C	0,137905	0,197063	-1,383307	C	1,571114	-0,019357	-0,543157

C	1,400788	0,633909	-0,625121	C	0,850685	1,337141	-0,408947
C	1,316946	0,024882	0,790026	C	-0,164139	1,233333	0,736681
C	-0,083677	0,047879	1,343495	C	-0,937914	-0,086373	0,571429
H	-1,656159	-1,104693	-0,094233	H	0,939024	-1,517673	1,360338
H	0,244854	-0,815701	-1,775375	H	2,473981	-0,055574	0,067110
H	-0,092941	0,859428	-2,217300	H	1,867654	-0,220323	-1,572490
H	2,310447	0,327526	-1,148662	H	1,560619	2,150768	-0,240960
H	1,429446	1,725315	-0,551031	H	0,327705	1,568255	-1,340578
H	1,535070	-1,052030	0,719638	H	0,367593	1,222828	1,692909
H	2,058974	0,430447	1,481917	H	-0,840237	2,094514	0,753115
H	-0,251055	0,941517	2,260363	H	-1,360205	-0,405274	1,526986
C	-0,164194	2,213262	2,206549	C	-2,067485	-0,002649	-0,460937
H	0,299433	2,654770	1,333375	H	-1,697197	0,266506	-1,453331
H	0,426788	2,381823	3,106482	H	-2,802816	0,752263	-0,167375
H	-1,201323	2,520134	2,313382	H	-2,586274	-0,957993	-0,557425

1P NH3 TS				**1P NH3 Product**			
16				16			
E(SCF)=	-554,513677			done:	-554,638462		
C	0,539244	0,244113	-1,705214	C	-0,961358	-0,042589	0,503695
C	1,786455	0,621090	-0,958673	C	-0,171422	1,250937	0,734259
C	1,963086	2,150639	-0,885269	C	0,897719	1,355620	-0,360491
C	1,561108	2,717052	-2,255869	C	1,616509	-0,004794	-0,462578
P	0,065404	1,659145	-2,773827	P	0,363926	-1,351719	0,033008
N	-0,990858	0,205184	-0,212689	N	-2,001347	0,153251	-0,507270
H	0,559241	1,100607	-3,987902	H	0,855422	-1,557446	1,358914
H	2,372426	2,612000	-2,978001	H	2,470357	-0,052673	0,213717
H	1,288250	3,770670	-2,204492	H	1,989110	-0,194048	-1,469107
H	2,984328	2,432631	-0,616583	H	1,603050	2,164124	-0,154224
H	1,303909	2,554389	-0,110234	H	0,425452	1,599791	-1,317154
H	2,592757	0,202384	-1,581271	H	0,316102	1,201035	1,711784
H	1,878968	0,121423	0,009183	H	-0,843525	2,112802	0,739600
H	-0,398937	-0,405276	-1,035566	H	-1,453801	-0,366134	1,421949
H	-1,607364	0,921330	-0,575653	H	-2,501367	-0,710236	-0,686062
H	-0,472951	0,547049	0,586392	H	-1,608035	0,453202	-1,392668

1P OH2 TS				**1P OH2 Product**			
15				15			
done:	-574,400123			done:	-574,516319		
C	-1,209686	0,361476	-0,101406	C	-0,956714	-0,015740	0,479771
P	0,105021	0,333987	-1,354385	P	0,325164	-1,385164	0,144003
C	1,470583	0,740683	-0,108347	C	1,655050	-0,115096	-0,338454
C	0,719688	1,565204	0,949674	C	0,958043	1,257164	-0,408575
C	-0,641503	0,880522	1,174003	C	-0,159057	1,273683	0,640146
O	-2,615897	1,881362	-0,640123	O	-1,824574	0,152041	-0,646647
H	0,188841	-1,080355	-1,485436	H	0,707426	-1,553643	1,508912
H	1,891782	-0,170269	0,320626	H	2,443816	-0,124227	0,414621
H	2,274194	1,301799	-0,583191	H	2,105317	-0,393412	-1,290758
H	1,294355	1,648484	1,874687	H	1,669460	2,071762	-0,254010
H	0,548048	2,578912	0,578209	H	0,515715	1,394879	-1,397048
H	-0,492950	-0,035878	1,770762	H	0,269040	1,300357	1,646401
H	-1,359876	1,487660	1,726677	H	-0,816120	2,140419	0,532567

H	-2,413222	0,732577	-0,395499	H	-1,536247	-0,250521	1,379058
H	-2,510142	1,946867	-1,599544	H	-2,210395	-0,702578	-0,869902

1P SiH4 TS				**1P SiH4 Product**			
17				17			
done:	-789,843318			done:	-789,982916		
C	0,397122	-1,116820	0,892315	C	-0,433032	-0,101925	0,763608
P	-0,910570	-0,672386	-0,282175	P	0,748138	-1,382278	0,008744
C	0,212086	0,280480	-1,475821	C	1,829170	-0,024087	-0,769734
C	1,294377	0,815236	-0,525880	C	1,177564	1,338683	-0,458212
C	1,596415	-0,314019	0,484598	C	0,371303	1,211821	0,839854
Si	-0,592172	0,648564	3,249635	Si	-2,054147	-0,002521	-0,233237
H	-1,074117	-1,945972	-0,888021	H	1,541113	-1,563469	1,184463
H	-0,331156	1,075802	-1,984465	H	1,915427	-0,193782	-1,842648
H	0,637210	-0,386241	-2,228563	H	2,831826	-0,096407	-0,347880
H	0,916103	1,688919	0,013252	H	0,506710	1,615736	-1,275635
H	2,189205	1,131414	-1,067786	H	1,927025	2,130551	-0,385519
H	2,224357	-0,003230	1,323960	H	-0,269275	2,085406	0,996233
H	2,179846	-1,097874	-0,032174	H	1,056521	1,163353	1,692766
H	-0,045056	-0,503206	2,355142	H	-0,715438	-0,451732	1,760308
H	0,138974	0,635021	4,546797	H	-2,889310	1,127579	0,268338
H	-0,403166	1,970467	2,593147	H	-1,793328	0,222088	-1,683077
H	-2,040634	0,399656	3,470666	H	-2,817578	-1,270595	-0,082980

1P C6H6 CC TS				**1P C6H6 CC Product**			
24				24			
done:	-730,252480			done:	-730,328295		
C	2,035597	0,802556	-1,042664	C	1,962126	0,265186	-1,267844
C	0,999039	1,334633	-0,219870	C	0,903915	1,092589	-0,668811
C	0,777426	0,718979	1,035498	C	0,717194	0,953012	0,876022
C	1,421144	-0,476744	1,365879	C	1,623402	0,017958	1,551700
C	2,328042	-1,041913	0,491384	C	2,457792	-0,790785	0,872948
C	2,649537	-0,375997	-0,712259	C	2,630501	-0,664569	-0,560529
C	-0,843464	0,649136	-0,949012	C	-0,360394	0,508487	-0,100504
C	-1,989569	1,097758	-0,082328	C	-1,631904	1,344955	-0,153667
C	-2,635918	-0,046603	0,726407	C	-2,693393	0,584667	0,645483
C	-2,622317	-1,290048	-0,176256	C	-2,642596	-0,893912	0,213145
P	-0,946079	-1,164083	-1,069423	P	-0,844058	-1,295852	-0,274324
H	-1,345069	-1,203093	-2,435725	H	-1,041493	-1,231608	-1,688173
H	-3,443428	-1,264929	-0,895079	H	-3,291616	-1,079900	-0,643322
H	-2,693771	-2,217345	0,391626	H	-2,962665	-1,559361	1,014869
H	-3,648888	0,202559	1,055157	H	-3,690555	1,009456	0,504289
H	-2,039510	-0,234735	1,623935	H	-2,461012	0,662407	1,711405
H	-2,716306	1,431058	-0,843178	H	-1,953868	1,451605	-1,196091
H	-1,773833	1,988860	0,513270	H	-1,469452	2,353584	0,239516
H	0,706964	2,363017	-0,366498	H	0,782576	2,082630	-1,098938
H	0,116476	1,186660	1,752466	H	0,467915	1,852634	1,430452
H	1,209177	-0,954598	2,314790	H	1,627600	0,019454	2,636090
H	2,820504	-1,973397	0,740114	H	3,091809	-1,486707	1,409106
H	3,405114	-0,794915	-1,366262	H	3,389006	-1,268977	-1,043648
H	2,293403	1,317932	-1,959312	H	2,223565	0,457599	-2,302385

1P C6H6 CH TS				1P C6H6 CH Product			
24				24			
done:	-730,250239			done:	-730,391623		
P	-0,251594	-0,963347	1,099815	P	-1,832613	-1,083083	-0,876744
H	0,503782	-2,169689	1,055441	H	-2,783234	-0,543092	-1,794534
C	-0,312791	-0,532751	-0,753575	C	-2,735317	-0,533126	0,707374
H	0,206304	-1,295058	-1,337107	H	-3,783856	-0,351941	0,469371
H	-1,343888	-0,482841	-1,102206	H	-2,704097	-1,333527	1,446961
C	0,400130	0,825215	-0,847664	C	-2,040829	0,744593	1,216970
H	-0,289214	1,626370	-0,566621	H	-1,231549	0,476097	1,900299
H	0,740038	1,029593	-1,866651	H	-2,731127	1,377024	1,780969
C	1,568999	0,798784	0,156451	C	-1,459825	1,490506	0,012033
H	2,035347	1,774202	0,304127	H	-0,793345	2,300238	0,320932
H	2,366572	0,152557	-0,243283	H	-2,272950	1,938639	-0,566915
C	1,199103	0,107205	1,441114	C	-0,720528	0,466307	-0,884692
C	0,185628	1,857297	2,584381	C	0,708896	0,212418	-0,448334
C	0,717300	3,132237	2,467503	C	1,737898	0,973869	-1,013637
C	-0,021958	4,220713	2,927096	C	3,059972	0,811785	-0,615364
C	-1,277405	4,018526	3,494334	C	3,384459	-0,121568	0,364004
C	-1,793866	2,730738	3,610194	C	2,375643	-0,891737	0,931520
C	-1,058681	1,639526	3,149636	C	1,054234	-0,727273	0,526923
H	1,700969	3,286262	2,039132	H	1,497789	1,702630	-1,780385
H	0,382686	5,222513	2,844270	H	3,837177	1,411689	-1,073761
H	-1,852769	4,865489	3,847865	H	4,413592	-0,253127	0,674982
H	-2,769808	2,574644	4,054496	H	2,616525	-1,630291	1,686808
H	-1,458856	0,634638	3,222692	H	0,291048	-1,359179	0,965289
H	1,007737	0,904779	2,457505	H	-0,692891	0,834959	-1,911607

1P C2H6 CC TS				1P C2H6 CC Product			
20				20			
done:	-577,695649			done:	-577,924778		
P	-0,309885	0,062033	-0,321301	P	-0,445419	-1,331674	0,104305
C	0,152605	-0,394928	1,485749	C	-1,921739	-0,135120	0,128665
C	1,657796	-0,098077	1,661191	C	-1,364635	1,306033	0,122973
C	2,075724	0,974664	0,620622	C	0,026707	1,287071	-0,517969
C	1,279475	0,915161	-0,656091	C	0,825935	0,095435	0,047141
H	-0,988850	1,281181	-0,025345	H	-0,454585	-1,562959	-1,305184
H	-0,455318	0,205897	2,163105	H	-2,540452	-0,330049	-0,747691
H	-0,079162	-1,441517	1,682283	H	-2,539362	-0,325434	1,006359
H	1,876008	0,247305	2,674671	H	-2,035309	1,988625	-0,404669
H	2,238779	-1,012384	1,522774	H	-1,293409	1,675842	1,148542
H	1,802908	1,961842	1,021902	H	-0,072798	1,163051	-1,601160
H	3,156864	1,013292	0,462380	H	0,558692	2,230629	-0,351401
C	2,258095	-0,922777	-1,425623	C	1,308722	0,378001	1,480046
H	1,770048	-1,518622	-2,189041	H	1,847357	-0,479770	1,887558
H	1,934899	-1,276777	-0,456174	H	0,486418	0,600401	2,163089
H	3,341152	-0,994359	-1,465373	H	1,987363	1,237065	1,486894
C	2,197222	0,703855	-2,427941	C	2,026607	-0,258964	-0,834850
H	1,290223	1,025251	-2,921477	H	2,545331	-1,148679	-0,469705
H	2,758456	0,092083	-3,152805	H	2,750471	0,562509	-0,839262

H	2,823796	1,551723	-2,179742	H	1,725075	-0,444339	-1,867977

1P C2H6 CH TS				**1P C2H6 CH Product**			
20				20			
done:	-577,787682			done:	-577,924732		
C	0,128163	0,664756	1,131774	C	-0,445106	0,264548	0,638600
C	1,619224	0,697469	0,906101	C	0,685957	1,306894	0,652543
C	2,091832	-0,382684	-0,090471	C	1,583843	1,058782	-0,565946
C	1,263163	-1,646383	0,184069	C	1,874407	-0,452658	-0,649672
P	-0,475571	-0,972743	0,569758	P	0,395465	-1,366329	0,126862
C	-0,607343	1,991303	-0,699579	C	-1,602974	0,631625	-0,304976
H	-0,674387	-1,510969	1,872253	H	1,003037	-1,615661	1,394289
H	1,238729	-2,320678	-0,671630	H	2,012694	-0,783323	-1,678917
H	1,657603	-2,197229	1,039707	H	2,778099	-0,717351	-0,099832
H	1,913550	-0,037969	-1,113671	H	1,068156	1,385100	-1,472830
H	3,164105	-0,577836	-0,002788	H	2,508002	1,639144	-0,506999
H	1,993226	1,696955	0,669338	H	0,288705	2,327221	0,657298
H	2,028480	0,457722	1,899533	H	1,275260	1,186817	1,566592
C	-2,097230	1,926138	-0,929184	C	-2,823306	-0,279201	-0,171142
H	-0,023963	1,410889	-1,406362	H	-1,259176	0,624707	-1,344709
H	-0,199639	2,999623	-0,607205	H	-1,901290	1,664850	-0,093256
H	-2,643502	2,519606	-0,193436	H	-3,226664	-0,246683	0,844688
H	-2,354641	2,305528	-1,923090	H	-3,618755	0,027019	-0,854011
H	-2,454613	0,895235	-0,869924	H	-2,570207	-1,317353	-0,395535
H	-0,462244	1,636006	0,516020	H	-0,852280	0,130865	1,644489

1P C2H4 CC TS				**1P C2H4 CC Product**			
18				18			
done:	-576,558649			done:	-576,680193		
C	0,990821	0,802983	-0,665903	C	0,699201	0,022646	-0,124481
P	-0,634410	0,347435	-0,008057	P	-0,555021	-1,291752	0,304851
C	-0,059663	0,109516	1,786699	C	-1,928187	0,017798	0,474045
C	1,410587	-0,297638	1,598951	C	-1,275006	1,404034	0,279073
C	1,966274	0,552967	0,436134	C	-0,053583	1,240090	-0,634343
C	1,563721	-0,611576	-2,545565	C	2,072827	-0,333868	-0,616342
C	1,523018	-1,750680	-1,840014	C	1,898748	0,204575	0,779053
H	-1,192032	1,654978	-0,014469	H	-0,856117	-1,659874	-1,043756
H	-0,645201	-0,656059	2,294398	H	-2,406507	-0,067366	1,449556
H	1,987622	-0,167448	2,518247	H	-1,989508	2,127428	-0,121506
H	2,100743	1,591067	0,796047	H	-0,378923	1,065396	-1,666021
H	2,956268	0,244087	0,091336	H	0,575079	2,135994	-0,637694
H	0,704059	-0,247983	-3,089749	H	2,331527	-1,379297	-0,731692
H	2,486796	-0,073340	-2,709942	H	2,517342	0,316387	-1,360883
H	0,605178	-2,312805	-1,721898	H	2,030562	-0,479905	1,607651
H	2,402961	-2,147316	-1,347572	H	2,226063	1,218830	0,976489
H	1,470554	-1,354701	1,321580	H	-0,942052	1,786112	1,247938
H	-0,145865	1,040956	2,349664	H	-2,691485	-0,175169	-0,280250

1P C2H4 CH TS				**1P C2H4 CH Product**			
18				18			

done:	-576,544715			done:	-576,688871		
P	-0,063737	0,996842	1,440107	P	-0,411809	-1,350891	-0,320507
C	1,712444	0,865272	0,998205	C	0,463311	0,250399	-0,863748
C	1,850335	-0,236839	-0,016621	C	-0,564892	1,372615	-0,605539
C	0,519272	-0,542244	-0,733517	C	-1,221182	1,091711	0,749778
C	-0,598286	-0,448102	0,317491	C	-1,627300	-0,394216	0,787259
C	1,920915	2,649695	-0,463053	C	1,770418	0,511803	-0,157293
C	1,079097	3,663137	-0,428601	C	2,469778	-0,319121	0,607642
H	0,085790	0,309948	2,678804	H	-1,251302	-1,411731	-1,472986
H	-1,570868	-0,247643	-0,130995	H	-1,596564	-0,797609	1,799111
H	-0,675791	-1,369273	0,897666	H	-2,638317	-0,544328	0,406910
H	0,356333	0,207423	-1,512870	H	-0,499510	1,292359	1,545786
H	0,531735	-1,521430	-1,219885	H	-2,079178	1,745500	0,924524
H	2,689893	-0,091675	-0,701182	H	-0,093433	2,360281	-0,629281
H	2,124761	-1,103601	0,604971	H	-1,321983	1,355549	-1,394669
H	2,599251	2,417868	-1,276979	H	2,166868	1,513275	-0,323374
H	0,405934	3,812435	0,410431	H	2,140707	-1,331587	0,810234
H	1,019104	4,385127	-1,238175	H	3,408721	-0,010304	1,050916
H	2,208166	2,022128	0,568950	H	0,667331	0,173715	-1,936410

1P C2H2 CC TS				**1P C2H2 CC Product**			
16				16			
done:	-575,297589			done:	-575,404881		
C	-0,308074	0,357023	-0,979025	C	0,743595	0,044606	-0,095880
P	0,461452	1,628475	0,064771	P	-0,524755	-1,287727	0,355138
C	1,974994	0,580946	0,540667	C	-1,939240	-0,017131	0,351088
C	1,422189	-0,850027	0,452785	C	-1,283406	1,377589	0,304520
C	0,482917	-0,893589	-0,771723	C	-0,025099	1,282058	-0,562365
C	-2,477218	-0,041516	-0,338704	C	2,131762	-0,284284	-0,551283
C	-2,260672	-0,331514	0,815816	C	2,045313	0,152896	0,659300
H	0,950565	2,431030	-1,002606	H	-0,723712	-1,768577	-0,976742
H	2,332568	0,831081	1,539001	H	-2,561690	-0,141012	1,237282
H	2,222489	-1,591802	0,386307	H	-1,982852	2,131189	-0,066232
H	1,102742	-0,879548	-1,687894	H	-0,310494	1,161650	-1,614641
H	-0,113678	-1,805442	-0,844381	H	0,595423	2,179769	-0,491826
H	-2,907791	0,174083	-1,285299	H	2,732623	-0,657992	-1,362826
H	-1,997449	-0,561120	1,819267	H	2,515617	0,413265	1,591538
H	0,841432	-1,080471	1,351894	H	-0,996467	1,679782	1,316584
H	2,792805	0,733513	-0,166284	H	-2,572535	-0,180203	-0,521480

1P C2H2 CH TS				**1P C2H2 CH Product**			
16				16			
done:	-575,276825			done:	-575,438341		
C	0,409794	0,345694	1,008875	C	0,543044	0,153656	-0,545519
C	1,749499	0,085950	0,368480	C	-0,190907	1,431341	-0,061173
C	1,553247	-0,612277	-0,996909	C	-1,679397	1,107902	0,074361
C	0,311042	-0,011951	-1,663784	C	-1,776590	-0,201231	0,863835
P	-0,910187	0,339885	-0,270116	P	-0,426589	-1,344561	0,206839
C	0,503404	2,573193	1,592203	C	1,953277	0,132663	-0,207669
C	0,678207	3,761120	1,452691	C	3,119285	0,117238	0,085216
H	-1,215519	-1,019281	0,060905	H	-1,103552	-1,676767	-1,006810

H	0,536250	0,948117	-2,135314	H	-1,579193	-0,027782	1,924229
H	-0,120172	-0,659740	-2,427766	H	-2,752226	-0,683005	0,787995
H	2,445970	-0,512562	-1,620020	H	-2,218304	1,922448	0,566646
H	1,393229	-1,681298	-0,832666	H	-2,126024	0,976413	-0,916179
H	2,268461	1,037941	0,230127	H	0,211550	1,720551	0,913019
H	2,375603	-0,501576	1,048043	H	-0,004933	2,261963	-0,745452
H	0,348906	1,318913	1,888240	H	0,442768	0,068643	-1,629693
H	0,816581	4,812249	1,360178	H	4,149819	0,097845	0,341004

1P CH3F CF TS				**1P CH3F CF Product**			
17				17			
done:	-637,686580			done:	-637,879763		
F	-0,083290	0,148634	-0,011861	F	-1,125715	0,248761	-1,470301
C	0,058888	-0,452361	1,645318	C	-2,120518	-0,193859	0,628058
C	1,654212	0,318965	0,332044	C	-0,812716	0,066505	-0,090901
C	1,866559	1,772776	0,041493	C	-0,053710	1,312228	0,355750
C	2,025968	2,013387	-1,474397	C	1,350626	1,244010	-0,248060
C	2,940250	0,903362	-2,017076	C	1,912929	-0,166598	0,017430
P	2,398403	-0,649694	-1,049000	P	0,444191	-1,371478	-0,037838
H	3,605382	-0,925807	-0,341993	H	0,326337	-1,568638	1,371004
H	3,991934	1,127990	-1,830453	H	2,389616	-0,226266	0,996412
H	2,811372	0,748134	-3,087891	H	2,654241	-0,453292	-0,727802
H	2,427595	3,007802	-1,686103	H	2,004577	2,016866	0,162187
H	1,043149	1,952272	-1,948837	H	1,283161	1,417496	-1,324034
H	2,813834	2,013091	0,546473	H	0,003304	1,311807	1,448446
H	1,103056	2,406249	0,499458	H	-0,596800	2,211075	0,050590
H	0,629881	-1,363481	1,711528	H	-2,606852	-1,089206	0,238969
H	-1,015679	-0,603841	1,590987	H	-2,797572	0,651434	0,482044
H	0,364587	0,308975	2,344172	H	-1,955647	-0,325062	1,698236

1P CH3F CH TS				**1P CH3F CH Product**			
17				17			
done:	-637,727523			done:	-637,874358		
C	1,468918	-0,471179	0,641488	C	-0,030984	1,120198	0,768035
C	1,299633	0,707735	-0,339729	C	0,880992	1,444193	-0,420397
C	0,075708	0,401138	-1,216369	C	1,921838	0,318283	-0,546875
P	-1,156817	-0,389367	-0,005650	P	1,064552	-1,293049	-0,014319
C	0,149891	-1,014413	1,118524	C	-0,455134	-0,353975	0,656378
C	-0,195552	0,420520	2,979208	C	-1,632227	-0,580066	-0,274691
F	1,011359	0,638084	3,593541	F	-2,769992	0,094825	0,204963
H	-1,412241	-1,633042	-0,648664	H	1,705598	-1,429473	1,251065
H	-0,345134	1,297964	-1,670023	H	2,296090	0,219495	-1,565635
H	0,327702	-0,298186	-2,015319	H	2,779060	0,497197	0,102713
H	1,129377	1,627967	0,227573	H	0,286489	1,500686	-1,336717
H	2,195738	0,868807	-0,944538	H	1,361104	2,418688	-0,303112
H	2,159520	-0,259285	1,460914	H	-0,901549	1,779357	0,808043
H	1,907530	-1,325143	0,101922	H	0,522170	1,259627	1,701099
H	-0,086288	-0,704180	2,345357	H	-0,715555	-0,767440	1,632508
H	-0,494334	1,284789	2,395775	H	-1,443021	-0,202479	-1,283148
H	-0,946879	0,111156	3,708979	H	-1,889537	-1,638762	-0,337180

1P CH3Cl CCl TS				1P CH3Cl CCl Product			
17				17			
done:	-998,037141			done:	-998,220138		
Cl	-0,518631	0,089573	-0,148258	Cl	1,310328	-0,500730	-1,375499
C	0,067495	-0,551071	1,915115	C	1,744058	0,641213	1,071379
C	1,701010	0,275651	0,469703	C	0,594304	0,096321	0,243541
C	1,918714	1,729300	0,199773	C	-0,159562	-1,070353	0,881773
C	2,135911	1,995945	-1,302901	C	-1,456910	-1,299675	0,103497
C	3,028545	0,867791	-1,849639	C	-2,103317	0,071812	-0,194208
P	2,510608	-0,692280	-0,872398	P	-0,730583	1,383543	-0,211207
H	3,698041	-0,876948	-0,098907	H	-0,906071	1,807097	1,144097
H	4,086422	1,078581	-1,684194	H	-2,834619	0,348157	0,565843
H	2,880073	0,706391	-2,916794	H	-2,617282	0,071352	-1,154724
H	2,578644	2,980112	-1,476442	H	-2,139248	-1,948844	0,656465
H	1,166145	1,982287	-1,805241	H	-1,222669	-1,804094	-0,834893
H	2,859661	1,929406	0,739800	H	-0,388124	-0,778200	1,912914
H	1,162819	2,375495	0,650538	H	0,462202	-1,967780	0,924853
H	0,699034	-1,422947	1,909642	H	2,239974	1,471538	0,568859
H	-0,988358	-0,761945	2,015142	H	2,486645	-0,137731	1,254886
H	0,420600	0,259685	2,529961	H	1,369378	0,994092	2,035523

1P CH3Cl CH TS				1P CH3Cl CH Product			
17				17			
done:	-998,070400			done:	-998,218754		
C	0,405088	-1,188514	1,109808	C	-1,139868	-0,662502	-0,343646
C	1,642318	-0,505180	0,597068	Cl	-2,737299	0,077168	0,184711
C	1,298395	0,670073	-0,350716	C	-0,015211	-0,366956	0,633909
C	0,089064	0,266633	-1,215111	P	1,555994	-1,282792	0,036822
P	-0,813347	-1,103181	-0,250501	C	2,383464	0,336163	-0,518598
C	-0,315312	0,374407	2,780712	C	1,312061	1,437563	-0,443566
Cl	0,908871	0,743841	4,020262	C	0,378743	1,115777	0,728832
H	-1,856281	-0,390122	0,405084	H	2,157393	-1,359336	1,327101
H	-0,564638	1,106118	-1,451594	H	2,783250	0,221401	-1,525909
H	0,408670	-0,172209	-2,161749	H	3,221102	0,553140	0,144807
H	1,045440	1,542904	0,256169	H	0,739664	1,460349	-1,375459
H	2,154049	0,953149	-0,968988	H	1,763885	2,426448	-0,335215
H	2,308685	-0,209410	1,409619	H	-0,502975	1,760584	0,739299
H	2,180756	-1,288003	0,040497	H	0,908754	1,279156	1,671229
H	0,047064	-0,796439	2,258343	H	-0,293114	-0,768750	1,609157
H	-0,420241	1,204416	2,094818	H	-0,952149	-0,261450	-1,337579
H	-1,254347	0,085023	3,246849	H	-1,330941	-1,728857	-0,422826