Supporting Information

for

Computational Studies on Aryl Ring Formation by the Cross-Linking of Acetylenes

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A. Spin-correction analysis

The energy of spin-corrected singlet species, ^{1}E(SC), can be calculated from the following relationship[1]

$^1E(SC) = {}^1E + f'_{sc}(n)[{}^1E - {}^3E]$,

where,

^{1}E = energy of spin-uncorrected singlet species

^{3}E = energy of triplet species

and,

$$f'sc(n) = \frac{^1\langle S^2\rangle}{^3\langle S^2\rangle - {}^1\langle S^2\rangle}$$

B. Spin-correction of species derived from phenylacetylene and methylacetylene

S-squared values of singlet species derived from phenylacetylene that required spin-correction are:

int1b_14eze: S-Squared = 1.085

int1b_14zez: S-Squared = .975

int1b_14zzz: S-Squared = 1.057

int2_12: S-Squared = 1.023

int2_13: S-Squared = .985

ts1b_14zzz0deg: S-Squared = .151

ts2b_14zzz_eze: S-Squared = 1.085

ts3b_14eze: S-Squared = .657

S-squared values of singlet species derived from methylacetylene that required spin-correction are:

int1b_12: S-Squared = .941

int1b_14eee: S-Squared = 1.041

int1b_14eez: S-Squared = 1.019

int1b_14eze: S-Squared = 1.033

int1b_14zez: S-Squared = .915

int1c: S-Squared = .102

int2r_14enyne: S-Squared = .764

int3bhh_12: S-Squared = 1.038

int3bhme_12: S-Squared = 1.041

int3bmeh_12: S-Squared = .988

int3bmehx_12: S-Squared = 1.037

int3bmeme_12: S-Squared = 1.041

int5crbhmeme_12: S-Squared = .246

ts1b_14zez: S-Squared = .230

ts2b_14eee_eze: S-Squared = 1.008

ts2b_14eez_eee: S-Squared = 1.037

ts2b_14zez_eez: S-Squared = .929

ts3b_14eze: S-Squared = .815

ts3strss_14eee: S-Squared = .542

ts4bcrbhh_12: S-Squared = .722

ts4bhh_12: S-Squared = .910

ts4bhh_13: S-Squared = .803

ts4bhme_12: S-Squared = .956

ts4bmeh_12: S-Squared = .996

ts4bmeme_13: S-Squared = .959

C. Barriers for carbene formation from vinylcyclobutene biradicals

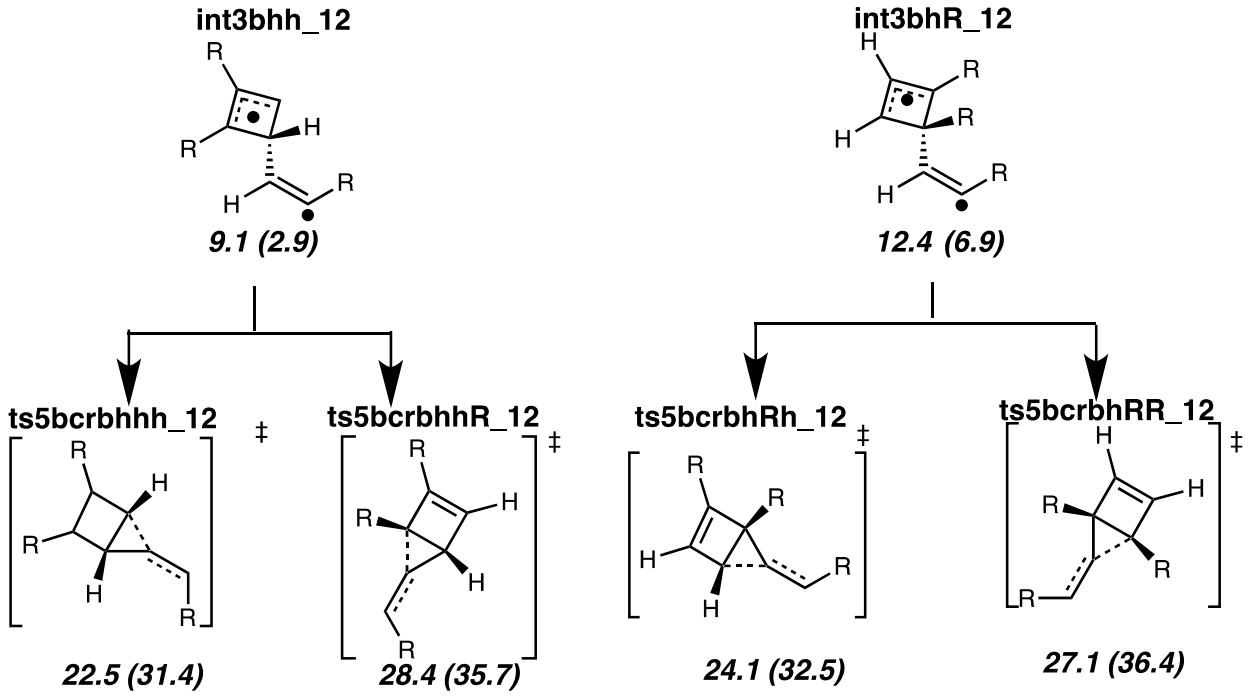

Figure S1. Structures and free energies of activation, in kcal/mol, for carbene formation from phenyl- and methyl-substituted (in parentheses) vinyl cyclobutene biradicals

The free energies shown in Figure S1 indicate that the barriers for carbene formation range from 23 -28 kcal/mol and from 31 -36 kcal/mol for reactions involving phenyl and methyl-substituted vinyl cyclobutene biradicals. These are at least 12 kcal/mol larger than barriers for rotation to form Dewar benzenes.

Phenylacetylene Stationary Points

123ph3ph
E [Hartrees] = -925.4508367649
Gcorr [kcal/mol] = 188.752

C	-0.00027416	-0.00004787	-3.47230845
C	0.00136039	-1.20203085	-2.77194127
C	0.01093066	-1.22211838	-1.36915065
C	-0.00012439	-0.00000900	-0.65355833
C	-0.01124182	1.22207776	-1.36919702
C	-0.00183683	1.20195997	-2.77198126
C	0.05785948	-2.55202947	-0.69459428
C	-0.00011838	0.00003100	0.84054176
C	-0.05794931	2.55198614	-0.69462445
C	-1.03489453	-0.61950152	1.55610166
C	-1.03718339	-0.61743400	2.95035261
C	-0.00017548	0.00021704	3.65261884
C	1.03688127	0.61774668	2.95031755
C	1.03465318	0.61962852	1.55606307
C	-1.04371096	2.86322399	0.25535871
C	0.87444836	3.54276682	-1.03903275
C	0.83103562	4.80491883	-0.44540909
C	-0.15186967	5.10001909	0.50012259
C	-1.09015158	4.12426317	0.84600056
C	-0.87417679	-3.54307698	-1.03920056
C	-0.83038517	-4.80528425	-0.44573993
C	0.15253173	-5.10019189	0.49985335
C	1.09037727	-4.12411615	0.84600496
C	1.04358190	-2.86302667	0.25551947
H	-0.00035613	-0.00006370	-4.55897132
H	0.02497220	-2.14620621	-3.30864451
H	-0.02548395	2.14613376	-3.30868789
H	-1.83444315	-1.11227875	1.01065274
H	-1.84838290	-1.10103267	3.48822364
H	-0.00020154	0.00032206	4.73939526
H	1.84806248	1.10143123	3.48814192
H	1.83422317	1.11234591	1.01059245
H	-1.77210713	2.10810588	0.53269356
H	1.64802341	3.31166952	-1.76687754
H	1.56822623	5.55512668	-0.71971994
H	-0.18720611	6.08181454	0.96472200
H	-1.86233092	4.34589106	1.57801758
H	-1.64775241	-3.31218538	-1.76711506
H	-1.56725702	-5.55573120	-0.72023717
H	0.18821216	-6.08205402	0.96426316
H	1.86256496	-4.34557096	1.57807365

H	1.77166926	-2.10768974	0.53307016

124ph3ph
E [Hartrees] = -925.4543796407
Gcorr [kcal/mol] = 189.640

H	1.57369804	1.54193244	5.60271541
C	1.68539112	1.42481890	4.52809169
C	0.58102585	1.57667392	3.68564877
H	-0.39324275	1.81793455	4.10251770
C	0.72129813	1.42260034	2.30818412
H	-0.14062269	1.53934373	1.65881135
C	1.97004404	1.11483862	1.74363184
C	3.07293081	0.97008883	2.60002515
H	4.04258489	0.71986696	2.17745971
C	2.93242715	1.12104009	3.98010729
H	3.79732395	0.99644598	4.62653093
C	2.14291508	0.98435976	0.27070156
C	3.16624613	1.71819139	-0.35010430
H	3.80678096	2.34211814	0.26725756
C	3.36158358	1.68962773	-1.72619981
H	4.17682251	2.25712334	-2.16599124
C	2.52621880	0.91762893	-2.54732209
H	0.85557455	-0.43597022	-2.54205897
C	1.51059132	0.17634693	-1.92896769
C	2.71384448	0.87858180	-4.01846464
C	2.54668710	-0.31676744	-4.73811077
H	2.30317163	-1.23116987	-4.20418981
C	2.72122757	-0.35012402	-6.12083276
H	2.59427929	-1.28747132	-6.65618176
C	3.06862020	0.81098188	-6.81449206
H	3.20503209	0.78492983	-7.89221920
C	3.23968481	2.00576565	-6.11229056
H	3.50209853	2.91726357	-6.64310550
C	3.06361854	2.03890587	-4.72975338
H	3.17224613	2.97884171	-4.19554675
C	1.30436292	0.18428010	-0.54284840
C	0.22262292	-0.68003761	0.00810834
C	0.47521923	-1.58613307	1.05067358
H	1.47026809	-1.63527172	1.48179779
C	-0.53523794	-2.41454217	1.53415351
H	-0.31911833	-3.11134386	2.33972872
C	-1.81929297	-2.35290623	0.98667199
H	-2.60745627	-2.99720411	1.36702157
C	-2.08305182	-1.45803412	-0.05127061

H	-3.07943590	-1.39896596	-0.48153714
C	-1.06957628	-0.63090819	-0.53732653
H	-1.28080546	0.07421892	-1.33702459

135ph3ph
E [Hartrees] = -925.4571702645
Gcorr [kcal/mol] = 190.466

H	5.89160093	-0.00167855	3.39915777
C	4.95022175	-0.00126903	2.85637818
C	3.87835893	0.77165756	3.30755402
H	3.98469783	1.38294226	4.19998188
C	2.67080614	0.77258249	2.61062420
H	1.85074336	1.39727820	2.95393856
C	2.50863856	0.00012150	1.44848873
C	3.59512132	-0.77303586	1.00632164
H	3.48104873	-1.39716765	0.12425622
C	4.80320095	-0.77346586	1.70227342
H	5.62826100	-1.38538819	1.34701148
C	1.22218402	0.00048262	0.70621228
C	-0.00006946	0.00001786	1.39233092
H	-0.00004973	0.00006024	2.47816402
C	-1.22228443	-0.00054963	0.70612153
H	2.14567192	0.00149855	-1.23821830
C	-1.20525698	-0.00085943	-0.69543189
H	-2.14556935	-0.00154420	-1.23840841
C	0.00005069	-0.00002432	-1.41078602
C	0.00008118	0.00003305	-2.89602771
C	0.92360729	0.77557531	-3.61648552
H	1.62917003	1.40145723	-3.07702083
C	0.92413867	0.77555937	-5.01071764
H	1.64228393	1.38926144	-5.54828107
C	0.00002796	0.00038877	-5.71425802
H	0.00003948	0.00046062	-6.80090034
C	-0.92400690	-0.77502121	-5.01085765
H	-1.64216143	-1.38859690	-5.54849858
C	-0.92349911	-0.77530671	-3.61661986
H	-1.62912508	-1.40130190	-3.07729546
C	1.20530232	0.00080478	-0.69533893
C	-2.50878902	-0.00035956	1.44830958
C	-2.67046459	-0.77192354	2.61109726
H	-1.85010164	-1.39597907	2.95482628
C	-3.87790030	-0.77094261	3.30822437
H	-3.98379606	-1.38149695	4.20114839
C	-4.95016602	0.00109470	2.85655197

H	-5.89143198	0.00160719	3.39952568
C	-4.80371009	0.77230157	1.70173775
H	-5.62907704	1.38352245	1.34609452
C	-3.59570567	0.77187283	1.00566493
H	-3.48209210	1.39533058	0.12307309

int1b_14eze
E [Hartrees] = -616.7811063604

C	-3.04670534	0.10081168	-0.06198428
C	-1.78102200	-0.24415001	-0.03067932
C	-2.96561500	2.59244998	-0.37048681
C	-3.61466288	1.46354762	-0.20870892
C	-0.58532566	-0.92620138	0.04211372
C	-2.60401799	3.91059169	-0.54851258
H	-3.80275950	-0.68888943	0.03000501
H	-4.71080416	1.49495204	-0.17428224
C	0.06171144	-1.15283688	1.29940329
C	0.06225319	-1.41347023	-1.13849645
C	-2.34884843	4.76595993	0.57126714
C	-2.45018288	4.46505443	-1.85990845
H	-2.45418058	4.35953989	1.57241831
C	-1.98448071	6.08843990	0.37893186
H	-0.41133804	-1.24399859	-2.10056083
C	1.26432497	-2.09624878	-1.05182568
H	-0.41257027	-0.78409571	2.20365987
C	1.26368243	-1.83860041	1.35967982
H	-2.63347434	3.82831371	-2.71988069
C	-2.08487165	5.79080964	-2.02587886
C	-1.85034375	6.61488262	-0.91474797
H	-1.98239642	6.19528731	-3.02965214
H	-1.80373078	6.72392567	1.24213868
C	1.87575648	-2.31760394	0.19151163
H	1.73424785	-2.00849928	2.32475157
H	2.81745624	-2.85567889	0.24928262
H	1.73559031	-2.46597834	-1.95894056
H	-1.56622733	7.65371879	-1.05528195

int1b_14zez
E [Hartrees] = -616.7879105579
Gcorr [kcal/mol] = 114.872

C	-0.80588211	1.38463142	-0.13515625
C	0.49382522	1.22380096	-0.08433156
C	-2.76383908	2.89313898	-0.25896165
C	-1.46415258	2.73241137	-0.20697466

C	1.82967431	1.61035340	-0.05162792
C	-4.09936175	2.50557827	-0.29409617
H	-1.48620573	0.53275441	-0.12782683
H	-0.78384414	3.58431507	-0.21333541
C	2.58659040	1.74182060	-1.25448491
C	2.50000013	1.83416155	1.18838606
C	-4.85827479	2.37227486	0.90728167
C	-4.76727087	2.28235586	-1.53550767
H	-4.36442238	2.54568034	1.85852560
C	-6.19892015	2.02100642	0.85935702
H	1.93783893	1.73125339	2.11154299
C	3.84188505	2.18327753	1.21179418
H	2.09084646	1.56801714	-2.20467414
C	3.92768994	2.09169366	-1.20929202
H	-4.20355841	2.38678422	-2.45754661
C	-6.10874429	1.93191986	-1.56165835
C	-6.83514423	1.79872735	-0.36998776
H	-6.59857528	1.75819528	-2.51628903
H	-6.75886154	1.91649530	1.78510130
C	4.56633158	2.31448565	0.01871459
H	4.48608718	2.19469797	-2.13613379
H	5.61768093	2.58613888	0.04564174
H	4.33359217	2.35750955	2.16537180
H	-7.88613923	1.52594943	-0.39901830

int1b_14zzz
E [Hartrees] = -616.7855532420
Gcorr [kcal/mol] = 115.657

C	-0.80171562	1.39404058	-0.04425520
C	0.46723178	1.05551563	-0.02211395
C	-0.62464977	3.89541040	-0.15515496
C	-1.34084929	2.79452501	-0.12284325
C	1.83261514	1.33912062	-0.03169526
C	0.58915334	4.58378204	-0.15727796
H	-1.57167003	0.62094508	-0.00504873
H	-2.43061758	2.85267328	-0.15215506
C	2.56113827	1.39825320	-1.25499542
C	2.54558640	1.54948524	1.18414161
C	1.25373703	4.89276121	-1.37903109
C	1.18606683	5.02087377	1.06024754
H	0.80650012	4.56767140	-2.31333437
C	2.46331468	5.57081422	-1.37115086
H	2.00177161	1.50446690	2.12264794
C	3.90251785	1.83397165	1.16519652

H	2.02959042	1.23587292	-2.18762473
C	3.91809305	1.68377758	-1.25378741
H	0.68657025	4.79483081	1.99733084
C	2.39616132	5.69801339	1.04827339
C	3.04447465	5.97704521	-0.16240767
H	2.84614916	6.00887107	1.98754453
H	2.96554207	5.78237954	-2.31154577
C	4.59893896	1.90463195	-0.04890580
H	4.45468564	1.74142041	-2.19725274
H	5.66154842	2.12996022	-0.05594370
H	4.42683511	2.00889486	2.10107837
H	3.99330232	6.50586719	-0.16396020

int1c

E [Hartrees] = -616.7490278780

C	-0.96004360	0.68478848	0.22778063
C	-1.15127220	-0.16047594	1.37752150
C	0.35851189	0.86512772	-0.29103909
C	1.11522728	-0.47350118	-0.62544206
C	0.88921633	-1.57710434	-1.52159707
C	1.69596278	0.24575541	0.26389753
H	0.48815030	1.64578183	-1.04485102
H	2.51097808	0.44992824	0.93859738
C	-0.39529749	-0.02943537	2.56983552
C	-2.19736464	-1.11486236	1.36064096
C	-0.32843297	-1.67052451	-2.21634130
C	1.87119837	-2.56915106	-1.69838862
H	-1.07944641	-0.90069959	-2.05984161
C	-0.56001296	-2.74374067	-3.07363689
H	2.81138554	-2.49271026	-1.15993926
C	1.63128077	-3.63770416	-2.55678172
H	0.39027228	0.71899158	2.61770068
C	-0.68596347	-0.80582589	3.68775764
H	-2.80784968	-1.19388159	0.46568619
C	-2.42472567	-1.94662014	2.45089399
C	0.41727959	-3.72696292	-3.24625275
H	-1.50388298	-2.81365875	-3.60683302
H	2.39074594	-4.40309686	-2.69046222
H	-3.20897814	-2.69787755	2.40325465
C	-1.68207708	-1.78511246	3.62647613
H	-0.11776966	-0.66673284	4.60440966
H	0.23478554	-4.56293628	-3.91589823
H	-1.89017841	-2.40659267	4.49329258

int2_12
E [Hartrees] = -616.8350641243
Gcorr [kcal/mol] = 117.194

H	-2.39671564	-3.68419832	-0.17762534
C	-1.76572424	-2.80847385	-0.08894521
C	-0.64418733	-2.33085463	-0.77180523
H	-0.07853134	-2.66178467	-1.63398330
C	-0.57332451	-1.14970235	0.11179449
C	-1.71168137	-1.67258825	0.85323964
C	-2.43654663	-1.38214326	2.05456722
C	-3.68278671	-2.01444799	2.28866092
H	-4.08141466	-2.68975723	1.53640273
C	-4.40489209	-1.76632947	3.44958719
H	-5.36339616	-2.25591576	3.60159455
C	-3.90530384	-0.89012968	4.41979072
H	-4.47111461	-0.69732949	5.32692786
C	-2.66616048	-0.27276316	4.21595086
H	-2.26031185	0.39273724	4.97355420
C	-1.93864861	-0.51304907	3.05594065
H	-0.96227291	-0.05896239	2.92741570
C	0.23082891	0.03556428	0.07175655
C	1.44146821	0.03302507	-0.66428600
H	1.75374191	-0.88031492	-1.16333923
C	2.23777399	1.16945826	-0.73705037
H	3.16716404	1.13953131	-1.29992173
C	1.84980163	2.34777036	-0.08921256
H	2.47341445	3.23545367	-0.14694660
C	0.64682754	2.37557078	0.62510901
H	0.32694814	3.29231829	1.11380424
C	-0.15422547	1.24221847	0.70540923
H	-1.10263037	1.28799677	1.22920980

int2_13
E [Hartrees] = -616.8373482808
Gcorr [kcal/mol] = 115.549

H	-2.17456608	-0.00484987	-0.02778730
C	-1.09181090	-0.00161033	-0.01343171
C	-0.05711067	0.00060374	-1.02781731
C	0.95007458	0.00246734	0.01344108
H	2.03280915	0.00660622	0.02777107
C	-0.08461943	-0.00011720	1.02782008
C	-0.10342614	-0.00066776	2.45936742
C	-1.32637078	-0.00014828	3.17009380
H	-2.26127097	0.00010080	2.61602237

C	-1.34062534	0.00050752	4.55973965
H	-2.29030178	0.00134168	5.08844434
C	-0.13998760	0.00043392	5.27953153
H	-0.15415155	0.00137193	6.36583371
C	1.07890848	-0.00082143	4.59111466
H	2.01452673	-0.00132813	5.14433122
C	1.10067407	-0.00140146	3.20156553
H	2.04966037	-0.00247876	2.67197859
C	-0.03840395	0.00043704	-2.45936545
C	1.18453629	-0.00038126	-3.17010496
H	2.11948219	-0.00109353	-2.61611421
C	1.19878859	-0.00069387	-4.55976011
H	2.14843456	-0.00147737	-5.08851318
C	-0.00186304	-0.00018063	-5.27954884
H	0.01231564	-0.00041574	-6.36585181
C	-1.22073403	0.00056361	-4.59109418
H	-2.15636125	0.00097726	-5.14430140
C	-1.24250659	0.00081860	-3.20155436
H	-2.19144866	0.00143597	-2.67189382

int3bhh_12
E [Hartrees] = -925.2409448482
Gcorr [kcal/mol] = 184.029

C	0.79250809	0.33227713	0.50105136
C	-0.67483370	0.60318840	0.18775160
C	-1.56136339	-0.56733908	0.74233730
C	-1.93269129	-0.90308466	-0.58829674
C	-1.16535396	0.12219455	-1.14485703
C	1.73253140	1.19186351	0.72218990
C	2.73831373	2.08201205	0.99262980
H	0.96324460	-0.75292691	0.60044562
H	-0.96715999	1.62130099	0.46609325
C	-1.76938103	-1.01400879	2.07329744
C	-2.81084402	-1.90673817	-1.20766799
H	-0.98463294	0.46458653	-2.15698993
C	2.95617666	2.56536115	2.32687459
C	3.60425607	2.57183524	-0.04186729
C	-1.29702751	-0.22308403	3.15735952
C	-2.42483916	-2.23702425	2.38739678
C	-4.04847412	-2.24463441	-0.63633989
C	-2.43795829	-2.51008293	-2.41931779
H	-0.77535151	0.70459723	2.94138277
C	-1.48999636	-0.62306007	4.47201138
H	-2.76507303	-2.87929748	1.58267670

C	-2.60340190	-2.62824983	3.70620014
H	-1.48120781	-2.25180714	-2.86557301
C	-3.27256056	-3.44156468	-3.03509714
H	-4.35756926	-1.76239489	0.28621917
C	-4.88386822	-3.17370389	-1.25467465
H	2.31620525	2.19844843	3.12348851
C	3.95731870	3.48353861	2.58833655
H	3.45425056	2.21792038	-1.05711284
C	4.61358239	3.47074098	0.25287188
H	-2.96645930	-3.90707230	-3.96819982
H	-3.10089195	-3.57092450	3.92039377
H	4.09995548	3.84328249	3.60419887
C	-2.14650231	-1.82578172	4.76050570
H	-1.12448671	0.00311878	5.28204765
C	4.79866940	3.94175210	1.56240274
H	5.26421693	3.82297444	-0.54358387
C	-4.49718861	-3.77802682	-2.45334576
H	-5.84026623	-3.42253367	-0.80255074
H	-5.14751076	-4.50484844	-2.93253199
H	5.58884917	4.65390050	1.78054871
H	-2.29430013	-2.13711769	5.79059751

int3bhph_12
E [Hartrees] = -925.2363614199
Gcorr [kcal/mol] = 184.264

C	1.07171285	0.12353708	-0.57697825
C	-0.29694947	0.81849464	-0.44299607
C	-1.03769488	0.02192040	0.71453994
C	-1.95294146	-0.47003352	-0.23241299
C	-1.37933813	0.21971798	-1.29627416
C	2.22464259	0.61371803	-0.88504579
C	3.47195075	1.09794598	-1.19617008
H	0.96289448	-0.91863701	-0.22927752
C	-0.25842952	2.32788056	-0.43377031
C	-0.81887705	-0.07083119	2.11546148
H	-2.79572525	-1.15170908	-0.15756900
H	-1.58861695	0.31506308	-2.35479021
C	-0.91561633	3.07061974	0.55669113
C	0.42978729	3.01472216	-1.44565458
C	4.30012072	1.69912019	-0.19383799
C	3.98109053	1.03572263	-2.53374739
C	0.23766614	0.64920311	2.73299958
C	-1.65152595	-0.87174331	2.94116948
H	-2.46865372	-1.42744581	2.48853226

C	-1.42974387	-0.95085002	4.30823337
H	0.88046463	1.26946259	2.11635814
C	0.44646246	0.56443723	4.10307116
H	0.92449450	2.45550525	-2.23318702
C	0.47785445	4.40955800	-1.45334833
H	-1.45528575	2.55475291	1.34421831
C	-0.87020264	4.46488575	0.54585699
H	3.36589768	0.58309785	-3.30549050
C	5.23745267	1.53478319	-2.83184850
H	3.92825669	1.75302300	0.82459050
C	5.54160031	2.21434536	-0.52391240
H	6.15040231	2.67703359	0.24863803
C	6.02653105	2.13352657	-1.83814359
H	5.61013442	1.46978952	-3.85094934
C	-0.38093087	-0.23451542	4.90136471
H	1.26014745	1.12453366	4.55669499
H	-2.07735758	-1.57123845	4.92257744
C	-0.16921688	5.14013923	-0.45596047
H	1.02187927	4.92359664	-2.24154008
H	-1.38033571	5.02381914	1.32621410
H	-0.21276428	-0.29829141	5.97261754
H	-0.13083173	6.22624179	-0.46036168
H	7.00659848	2.53112482	-2.08439935

int3bphh_12
E [Hartrees] = -925.2150927109
Gcorr [kcal/mol] = 184.184

C	1.11129827	-0.31902443	-0.41444563
C	-0.24851399	0.46985086	-0.42780912
C	-1.35583213	-0.29909977	0.35126876
C	-2.06171024	-0.56046849	-0.78525025
C	-1.14091355	0.24090473	-1.60032424
C	2.19953236	0.19894312	0.11433148
H	2.44748720	1.24130281	0.31342816
C	1.06328486	-1.76018461	-0.83359428
H	-0.06542287	1.51131635	-0.15055266
H	-1.42164130	-0.64070871	1.37859843
C	-3.23298144	-1.39192004	-1.07857956
C	-1.10431651	0.77159868	-2.91557287
C	0.05890592	1.45645701	-3.36139031
C	-2.20732560	0.66994507	-3.80441876
C	-4.31529855	-1.44034246	-0.18629187
C	-3.26463582	-2.19007649	-2.23439269
C	0.68671943	-2.13104645	-2.13243899

C	1.40876732	-2.76942716	0.07879695
H	1.72134962	-2.47920420	1.07725970
C	1.34183421	-4.11234473	-0.28519532
H	0.47160632	-1.36761616	-2.87097112
C	0.62360334	-3.47885363	-2.49891063
H	-2.41371222	-2.17910978	-2.90879143
C	-4.35883362	-3.01420222	-2.49120958
H	-4.29582107	-0.81820354	0.70459869
C	-5.40919790	-2.26379247	-0.44707128
H	-3.10807571	0.16148580	-3.47868293
C	-2.14616122	1.24013818	-5.06857256
H	0.91897051	1.51268647	-2.69991496
C	0.11052574	2.00897435	-4.63239427
C	-0.99057642	1.90778884	-5.49338439
H	1.01148053	2.51981351	-4.96108391
H	-3.00293601	1.16450832	-5.73283385
C	-5.43511089	-3.05098604	-1.60105572
H	-6.24398798	-2.28863847	0.24819313
H	-4.36881068	-3.63354221	-3.38404019
C	0.94180716	-4.47370260	-1.57579482
H	0.33952115	-3.74594122	-3.51394186
H	1.59644364	-4.88043426	0.44087642
H	0.88940697	-5.52165218	-1.85935921
H	-6.28923821	-3.69104945	-1.80468337
H	-0.94656972	2.34252769	-6.48787940

int3bphph_12
E [Hartrees] = -925.2034553041
Gcorr [kcal/mol] = 183.561

C	1.13999031	-0.22860026	-0.56016799
C	-0.19236768	0.62736296	-0.50339695
C	-1.31630276	-0.18851188	0.24784912
C	-2.05155892	-0.31380941	-0.88093194
C	-1.09622057	0.43436585	-1.68446735
C	2.30446292	0.23215063	-0.16238502
H	2.69236426	1.23997310	-0.04675317
C	0.99765032	-1.68980120	-0.89532353
C	0.02570429	2.03117752	0.02823938
H	-1.38343294	-0.56348683	1.26189973
H	-2.98031457	-0.82241803	-1.11959581
C	-1.00629970	0.79207793	-3.05458533
C	0.18095588	1.36710554	-3.58410202
C	-2.09692530	0.57155618	-3.93599163
C	0.61168268	-2.11685367	-2.17279306

C	1.28741292	-2.65872817	0.07881342
H	1.61147632	-2.32652693	1.06066778
C	1.16088358	-4.01601752	-0.20577068
H	0.42910846	-1.38921943	-2.95413802
C	0.48974738	-3.47976424	-2.45956208
H	-3.00906282	0.12616753	-3.54903061
C	-2.00973145	0.93264425	-5.27297532
H	1.03458036	1.50412216	-2.92731928
C	0.25826428	1.71474571	-4.92485455
C	-0.83461083	1.50546460	-5.77664827
H	1.17560958	2.14644564	-5.31551144
H	-2.85700836	0.76540475	-5.93249111
C	0.75577079	-4.43304859	-1.47804239
H	0.19765720	-3.79215891	-3.45913864
H	1.37681238	-4.75091984	0.56579493
H	0.65941404	-5.49227956	-1.70192310
H	-0.76859217	1.77987187	-6.82548777
C	-0.21231524	3.18188128	-0.72911841
C	0.43721393	2.18296838	1.36369757
H	-0.54783576	3.09750250	-1.75598439
C	-0.02838579	4.45231105	-0.17337298
H	0.62584901	1.29608312	1.96293941
C	0.61480952	3.44655429	1.92075861
C	0.38545823	4.59029412	1.14986325
H	-0.21693003	5.33357296	-0.78109868
H	0.93022314	3.53980255	2.95665528
H	0.52494681	5.57801706	1.58115587

int4bhh_12
E [Hartrees] = -925.2409478606
Gcorr [kcal/mol] = 184.094

C	1.07316331	-0.89378597	0.66004825
C	-0.22415055	-0.19330435	0.27011538
C	-1.45562709	-1.02332679	0.77872863
C	-1.84469385	-1.25284958	-0.56915809
C	-0.77015588	-0.52553953	-1.08561110
C	2.22413337	-0.35918364	0.90617093
C	3.44473493	0.19403598	1.19105546
H	0.89526956	-1.97498841	0.78653967
H	-0.20315560	0.87061981	0.52919876
C	-1.85903170	-1.35797448	2.09771153
C	-2.95701771	-1.94603188	-1.23553082
H	-0.44142238	-0.27417100	-2.08714229
C	3.76063593	0.64537767	2.51672766

C	4.44877088	0.35233817	0.17762493
C	-1.21955345	-0.73164495	3.20345340
C	-2.87670991	-2.31137590	2.37956685
C	-4.26593481	-1.88012573	-0.73096599
C	-2.72680746	-2.64913103	-2.42888751
H	-0.42512403	-0.01591991	3.01348189
C	-1.59308019	-1.02641336	4.50690958
H	-3.35813094	-2.83260475	1.55956043
C	-3.23440765	-2.60193310	3.68796256
H	-1.71560546	-2.70294302	-2.82367926
C	-3.77499663	-3.28581649	-3.09157372
H	-4.45825955	-1.31474719	0.17596149
C	-5.31406257	-2.51455920	-1.39617427
H	3.01617944	0.52575752	3.29792667
C	4.98604245	1.22690524	2.78893396
H	4.22773902	0.01669938	-0.83079487
C	5.67513969	0.91425198	0.48408372
H	-3.57983991	-3.83356263	-4.00971784
H	-4.01024073	-3.33956576	3.87772120
H	5.20170035	1.57068488	3.79742020
C	-2.60465953	-1.96013251	4.76306014
H	-1.09223595	-0.52892269	5.33366999
C	5.95664736	1.36331926	1.78407231
H	6.42506015	1.01738040	-0.29615200
C	-5.07171080	-3.22248403	-2.57589585
H	-6.32240884	-2.45172029	-0.99574591
H	-5.88890322	-3.71949607	-3.09171270
H	6.91941303	1.81126558	2.01114969
H	-2.89378056	-2.18991152	5.78454771

int4bhph_12
E [Hartrees] = -925.2363702678
Gcorr [kcal/mol] = 183.923

C	0.63921412	-0.67470481	-0.24452664
C	-0.45216631	0.41292317	-0.23785952
C	-1.44986070	-0.02915565	0.91642331
C	-2.43237991	-0.28880263	-0.05502858
C	-1.63029796	0.10983779	-1.12006053
C	1.89844184	-0.58554894	-0.51054501
C	3.24538822	-0.52933928	-0.77457376
H	0.19950993	-1.60379963	0.15843550
C	0.04925987	1.83511206	-0.31569843
C	-1.32933617	-0.07576504	2.33149097
H	-3.44687068	-0.67289973	0.00740146

H	-1.75599230	0.18374314	-2.19341265
C	-0.39024356	2.81562279	0.58436624
C	0.95885697	2.20126292	-1.31959375
C	3.76238577	-0.84514123	-2.07274261
C	4.17866282	-0.13394333	0.23765637
C	-0.12856021	0.33144554	2.97049893
C	-2.40340427	-0.51613183	3.14936238
H	-3.33285064	-0.82791592	2.68002852
C	-2.27512933	-0.55244666	4.53013060
H	0.70073834	0.67410328	2.35975931
C	-0.01449571	0.29400093	4.35379406
H	1.29114450	1.45993980	-2.03902805
C	1.43400362	3.51072991	-1.40642157
H	-1.09642151	2.54982082	1.36424388
C	0.08222206	4.12508251	0.49414046
H	3.80210298	0.10769860	1.22667646
C	5.53023521	-0.04676258	-0.04760366
H	3.06838517	-1.14696231	-2.85131779
C	5.12184314	-0.77519121	-2.32435551
H	5.49581917	-1.02755425	-3.31336656
C	6.01748859	-0.37043147	-1.32301926
H	6.22125659	0.26635859	0.73085937
C	-1.08196113	-0.14784277	5.14457596
H	0.91294745	0.61119429	4.82364845
H	-3.10865844	-0.89451855	5.13831642
C	1.00009354	4.47710949	-0.49806591
H	2.14367289	3.77368787	-2.18659584
H	-0.26479702	4.87034475	1.20527322
H	-0.98732632	-0.17614281	6.22633232
H	1.37084460	5.49657325	-0.56418154
H	7.08106023	-0.30910049	-1.53353985

int4hhh_12

E [Hartrees] = -925.2270949676

H	0.25318540	-2.68831300	-1.33545026
C	-2.11571315	-1.04107465	-0.33758394
C	-0.76818970	-0.79065974	-0.39460912
C	0.13822397	0.31494313	-0.12772339
C	1.48862417	0.20113296	-0.51085245
H	1.82211668	-0.70286261	-1.01280890
C	2.39380992	1.22988060	-0.26012503
H	3.43029097	1.12319136	-0.56902107
C	1.97176759	2.39301289	0.38712177
H	2.67638957	3.19665384	0.58278077

C	0.63764999	2.51358386	0.78916663
H	0.30564087	3.40787302	1.31002176
C	-0.26974984	1.48943498	0.53664540
H	-1.29523104	1.58211754	0.87712899
C	-0.43329261	-2.26611378	-0.61300351
C	-3.36075984	-0.32971628	-0.09357602
C	-3.52933418	1.02775077	-0.42849875
H	-2.70900383	1.56748039	-0.89128304
C	-4.74419683	1.66905002	-0.20001615
H	-4.85724452	2.71614121	-0.46862819
C	-5.81756352	0.97027313	0.35977389
H	-6.76419732	1.47318615	0.53711731
C	-5.66938309	-0.38235440	0.67799694
H	-6.50102085	-0.93537689	1.10661075
C	-4.45792764	-1.02858752	0.44568972
H	-4.34402337	-2.08087648	0.69372657
C	-0.96582019	-3.08939465	0.59651084
H	-1.07443390	-2.53782344	1.53000694
C	-1.16924347	-4.50520112	0.63364930
C	-0.67855171	-5.32841114	-0.43927855
C	-1.53387111	-6.30423156	-1.01072495
H	-2.55520996	-6.37047832	-0.64701839
C	-1.08395306	-7.14144512	-2.02428099
H	-1.76638978	-7.85556604	-2.47786819
C	0.25733432	-7.10519039	-2.42514425
H	0.61740373	-7.79134930	-3.18679222
C	1.13627931	-6.19715533	-1.82690546
H	2.18179814	-6.17742861	-2.12434155
C	0.67130700	-5.29189760	-0.87768335
H	1.35221566	-4.57400797	-0.42936402
C	-1.90006868	-2.52593815	-0.56642316
H	-2.47469760	-3.19922957	-1.19282416

int4hhph_12

E [Hartrees] = -925.2214789715

C	0.23912189	-2.68077231	-1.77731983
C	-2.14741378	-0.66000982	-0.42776055
C	-0.79169002	-0.61190399	-0.40637518
C	0.23107830	0.36726033	-0.07970222
C	1.58602333	-0.00606282	-0.02695213
H	1.86444345	-1.03393370	-0.23750318
C	2.56754705	0.93270198	0.28674130
H	3.60988111	0.62736181	0.32532480
C	2.21693785	2.25877340	0.54700518

H	2.98349165	2.98988681	0.78913161
C	0.87267572	2.64294844	0.49029429
H	0.59275758	3.67422353	0.68918036
C	-0.10985567	1.70906425	0.17899211
H	-1.15283467	2.01189198	0.13178259
C	-0.68021448	-2.10524084	-0.76130999
H	-2.92399520	0.04446477	-0.14370661
C	-1.38980828	-2.91742078	0.38870926
H	-1.30203469	-2.41280536	1.35128652
C	-1.06032767	-4.32047058	0.39259258
C	-1.74222568	-5.23477078	-0.47703746
C	-3.15312131	-5.21635200	-0.64499085
H	-3.73102926	-4.43436969	-0.16226411
C	-3.79835067	-6.21615998	-1.36655631
H	-4.88196016	-6.20761353	-1.45250692
C	-3.05410052	-7.20793886	-2.01164329
H	-3.55792404	-7.96908925	-2.60135769
C	-1.65851217	-7.22952858	-1.88399100
H	-1.08077024	-8.00541517	-2.37912887
C	-1.01755331	-6.29186309	-1.08724107
H	0.05735408	-6.32649120	-0.94279301
C	-2.18898117	-2.14118370	-0.71334681
H	-2.81229611	-2.66617655	-1.42686984
C	0.13458125	-2.25663626	-3.11072248
C	1.24927078	-3.58866675	-1.43108419
H	-0.63919176	-1.54219432	-3.37941745
C	1.00715230	-2.74664988	-4.07952651
H	1.32885348	-3.91676527	-0.39833558
C	2.12109524	-4.08289076	-2.40437479
H	0.90961145	-2.41570921	-5.11015713
C	2.00326683	-3.66388975	-3.72944617
H	2.89402962	-4.79326807	-2.12261595
H	2.68353680	-4.04512626	-4.48632354

int4hphph_12
E [Hartrees] = -925.2057444784
Gcorr [kcal/mol] = 187.157

C	0.42655819	-2.58004415	-1.71582177
C	-2.25205423	-1.20235175	-0.07113249
C	-0.93123491	-0.96707740	-0.08131672
H	-0.28059277	-0.19110348	0.30857896
C	-0.60973056	-2.33793830	-0.68281513
H	-3.11674284	-0.67823745	0.32495955
C	-1.15735448	-3.41876022	0.33130655

H	-1.13811903	-3.02893842	1.35060635
C	-0.68675463	-4.78868828	0.24556148
C	-1.04120282	-5.74374803	-0.76461377
C	-1.16794092	-5.56552061	-2.17026430
H	-0.93498640	-4.60676943	-2.61205215
C	-1.55263256	-6.61685182	-2.98931708
H	-1.62619548	-6.45764574	-4.06175075
C	-1.89419993	-7.85932439	-2.44015078
H	-2.22765496	-8.66701385	-3.08643943
C	-1.77604124	-8.06497995	-1.06365750
H	-2.01189339	-9.03503401	-0.63383426
C	-1.29072806	-7.04535939	-0.24966369
H	-1.12481657	-7.21043085	0.81030863
C	-2.10826730	-2.61826880	-0.63035800
C	-3.04298917	-3.23873266	-1.60283382
C	0.42761023	-1.79782170	-2.88355335
C	1.43947559	-3.53294799	-1.54256187
H	-0.32991203	-1.02884413	-3.00802846
C	1.39038345	-1.99672490	-3.87016684
H	1.45727977	-4.12368438	-0.62951723
C	2.40190991	-3.73411688	-2.53310931
H	1.37069867	-1.39063415	-4.77211252
C	2.37899282	-2.97093296	-3.70066241
H	3.17169234	-4.48695195	-2.38701928
H	3.12985882	-3.12595162	-4.47071258
C	-3.10783292	-2.79299191	-2.93087253
C	-3.91247308	-4.25781355	-1.19105976
H	-3.85511315	-4.61740835	-0.16796654
C	-4.80891335	-4.83583399	-2.08825926
H	-2.44193046	-2.00119596	-3.25936412
C	-4.00081847	-3.37227941	-3.83164144
H	-4.03082395	-3.02466806	-4.86111824
C	-4.85153734	-4.39858885	-3.41350223
H	-5.46344331	-5.63714906	-1.75632861
H	-5.54293674	-4.85470952	-4.11710811

int5hhh_12

E [Hartrees] = -925.2315291485

H	0.60802424	-2.96069197	-0.62930016
C	-1.96959883	-1.37720413	-0.18635947
C	-0.65175999	-1.01981024	-0.11386177
C	0.14415672	0.17680612	0.10717072
C	1.53766146	0.12012148	-0.08843172
H	1.98889389	-0.81223990	-0.41611958

C	2.33819109	1.23978190	0.12749012
H	3.41086938	1.17408001	-0.03438081
C	1.76597560	2.44090383	0.55097099
H	2.38890601	3.31529359	0.71836657
C	0.38554554	2.50818595	0.76566009
H	-0.06598684	3.43389557	1.11304153
C	-0.41701449	1.39250674	0.54866204
H	-1.48213138	1.44874472	0.74557775
C	-0.20724651	-2.48585927	-0.09858447
C	-3.27514304	-0.73889859	-0.22503427
C	-3.46731408	0.54581974	-0.77019405
H	-2.61741369	1.07979442	-1.18341199
C	-4.73599294	1.11787895	-0.80904175
H	-4.86556809	2.10859333	-1.23679342
C	-5.84104027	0.42003985	-0.31242413
H	-6.83003551	0.86889646	-0.34398423
C	-5.66794157	-0.86368941	0.21146642
H	-6.52318953	-1.41722853	0.59014882
C	-4.40130922	-1.44165569	0.24535758
H	-4.26817029	-2.44259865	0.64757341
C	-0.82695742	-3.17445181	1.16592370
H	-1.00651383	-2.49507732	2.01012151
C	-0.40604637	-4.54620360	1.28130365
C	-0.23623242	-5.05931075	2.62339692
C	0.66455392	-6.13954304	2.79352270
H	1.17560060	-6.51061720	1.91006429
C	0.89886288	-6.69399258	4.04708466
H	1.61578989	-7.50242084	4.16265954
C	0.17375684	-6.23774185	5.15326624
H	0.32671434	-6.69430308	6.12788505
C	-0.76141517	-5.20631362	5.00687824
H	-1.33114126	-4.86580834	5.86778403
C	-0.94166548	-4.60217911	3.76765463
H	-1.65731559	-3.79127518	3.66605624
C	-1.63651695	-2.86941401	-0.13343194
H	-2.08957925	-3.67850136	-0.69327375

int5hhph_12

E [Hartrees] = -925.2246688708

C	0.28253338	-2.93589238	-1.64535930
C	-2.23141708	-0.94204762	-0.45906575
C	-0.88455409	-0.82788887	-0.44621520
C	0.07408433	0.22455718	-0.15270703
C	1.42417143	-0.08896825	0.08838727

H	1.74614447	-1.12426199	0.03586825
C	2.34187000	0.91674971	0.38743827
H	3.38091428	0.65838248	0.57345880
C	1.93110345	2.24999485	0.44286330
H	2.64829808	3.03367759	0.67131446
C	0.59234715	2.57445523	0.19592458
H	0.26834673	3.61121867	0.23220585
C	-0.32667955	1.57377613	-0.10124372
H	-1.36421195	1.82805431	-0.30203830
C	-0.68657342	-2.35352497	-0.67706238
H	-3.04667079	-0.26747681	-0.21714444
C	-1.33970293	-3.05112162	0.56297499
H	-1.35161347	-2.42237129	1.46284624
C	-1.42121022	-4.48623800	0.60702723
C	-1.38857085	-5.08722482	1.92134226
C	-0.73129494	-4.53234832	3.05113440
H	-0.22619979	-3.57508267	2.95899402
C	-0.68523236	-5.21933996	4.25901137
H	-0.15088566	-4.79766913	5.10646080
C	-1.34755749	-6.44545524	4.39206234
H	-1.32617908	-6.97044778	5.34370646
C	-2.02143831	-7.00572711	3.30109109
H	-2.52471776	-7.96303744	3.40611336
C	-2.00607940	-6.35327641	2.07344683
H	-2.47698441	-6.79088533	1.19812743
C	-2.18034790	-2.44106286	-0.63776754
H	-2.80573398	-3.10117932	-1.22529742
C	0.88895022	-2.07808742	-2.58107797
C	0.61574739	-4.29943903	-1.68187835
H	0.65342604	-1.01890695	-2.57264313
C	1.79559659	-2.56814334	-3.52117059
H	0.12167767	-4.97078865	-0.98496408
C	1.52551021	-4.78463160	-2.61944674
H	2.24954435	-1.88333770	-4.23296416
C	2.12227481	-3.92407103	-3.54373446
H	1.76802330	-5.84439735	-2.62642928
H	2.83323322	-4.30601628	-4.27173079

int5hphph_12
E [Hartrees] = -925.2147940188
Gcorr [kcal/mol] = 186.317

C	0.17583113	-2.97987440	-1.60419794
C	-2.44245254	-1.07980440	-0.51890275
C	-1.11594281	-0.90150946	-0.52485670

H	-0.46041656	-0.05690753	-0.33958865
C	-0.83880687	-2.40183861	-0.69603039
H	-3.30435890	-0.44270757	-0.34623421
C	-1.50499000	-3.11199345	0.58010776
H	-1.57791991	-2.44770552	1.45118162
C	-1.32228551	-4.53072444	0.68366765
C	-1.17809961	-5.07337364	2.01066363
C	-0.62243280	-4.37917084	3.11870351
H	-0.28194973	-3.35560880	2.99133610
C	-0.46378737	-5.00904042	4.34745094
H	-0.00596464	-4.47708836	5.17752134
C	-0.91707262	-6.32183659	4.52594296
H	-0.81077650	-6.80336562	5.49464162
C	-1.48837596	-7.02172749	3.45738590
H	-1.82709498	-8.04481993	3.59672420
C	-1.57488589	-6.42021433	2.20696527
H	-1.96171569	-6.96057635	1.34802222
C	-2.32705621	-2.60558151	-0.65565609
C	-3.17875167	-3.45609858	-1.52615180
C	1.23794101	-2.16607812	-2.02921192
C	0.08979019	-4.29172928	-2.10445852
H	1.31795468	-1.14845906	-1.65744067
C	2.19460777	-2.64557755	-2.92518798
H	-0.71310206	-4.93113722	-1.75852319
C	1.04825749	-4.76656067	-2.99641528
H	3.00940828	-1.99853347	-3.23985124
C	2.10319370	-3.94893309	-3.41291730
H	0.96843319	-5.78342317	-3.37224812
H	2.84616475	-4.32574344	-4.11107166
C	-3.24129151	-3.16164239	-2.89608237
C	-3.95391817	-4.50805068	-1.02380049
H	-3.90091294	-4.74791828	0.03378975
C	-4.77225138	-5.25321580	-1.87250639
H	-2.63517717	-2.35047180	-3.29049205
C	-4.05787152	-3.90710685	-3.74574786
H	-4.08801445	-3.67322495	-4.80672818
C	-4.82713832	-4.95540653	-3.23597104
H	-5.36595214	-6.06909106	-1.46842941
H	-5.46231605	-5.53879728	-3.89730312

int6hh_124

E [Hartrees] = -925.3457691944

C	-2.93845523	2.28410688	0.09389261
C	-4.16883869	1.39667294	0.25052667

C	-3.17136877	0.19357043	0.15576497
C	-3.91934063	-0.20292887	-1.12037384
C	-4.79844161	0.83407717	-1.03284565
C	-5.93379906	1.34900119	-1.78769657
C	-3.59314449	-1.25693709	-2.07702097
C	-3.82543397	-1.11178357	-3.45778858
H	-4.26808427	-0.19208124	-3.82712595
C	-3.46759550	-2.12023542	-4.34913576
H	-3.64754028	-1.98560056	-5.41258783
C	-2.86848221	-3.29479419	-3.88448088
H	-2.59031689	-4.07979143	-4.58238095
C	-2.62309380	-3.44916431	-2.51832729
H	-2.15481230	-4.35716901	-2.14736960
C	-2.97762342	-2.43932108	-1.62554974
H	-2.78941121	-2.56533781	-0.56231210
H	-3.08318858	-0.53157598	0.96970686
H	-4.82072653	1.53594130	1.11785416
C	-2.07089346	1.25326988	-0.00424316
C	-0.64403362	1.11174963	-0.26602456
H	-2.83225180	3.36051428	-0.01054791
C	2.10132618	0.81832203	-0.80501551
C	1.58231464	2.07090198	-0.46079341
C	0.22436256	2.21675281	-0.19388390
C	-0.10980301	-0.14222009	-0.60744099
C	1.25010335	-0.28586956	-0.87847412
H	3.16197449	0.70596891	-1.01310200
H	2.24020453	2.93391928	-0.39900189
H	-0.17535966	3.18959810	0.08043456
H	-0.77193714	-0.99998210	-0.68158660
H	1.64504219	-1.26151093	-1.14941566
C	-6.32816302	2.68730897	-1.60565686
C	-6.68379116	0.54520623	-2.66823543
H	-6.41530015	-0.49878061	-2.79455943
C	-7.77159498	1.07241990	-3.35864082
H	-5.76886065	3.31382009	-0.91548722
C	-7.41326973	3.21494163	-2.30273982
H	-8.34069284	0.43583420	-4.03121841
C	-8.13844059	2.41054966	-3.18445134
H	-7.69607525	4.25393844	-2.15477032
H	-8.98719735	2.81951601	-3.72588303

int6hph_123

E [Hartrees] = -925.3397242881

C	-2.89720314	2.24654597	0.21157905

C	-4.11900837	1.35138367	0.36378139
C	-3.10048289	0.13536862	0.24300639
C	-3.87414213	-0.21192489	-1.05027043
C	-4.74144746	0.81227402	-0.91816297
H	-5.55275508	1.18588333	-1.53679838
C	-3.65343548	-1.24880279	-2.05480178
C	-4.28413529	-1.17508377	-3.31129128
H	-4.92783549	-0.32796979	-3.53300316
C	-4.07734222	-2.16066176	-4.27137877
H	-4.56868049	-2.08362680	-5.23780950
C	-3.23424233	-3.24300874	-3.99877182
H	-3.07082024	-4.01055171	-4.75041517
C	-2.60395013	-3.32989301	-2.75658100
H	-1.95070028	-4.16952817	-2.53415278
C	-2.81102880	-2.34352222	-1.79288499
H	-2.33974291	-2.43265919	-0.81971707
C	-2.99327719	-0.87430637	1.34977181
C	-3.92925010	-1.91716643	1.45228085
H	-4.70175300	-2.01329260	0.69486996
C	-3.87292789	-2.82903888	2.50486319
H	-4.60666069	-3.62899893	2.56252094
C	-2.87621791	-2.72002606	3.47761075
H	-2.82814078	-3.43412216	4.29540587
C	-1.93924573	-1.69015071	3.38573916
H	-1.15601259	-1.59683920	4.13374898
C	-1.99694504	-0.77600585	2.33252985
H	-1.25889009	0.01686046	2.26958642
H	-4.74561755	1.45177220	1.25443713
C	-2.02099944	1.23005032	0.07962006
C	-0.59057161	1.13338575	-0.19182450
H	-2.80193567	3.32592730	0.13278034
C	2.16558500	0.93860308	-0.72596944
C	1.59210440	2.18052576	-0.43285404
C	0.22983933	2.27716106	-0.16708342
C	-0.00095554	-0.10848497	-0.48147182
C	1.36380821	-0.20374882	-0.74932659
H	3.22991741	0.86427670	-0.93212775
H	2.21103267	3.07371263	-0.40957734
H	-0.21067609	3.24271595	0.06729108
H	-0.62116477	-0.99777234	-0.50353717
H	1.80106793	-1.17250378	-0.97597016

int6phh_124
E [Hartrees] = -925.3382610946

Gcorr [kcal/mol] = 187.918

H	1.11072091	-3.42517855	-1.55501621
C	0.20536124	-3.34917007	-0.95955811
C	-1.05561657	-3.79674403	-1.13011824
C	-1.75980611	-4.58245804	-2.13579865
C	-1.07763898	-5.15571818	-3.22544430
H	-0.00379914	-5.01348273	-3.31523137
C	-1.76416882	-5.89714991	-4.18168570
H	-1.22327086	-6.33244535	-5.01794259
C	-3.14638198	-6.08293211	-4.06904383
H	-3.68096286	-6.66340900	-4.81613915
C	-3.83395256	-5.52205125	-2.99146840
H	-4.90701430	-5.66512950	-2.89569691
C	-3.14746676	-4.78003624	-2.03108863
H	-3.68227893	-4.35548975	-1.18674797
C	-1.59597209	-3.09624052	0.13874834
C	-1.97461816	-1.62658533	-0.04811137
H	-2.92707101	-1.16157043	-0.28857036
C	-0.71754062	-1.15747858	0.08829062
C	-0.06858682	0.14244389	-0.01252126
C	1.32935795	0.23810703	0.08877862
H	1.91231382	-0.66525972	0.24934157
C	1.96902640	1.47263093	-0.01541522
H	3.05156438	1.52842458	0.06329018
C	1.22111787	2.63384422	-0.21776661
H	1.71804950	3.59696570	-0.29670263
C	-0.17226479	2.55266327	-0.31659858
H	-0.75934234	3.45380737	-0.47343116
C	-0.81099196	1.32091721	-0.21529781
H	-1.89348707	1.26102403	-0.29243850
C	-0.10965430	-2.55241181	0.29702265
H	0.44830141	-2.74832706	1.21667105
C	-2.25373456	-3.91189171	1.21356077
C	-2.07134440	-5.30282140	1.27645932
H	-1.47762648	-5.79773727	0.51393087
C	-2.64924433	-6.05389680	2.29909673
H	-2.49649895	-7.12979639	2.32722992
C	-3.42577577	-5.43090040	3.27863531
H	-3.88045331	-6.01737832	4.07262718
C	-3.61796422	-4.04939422	3.22517909
H	-4.22262791	-3.55305230	3.98005738
C	-3.03838762	-3.29867119	2.20186466
H	-3.18886802	-2.22324556	2.16892652

int6phph_124
E [Hartrees] = -925.3314291460
Gcorr [kcal/mol] = 187.961

H	-2.47473784	-3.99416655	-1.32365825
C	-2.32601696	-3.17076694	-0.62994634
C	-2.72420563	-1.89458313	-0.61292463
H	-3.31839249	-1.28455089	-1.28804463
C	-1.95875738	-1.52051099	0.65889793
C	-0.46680821	-1.20151211	0.44036091
C	-0.07773994	-2.49092289	0.44010963
H	0.87669087	-2.98292680	0.27198501
C	-1.47297579	-3.07756506	0.64244553
C	-1.75347654	-3.97508186	1.80358571
C	-2.95142438	-4.70196389	1.87891356
H	-3.66101794	-4.64461226	1.05856554
C	-3.24314105	-5.48629757	2.99429420
H	-4.17682010	-6.04169809	3.03226241
C	-2.34179086	-5.55872891	4.05810928
H	-2.56771781	-6.17170487	4.92663345
C	-1.14764838	-4.83792242	3.99674896
H	-0.43950433	-4.88512408	4.82019427
C	-0.85747964	-4.05413196	2.88076323
H	0.06998416	-3.48988658	2.84227673
C	0.18883563	0.08342257	0.23164066
C	-0.56772751	1.26798688	0.21843034
H	-1.63978337	1.21505082	0.38281915
C	0.04789805	2.50176142	0.01069068
H	-0.55155064	3.40819160	0.00347181
C	1.42842615	2.57383097	-0.18247036
H	1.90848851	3.53559323	-0.34180599
C	2.19302030	1.40204310	-0.16643257
H	3.26853928	1.45232274	-0.31485677
C	1.58066043	0.17006212	0.03924118
H	2.17726578	-0.73840694	0.05147750
C	-2.68213401	-0.97262420	1.84602552
C	-4.08198657	-1.03173364	1.92264234
H	-4.64392177	-1.43717429	1.08620413
C	-4.75588388	-0.58738105	3.05991054
H	-5.84083435	-0.64235889	3.09810513
C	-4.04180002	-0.07485998	4.14431302
H	-4.56625229	0.27387430	5.02997760
C	-2.64832254	-0.01130924	4.08074411
H	-2.08185182	0.38667895	4.91875069
C	-1.97545776	-0.45519778	2.94355605

H	-0.89224739	-0.39821482	2.90189274

int7hh_124
E [Hartrees] = -925.3118653093
Gcorr [kcal/mol] = 187.911

C	-2.39068061	2.15663256	-1.03751128
C	-3.82089090	2.32369927	-1.33126291
C	-3.09902047	0.16549596	-0.15398866
C	-3.93064097	0.01637768	-1.24354637
C	-4.73521850	1.28388271	-1.35127430
C	-6.15722357	1.37123802	-1.68795836
C	-3.50756241	-0.69989235	-2.44443699
C	-3.97924469	-0.37876308	-3.73523215
H	-4.68029686	0.44009973	-3.85920957
C	-3.53474325	-1.08393816	-4.84802522
H	-3.90532708	-0.81971718	-5.83511127
C	-2.60903692	-2.12390066	-4.70459491
H	-2.26727774	-2.67437543	-5.57706468
C	-2.14097745	-2.46158190	-3.43256365
H	-1.43149978	-3.27592339	-3.31084853
C	-2.60056081	-1.77251462	-2.31374314
H	-2.27660568	-2.05925271	-1.31773833
H	-3.60473298	0.63033871	0.70234165
H	-4.13742078	3.32613156	-1.61707444
C	-1.88674783	0.98881864	-0.50674196
C	-0.49917130	0.68755350	-0.17524773
H	-1.74677860	3.01460518	-1.22454851
C	2.15648070	0.02282646	0.49970660
C	1.88736425	1.15846047	-0.27227398
C	0.57853062	1.48747919	-0.60766146
C	-0.21050606	-0.45809331	0.59011252
C	1.10065693	-0.78425048	0.92785990
H	3.18082394	-0.23202206	0.75753385
H	2.70466934	1.78542263	-0.61913803
H	0.38878602	2.35994446	-1.22586503
H	-1.03735506	-1.08315779	0.91674114
H	1.29900727	-1.67106346	1.52412465
C	-6.83232337	2.59632729	-1.86591689
C	-6.89834836	0.18194190	-1.82832387
H	-6.39442097	-0.76834327	-1.67802295
C	-8.25156185	0.21235574	-2.15675652
H	-6.29778211	3.53332730	-1.74136620
C	-8.18500122	2.62476114	-2.18862226
H	-8.79951296	-0.71996491	-2.26424557

C	-8.90255933	1.43356630	-2.34020240
H	-8.68513367	3.58079932	-2.31992291
H	-9.95941270	1.45996616	-2.59096162

int7hph_123
E [Hartrees] = -925.3125738785
Gcorr [kcal/mol] = 188.206

C	-2.47034081	1.69004731	1.19416202
C	-3.62077494	1.70837170	0.45432748
C	-2.32672636	-0.53837562	0.48745020
C	-3.09614639	-0.37557045	-0.80438834
C	-3.86864134	0.74729414	-0.64184920
H	-4.67244160	0.98050715	-1.33849733
C	-3.12210436	-1.31997549	-1.91741801
C	-3.71539049	-1.00981006	-3.15738764
H	-4.14407307	-0.02450435	-3.31555979
C	-3.72947566	-1.94037163	-4.19090180
H	-4.18731976	-1.68089730	-5.14191147
C	-3.14459153	-3.19956355	-4.01692151
H	-3.15274761	-3.92206667	-4.82846633
C	-2.54094345	-3.51615600	-2.79864884
H	-2.07942646	-4.48960461	-2.65514187
C	-2.52636108	-2.58581905	-1.76159349
H	-2.06243004	-2.83122297	-0.81066351
C	-2.97215691	-1.20225849	1.60445814
C	-4.13645127	-1.99236532	1.45147085
H	-4.59736143	-2.07388597	0.47220595
C	-4.70206514	-2.64223131	2.54051703
H	-5.59905810	-3.24078875	2.40329692
C	-4.12611518	-2.52940248	3.81273346
H	-4.56845028	-3.04645126	4.65999176
C	-2.96246102	-1.77335829	3.97903475
H	-2.49690689	-1.69950015	4.95852944
C	-2.37883638	-1.13861300	2.88744077
H	-1.44385574	-0.59758403	2.99951542
H	-4.34579207	2.50989747	0.58997346
C	-1.55781596	0.62822022	0.69218495
C	-0.47634645	0.97409579	-0.21547813
H	-2.19536104	2.51635260	1.84787419
C	1.64684826	1.54724364	-1.98608024
C	0.93652437	2.58748703	-1.37439200
C	-0.11397197	2.30895463	-0.50843047
C	0.27632393	-0.06241501	-0.81492009
C	1.30513232	0.22122844	-1.70698692

H	2.46632446	1.77036752	-2.66391382
H	1.19816201	3.62078631	-1.58808231
H	-0.68554505	3.12290768	-0.07305279
H	0.04207720	-1.09055258	-0.55441527
H	1.85821459	-0.59272435	-2.16850944

int7phhz_124
E [Hartrees] = -925.3118717105
Gcorr [kcal/mol] = 188.498

H	0.62829317	-4.00026403	-2.27979133
C	-0.10507156	-3.36324125	-1.78675321
C	-1.44439707	-3.71430108	-1.81031730
C	-2.03659874	-4.87056166	-2.48493309
C	-1.31915107	-5.68685865	-3.38337061
H	-0.28215107	-5.45998712	-3.61230442
C	-1.92635239	-6.77796162	-3.99611323
H	-1.35431556	-7.39254044	-4.68637128
C	-3.26581751	-7.08358638	-3.73288387
H	-3.73718983	-7.93562217	-4.21493855
C	-3.99359880	-6.27836889	-2.85492994
H	-5.03720102	-6.50037994	-2.64836947
C	-3.38891741	-5.18206066	-2.24464226
H	-3.95805776	-4.55159711	-1.56779987
C	-2.12166654	-2.84850714	-0.78204719
C	-1.76086751	-1.54711403	-1.05958952
H	-1.77436262	-1.32533143	-2.13468525
C	-0.38834897	-1.23916031	-0.51773229
C	0.00764856	-0.05669859	0.23803176
C	1.30347181	0.10927801	0.76863082
H	2.04647608	-0.67085853	0.63209110
C	1.63566963	1.25141062	1.48903230
H	2.63867223	1.35842936	1.89386972
C	0.68517201	2.25600750	1.70158409
H	0.94817282	3.14590039	2.26692898
C	-0.60496167	2.10200940	1.19028896
H	-1.35220413	2.87415606	1.35369120
C	-0.94053359	0.95706393	0.47183161
H	-1.94374029	0.82778083	0.07445306
C	0.43134177	-2.21347739	-1.04527126
H	1.51482577	-2.14386364	-0.96234376
C	-2.30158903	-3.32297789	0.58779354
C	-2.04985502	-4.65595277	0.97729694
H	-1.69662047	-5.37005896	0.24056615
C	-2.22495202	-5.05344295	2.29808597

H	-2.02175115	-6.08311515	2.58092170
C	-2.65214770	-4.13488507	3.26389019
H	-2.79072850	-4.45126947	4.29428232
C	-2.91614648	-2.81443570	2.89241393
H	-3.25994840	-2.09765258	3.63357492
C	-2.76372581	-2.41831448	1.56670469
H	-3.01128176	-1.40594686	1.26168755

int7phph_124
E [Hartrees] = -925.3027041130
Gcorr [kcal/mol] = 187.723

H	-2.84570443	-3.65571422	-0.48634252
C	-2.51497716	-2.78609312	0.08073687
C	-2.72013139	-1.51031735	-0.33981159
H	-2.96846144	-1.19598941	-1.34970670
C	-2.24243493	-0.66896454	0.77736626
C	-0.77226956	-0.73670011	0.88274445
C	-0.54219383	-2.00107031	1.40442603
H	0.43358280	-2.32330222	1.76864693
C	-1.59727188	-2.97139854	1.22570437
C	-1.61298401	-4.20620627	2.00127264
C	-2.50032044	-5.26842452	1.70324730
H	-3.22701542	-5.15740666	0.90624951
C	-2.47401822	-6.45827534	2.42244354
H	-3.16501839	-7.25601289	2.16231011
C	-1.57843209	-6.62692778	3.48206988
H	-1.56604338	-7.55362201	4.04916792
C	-0.71977311	-5.57797119	3.82221528
H	-0.03866784	-5.68312390	4.66278772
C	-0.74442435	-4.38703979	3.10526171
H	-0.10148489	-3.57127986	3.41758373
C	0.16103336	0.19696093	0.28438108
C	-0.26822174	1.50379151	-0.03111493
H	-1.29307457	1.78746528	0.19583641
C	0.60642822	2.42766655	-0.59813543
H	0.25281134	3.42702969	-0.83861542
C	1.93777611	2.07995988	-0.83685183
H	2.62436020	2.80366004	-1.26749212
C	2.38219823	0.79074984	-0.51833761
H	3.41441321	0.51016922	-0.71221918
C	1.50583731	-0.14372220	0.02061569
H	1.84636317	-1.15567653	0.21990007
C	-3.05745014	-0.40086298	1.93110808
C	-4.45926357	-0.62426375	1.91920973

H	-4.91002376	-1.06298665	1.03496851
C	-5.23673862	-0.30481875	3.02149379
H	-6.30698969	-0.49276103	2.99938754
C	-4.65208325	0.26951628	4.15926179
H	-5.26855571	0.53328454	5.01422075
C	-3.27762914	0.53311782	4.17555780
H	-2.82493953	0.99919787	5.04675230
C	-2.49090985	0.22019711	3.07531235
H	-1.42967883	0.44626468	3.07506714

phactlen
E [Hartrees] = -308.4006856781
Gcorr [kcal/mol] = 50.107

C	-0.36387672	-0.63026128	0.00004771
C	1.04379219	-0.61916396	-0.00003589
C	1.73620969	0.58931009	-0.00010789
C	1.03953034	1.80042608	-0.00009885
C	-0.35765354	1.79830502	0.00000736
C	-1.05804267	0.59442441	0.00008181
C	-1.07862388	-1.86808492	0.00005780
C	-1.68354652	-2.91593281	0.00012006
H	1.58072546	-1.56273248	-0.00003997
H	2.82282193	0.58612788	-0.00017235
H	1.58284576	2.74141601	-0.00017091
H	-0.90368940	2.73777173	0.00002628
H	-2.14367975	0.58769559	0.00016644
H	-2.21681288	-3.83930139	0.00011840

ts1b_14zez
E [Hartrees] = -616.7718927211

C	-0.79390643	1.22383252	0.07441606
C	0.46214715	1.12887538	0.05402912
C	-2.74053142	2.99441350	-0.13222875
C	-1.48953129	2.90458727	-0.01413803
C	1.80500257	1.53851359	-0.00122538
C	-4.07743523	2.57922039	-0.25200052
H	-1.62887635	0.54508128	0.13173481
H	-0.65900922	3.58795938	0.05216692
C	2.47449975	1.66678535	-1.24536763
C	2.52711791	1.82228539	1.18640042
C	-4.88188022	2.38105951	0.89954481
C	-4.65856779	2.35971654	-1.52741516
H	-4.44666836	2.55170808	1.87945383
C	-6.20340877	1.97099323	0.77326902

H	2.02399728	1.72164782	2.14321539
C	3.85501617	2.22632855	1.12357874
H	1.93028867	1.44797058	-2.15897302
C	3.80309407	2.07014681	-1.29166246
H	-4.05105637	2.51264687	-2.41412167
C	-5.98192737	1.95158497	-1.63734827
C	-6.76158101	1.75467590	-0.49171277
H	-6.41141415	1.78330381	-2.62141983
H	-6.80513881	1.81795716	1.66526350
C	4.50088763	2.35213229	-0.11154568
H	4.30078589	2.16800090	-2.25285917
H	5.54002267	2.66597658	-0.15409140
H	4.39307921	2.44546465	2.04206762
H	-7.79616045	1.43656040	-0.58421656

ts1b_14zzz0deg
E [Hartrees] = -616.7694317831
Gcorr [kcal/mol] = 114.371

C	-0.66120174	1.32752403	0.31073916
C	0.54775419	0.99960293	0.21382217
C	-0.58777597	3.97084005	-0.38375628
C	-1.27338719	2.92143351	-0.46796336
C	1.91809477	1.16350964	-0.06969878
C	0.54626575	4.76303067	-0.11654921
H	-1.55466233	0.91840520	0.75536211
H	-2.21803641	2.63079401	-0.89981833
C	2.49578108	0.64227540	-1.25217178
C	2.74258115	1.88864783	0.82660985
C	1.63223694	4.77185825	-1.02730726
C	0.64446283	5.53820251	1.06381221
H	1.56684888	4.16852585	-1.92703000
C	2.78118308	5.49649060	-0.74356935
H	2.30103618	2.30163956	1.72785993
C	4.07878942	2.11309776	0.52688316
H	1.87279267	0.07719028	-1.93873444
C	3.83568124	0.87667515	-1.54065964
H	-0.18750010	5.54441142	1.76137973
C	1.80264890	6.25785318	1.33616676
C	2.87669944	6.23909073	0.43983328
H	1.87198059	6.83604243	2.25387598
H	3.61508801	5.47287794	-1.43981543
C	4.63272129	1.61426539	-0.65854558
H	4.26323115	0.48495006	-2.45992675
H	5.67828831	1.79653165	-0.89089950

H	4.69147000	2.69265069	1.21204680
H	3.78019707	6.80103941	0.65960975

ts1b_14zzz90deg
E [Hartrees] = -616.7719504035
Gcorr [kcal/mol] = 111.373

C	-0.69304290	1.33515867	-0.44961784
C	0.40460595	0.80503130	-0.13229799
C	-0.91377267	3.86657896	0.12901442
C	-1.24428190	2.71531477	0.51878975
C	1.66493314	0.62699253	0.45932955
C	-0.23930514	4.88558401	-0.56156712
H	-1.44289540	1.16426609	-1.20832553
H	-1.81283138	2.31263558	1.34441377
C	1.88858213	-0.37778528	1.43388186
C	2.75542342	1.45154823	0.07578187
C	1.13509465	5.13236769	-0.30415120
C	-0.90425368	5.69824951	-1.51375003
H	1.65208784	4.50773215	0.41816865
C	1.80580171	6.14567103	-0.97709583
H	2.58853255	2.22846722	-0.66434344
C	4.00772952	1.27351380	0.64977647
H	1.06334032	-1.01972649	1.72680310
C	3.14429712	-0.53472503	2.00780158
H	-1.95770862	5.52370510	-1.71036326
C	-0.21585605	6.69965343	-2.18772311
C	1.13849328	6.93278884	-1.92314638
H	-0.73769411	7.30877895	-2.92108772
H	2.85845943	6.32103510	-0.77074760
C	4.21065334	0.28408976	1.61915456
H	3.29769370	-1.30424189	2.75983952
H	5.19123519	0.15246635	2.06779561
H	4.83222025	1.91395910	0.34724235
H	1.66944154	7.72092142	-2.44948915

ts1c
E [Hartrees] = -616.7412492196

C	-0.99716164	0.65281424	0.24737569
C	-1.21358146	-0.17436080	1.39466922
C	0.17227389	0.81176655	-0.40856138
C	1.11673616	-0.44163404	-0.62566817
C	0.88734153	-1.54969179	-1.54114332
C	1.87702486	0.10545056	0.22568767
H	0.38787155	1.60778038	-1.11520620

H	2.58495007	0.48206027	0.93107226
C	-0.42326358	-0.05362686	2.56451907
C	-2.27494780	-1.11189667	1.40406607
C	-0.33993363	-1.67919240	-2.20574840
C	1.89639242	-2.50585890	-1.74800223
H	-1.11372863	-0.93723634	-2.03217215
C	-0.55636107	-2.75551402	-3.06500518
H	2.84409629	-2.39865074	-1.22804096
C	1.67486048	-3.57615164	-2.60885387
H	0.37164355	0.68589344	2.58379780
C	-0.68410860	-0.83798825	3.68440864
H	-2.90695808	-1.19040445	0.52415771
C	-2.48743329	-1.93452234	2.50373396
C	0.44828409	-3.70337434	-3.26965797
H	-1.51052849	-2.85351911	-3.57512989
H	2.45750288	-4.31331001	-2.76573144
H	-3.28707405	-2.67058028	2.47874105
C	-1.70257088	-1.79486310	3.65493881
H	-0.08004468	-0.71571365	4.58037863
H	0.27794866	-4.54047903	-3.94116024
H	-1.89521586	-2.41531363	4.52596216

ts2b_14zzz_eze

E [Hartrees] = -616.7810636545

C	-0.86033952	1.37536743	-0.04962456
C	0.39399492	0.99055346	-0.01985765
C	-0.69929975	3.87979569	-0.15594932
C	-1.38474742	2.76129814	-0.11393229
C	1.56477644	0.26387294	0.02507773
C	-0.31403628	5.20292579	-0.21020230
H	-1.64069167	0.60452750	-0.02475198
H	-2.48013051	2.82302967	-0.12579646
C	2.18555584	-0.06211382	1.27359852
C	2.21271554	-0.17108724	-1.17549328
C	-0.10351991	5.96204743	0.98535385
C	-0.08895680	5.85693680	-1.46377292
H	-0.26291316	5.47906903	1.94447349
C	0.28572013	7.28976364	0.91755820
H	1.75882280	0.07346285	-2.13087824
C	3.39006280	-0.89854122	-1.11681322
H	1.71088148	0.26604386	2.19315500
C	3.36327589	-0.79061943	1.30585430
H	-0.23736503	5.29349743	-2.37979527
C	0.29993380	7.18585983	-1.50534037

C	0.48941671	7.91512402	-0.32177785
H	0.45652195	7.66713808	-2.46736414
H	0.43137115	7.85169822	1.83662170
C	3.97587850	-1.21692730	0.11773490
H	3.81404309	-1.03566040	2.26419055
H	4.89821621	-1.78935929	0.15339223
H	3.86161369	-1.22752994	-2.03934043
H	0.79263990	8.95719258	-0.36455118

ts2b_trmr
E [Hartrees] = -925.1767150398
E [Hartrees] = -925.1767150398
Gcorr [kcal/mol] = 177.852

H	-4.31671589	1.25912887	-0.09109834
C	-4.08790966	0.20068056	-0.03087824
C	-2.90623665	-0.33404618	-0.12911008
C	-2.26397065	-1.59935896	-0.17356636
C	-2.36863033	-2.41469812	-1.32584091
H	-2.98019097	-2.07337627	-2.15572208
C	-1.69448463	-3.62989277	-1.39365983
H	-1.78865314	-4.24865517	-2.28231109
C	-0.89356844	-4.05291210	-0.32796351
H	-0.35777077	-4.99603469	-0.39026721
C	-0.77884338	-3.25608099	0.81599738
H	-0.14648343	-3.57516073	1.63963052
C	-1.45070716	-2.04263536	0.89565879
H	-1.34526023	-1.40964481	1.77061345
C	-5.34861558	-0.71088679	0.20265479
H	-5.11137018	-1.77076452	0.24959647
C	-6.51690853	-0.17388884	0.30555975
C	-7.42986761	0.87524007	0.33970380
C	-7.77438166	1.51054988	1.56933190
H	-7.29637080	1.17181483	2.48336008
C	-8.69816724	2.54454608	1.59427881
H	-8.94328389	3.02129995	2.53988566
C	-9.31470964	2.97949433	0.41327458
H	-10.03935579	3.78810912	0.44165709
C	-8.99366711	2.36381435	-0.80407693
H	-9.46853314	2.69987955	-1.72226968
C	-8.07316468	1.32761933	-0.85018320
H	-7.82487453	0.84806631	-1.79209416
C	-1.22472653	1.30775041	-0.35972162
C	-0.11791296	0.78825073	-0.25293357
C	0.97631437	-0.10025923	-0.11156990

H	-1.92571195	2.09713141	-0.52706667
C	2.34366983	-1.90056206	-1.00426699
C	1.31475980	-0.97973507	-1.16370501
C	1.71548187	-0.15828183	1.09046612
C	2.74514186	-1.08188324	1.23700017
C	3.06258539	-1.95820399	0.19421832
H	2.58281141	-2.58316658	-1.81522618
H	0.73696700	-0.94833295	-2.08158392
H	1.46003140	0.51803018	1.90059210
H	3.30284264	-1.12140859	2.16899554
H	3.86519739	-2.68060595	0.31457313

ts2c_12

E [Hartrees] = -616.7370216970

C	-0.68955460	0.44568485	0.10926356
C	-1.00040168	-0.30856073	1.32944742
C	0.57614812	1.01967506	-0.10238597
C	0.90741730	-0.56201255	-0.46682374
C	0.72508178	-1.60031403	-1.45859097
C	1.77374767	0.18509818	0.19319300
H	0.71065288	1.84666359	-0.81335143
H	2.84778932	0.30550956	0.28146386
C	-0.59284558	0.15399761	2.59891066
C	-1.81940011	-1.45496659	1.27852706
C	-0.45665536	-1.67769936	-2.21554695
C	1.73948531	-2.55714805	-1.64838872
H	-1.23112896	-0.93815911	-2.03721225
C	-0.60633808	-2.68572342	-3.16532237
H	2.64858692	-2.50055949	-1.05613536
C	1.57077865	-3.57300164	-2.58434391
H	0.03552207	1.03861699	2.66283199
C	-0.99803361	-0.49728896	3.76344249
H	-2.15799188	-1.81186186	0.30979522
C	-2.18526283	-2.12765887	2.44033290
C	0.40089546	-3.63633568	-3.34841684
H	-1.51716873	-2.73645269	-3.75517887
H	2.35379744	-4.31314225	-2.72367076
H	-2.80269970	-3.02030063	2.37270592
C	-1.78495350	-1.64864085	3.69248253
H	-0.68624352	-0.11039573	4.73106029
H	0.27474619	-4.42833797	-4.08146319
H	-2.09141882	-2.16144332	4.60029011

ts2c_13

E [Hartrees] = -616.7362910048

C	-0.74303813	0.30768910	-0.03961039
C	-0.96589330	-0.32016744	1.27030090
C	0.50965443	0.87147208	-0.36136636
C	0.83951251	-0.69537802	-0.60349240
H	0.68402020	-1.47307717	-1.33749119
C	1.74292492	0.07760166	-0.03153528
H	0.61686186	1.62871319	-1.14844382
C	3.14502200	0.27072046	0.24072506
C	-0.47758244	0.26116257	2.46024865
C	-1.78282170	-1.46336468	1.38516136
H	0.15198492	1.14528627	2.39756801
C	-0.80437730	-0.27246599	3.70640438
H	-2.18625752	-1.90315296	0.47686505
C	-2.07149145	-2.01939287	2.62765859
H	-2.69080050	-2.91132615	2.68773904
C	-1.59130470	-1.42252779	3.79865710
H	-0.43137386	0.20486700	4.60988900
H	-1.83687590	-1.84337033	4.77007765
C	3.60290080	1.53355193	0.65550203
C	4.05963289	-0.79325260	0.12392276
H	3.70223030	-1.77098378	-0.18689516
C	5.40537135	-0.59053326	0.40958022
H	2.88930246	2.34531620	0.76512628
C	4.95392305	1.73399952	0.92736651
H	6.10733991	-1.41491021	0.32127785
C	5.85580589	0.67357224	0.80693425
H	5.30303558	2.71319361	1.24233507
H	6.90822177	0.82875908	1.02765405

ts3b_14eze

E [Hartrees] = -616.7741316635

Gcorr [kcal/mol] = 115.629

C	-1.12097021	1.35270889	-0.03253522
C	0.20433164	1.29709945	-0.01086602
C	-0.61847339	3.61170302	-0.14932787
C	-1.61156122	2.73286606	-0.11204645
C	1.41094163	0.57699207	0.04677068
C	-0.13712420	4.93112941	-0.22147144
H	-1.77406694	0.47513220	0.00203772
H	-2.67217055	3.00189438	-0.13649989
C	2.02473232	0.27986086	1.29346349
C	2.08427951	0.18604228	-1.14190836
C	0.14732586	5.67007917	0.95843817

C	0.14242002	5.53746045	-1.47584474
H	-0.05176089	5.21209884	1.92265475
C	0.66421478	6.95668249	0.87936966
H	1.62987570	0.41830293	-2.10038484
C	3.29790643	-0.48606446	-1.07858544
H	1.52438426	0.58404691	2.20792192
C	3.23865922	-0.39319004	1.34117602
H	-0.06041573	4.97737394	-2.38372575
C	0.65931679	6.82491389	-1.53931693
C	0.92354450	7.54209545	-0.36599912
H	0.85864894	7.27688031	-2.50752383
H	0.86717861	7.51120199	1.79191985
C	3.88265571	-0.77983917	0.15944447
H	3.68943056	-0.62070923	2.30371769
H	4.83358935	-1.30344069	0.20286579
H	3.79486782	-0.78571222	-1.99763235
H	1.33064852	8.54781476	-0.42166265

ts4bhh_12
E [Hartrees] = -925.2209978616
Gcorr [kcal/mol] = 178.040

C	1.14923773	-0.16724340	-0.10541190
C	-0.64769181	0.63993336	-0.45350039
C	-1.49307601	-0.41168696	0.38197304
C	-1.99638343	-0.89721346	-0.80743025
C	-1.25007191	0.12675725	-1.59227901
C	1.99593246	0.55237124	0.45821164
C	2.69557126	1.60072729	1.08037037
H	0.93996918	-1.19205175	-0.36137007
H	-0.41810989	1.67422369	-0.22160750
C	-1.49548616	-0.67686085	1.79055669
C	-2.91596538	-1.93859375	-1.24317109
H	-1.25275520	0.41441239	-2.63677552
C	2.56616474	1.80348669	2.47847177
C	3.53678895	2.47091598	0.34346347
C	-0.91409184	0.27465175	2.66323977
C	-2.02427512	-1.85978528	2.36213539
C	-3.98478654	-2.38369470	-0.44099734
C	-2.77375307	-2.48729958	-2.53240270
H	-0.48240667	1.17867795	2.24600238
C	-0.89023558	0.06669032	4.03848758
H	-2.43390981	-2.62784045	1.71547072
C	-1.98734351	-2.06339822	3.73576068
H	-1.96220786	-2.14099980	-3.16701073

C	-3.64406796	-3.47488361	-2.98783742
H	-4.14230997	-1.93116144	0.53263805
C	-4.85707806	-3.36614790	-0.90145012
H	1.93529378	1.12811659	3.04840533
C	3.23752417	2.84914182	3.10108223
H	3.64177382	2.32013886	-0.72660324
C	4.21198685	3.50314015	0.98315032
H	-3.51039110	-3.89512719	-3.98121479
H	-2.39190176	-2.98333440	4.15030953
H	3.12416205	2.99782217	4.17175391
C	-1.42833637	-1.10119551	4.58604961
H	-0.44739735	0.81884568	4.68684105
C	4.06459586	3.70141686	2.36110652
H	4.85422883	4.16325463	0.40611556
C	-4.68751036	-3.92173229	-2.17331898
H	-5.67942566	-3.69303444	-0.27041270
H	-5.36952438	-4.68875011	-2.52990217
H	4.59395011	4.51167486	2.85456910
H	-1.40780270	-1.26477736	5.65983397

ts4bhph_12
E [Hartrees] = -925.2207396580
Gcorr [kcal/mol] = 179.324

C	1.18279870	-0.25580438	-0.47381472
C	-0.50268294	0.80736365	-0.45053809
C	-1.19724893	-0.03402508	0.73891364
C	-2.00883879	-0.60444534	-0.20318827
C	-1.43798712	0.18713482	-1.29230852
C	2.28325480	0.26637666	-0.73731008
C	3.35696287	1.09436881	-1.10729465
H	0.74932295	-1.17369159	-0.09980147
C	-0.10164505	2.22466383	-0.48850374
C	-0.97316267	-0.12833923	2.15196512
H	-2.76672341	-1.38064166	-0.16180717
H	-1.69546709	0.33773767	-2.33381848
C	-0.33586520	3.07969056	0.59957178
C	0.53019401	2.74196480	-1.63181883
C	3.96776400	1.94879790	-0.15645983
C	3.84493915	1.10343893	-2.43760412
C	0.16004080	0.47411738	2.74539395
C	-1.87468197	-0.83028548	2.98711793
H	-2.75837554	-1.28573879	2.54782841
C	-1.64515074	-0.92936940	4.35272212
H	0.86808162	0.99918679	2.11297410

C	0.37887204	0.37382112	4.11617397
H	0.73544535	2.07986684	-2.46781212
C	0.92136121	4.07682013	-1.68422302
H	-0.82969407	2.69722189	1.48665553
C	0.05316559	4.41920768	0.54145673
H	3.38362759	0.44931098	-3.17137374
C	4.89394141	1.94091269	-2.79617181
H	3.59597688	1.95062296	0.86337554
C	5.00701327	2.78994621	-0.53279878
H	5.45609620	3.44992828	0.20468606
C	5.47850607	2.79094446	-1.85050863
H	5.25718824	1.93719106	-3.82058134
C	-0.51848868	-0.32607914	4.92718129
H	1.25723758	0.84048659	4.55438127
H	-2.34890765	-1.47150035	4.97900500
C	0.68647585	4.92214156	-0.59585537
H	1.42417511	4.45500255	-2.57035755
H	-0.13808924	5.06912933	1.39164715
H	-0.34526625	-0.40144182	5.99705339
H	0.99773112	5.96259189	-0.63440189
H	6.29510663	3.44740068	-2.13758723

ts4bphh_12
E [Hartrees] = -925.2082875426
Gcorr [kcal/mol] = 179.610

C	1.20178144	-0.37959244	-0.20265153
C	-0.27249262	0.76365502	-0.43187604
C	-1.36138692	0.07516052	0.43673714
C	-1.99082933	-0.39927487	-0.66305070
C	-1.04978120	0.39483654	-1.55972247
C	2.11678480	0.05006582	0.56600383
H	2.48948126	0.92084924	1.07802118
C	0.92732897	-1.67073688	-0.86234032
H	0.15210808	1.75126937	-0.27362865
H	-1.43596814	-0.11922648	1.50086502
C	-3.03313761	-1.39183793	-0.89396554
C	-1.02070904	0.78182762	-2.93056168
C	0.09704521	1.48765108	-3.44666321
C	-2.09471002	0.49821363	-3.80874702
C	-4.10960357	-1.52494396	0.00075976
C	-2.94189259	-2.27582443	-1.98475427
C	1.03445103	-1.79207033	-2.25545155
C	0.49899289	-2.77531632	-0.11287613
H	0.41234392	-2.67868490	0.96464335

C	0.17273595	-3.97456427	-0.74625049
H	1.36217317	-0.94146433	-2.84262562
C	0.72472883	-2.99845313	-2.88540662
H	-2.09299925	-2.20253959	-2.65694944
C	-3.90492532	-3.26607458	-2.17082995
H	-4.18962270	-0.83639247	0.83789171
C	-5.06968184	-2.51530002	-0.19025774
H	-2.96492872	-0.02774153	-3.43167569
C	-2.04807356	0.90595131	-5.13795455
H	0.93689172	1.69531301	-2.78853680
C	0.13642079	1.88153034	-4.77577510
C	-0.93586479	1.59366410	-5.63218272
H	1.00570573	2.41286934	-5.15442918
H	-2.88499065	0.68453759	-5.79516869
C	-4.97241912	-3.38823726	-1.27832111
H	-5.89919487	-2.60412709	0.50641114
H	-3.81620469	-3.94934975	-3.01140472
C	0.28461895	-4.08975974	-2.13366996
H	0.82448933	-3.08137026	-3.96447537
H	-0.17741471	-4.81683920	-0.15576217
H	0.02878285	-5.02442157	-2.62565585
H	-5.72423267	-4.15849746	-1.42792134
H	-0.90088005	1.90191631	-6.67327124

ts4bphph_12
E [Hartrees] = -925.1992417387
Gcorr [kcal/mol] = 178.608

C	1.22540905	-0.49193544	-0.14921393
C	-0.12053180	0.83145996	-0.45535794
C	-1.25000547	0.17573721	0.42314430
C	-1.93036915	-0.19700142	-0.67381350
C	-0.95859562	0.51299128	-1.57154695
C	2.08703995	-0.19775295	0.73473398
H	2.53402229	0.58763045	1.31728197
C	0.90739366	-1.73800374	-0.86729771
C	0.43645978	2.18873525	-0.18812289
H	-1.33304085	0.01050721	1.49114851
H	-2.80771364	-0.80879503	-0.85283944
C	-1.00453337	0.84131981	-2.96199467
C	0.00284700	1.60972223	-3.59642223
C	-2.08525848	0.37973266	-3.75127397
C	0.90119955	-1.77915618	-2.26838482
C	0.60714727	-2.90627001	-0.14970835
H	0.61860330	-2.87075198	0.93521419

C	0.29519564	-4.08668565	-0.82151638
H	1.14845231	-0.88720241	-2.83212667
C	0.59616572	-2.96486636	-2.93903611
H	-2.86392037	-0.21724533	-3.28591695
C	-2.15791891	0.67749542	-5.10743444
H	0.83759968	1.97751600	-3.01121313
C	-0.07541194	1.89807890	-4.95167726
C	-1.15399618	1.43544261	-5.71720478
H	0.70730484	2.48915491	-5.41986350
H	-2.99705948	0.31347591	-5.69435727
C	0.28648470	-4.11927144	-2.21903974
H	0.60390280	-2.98289797	-4.02558979
H	0.05393627	-4.98157306	-0.25360147
H	0.04239312	-5.04036301	-2.74181730
H	-1.20837700	1.66317445	-6.77804750
C	-0.34632398	3.11108074	0.52280220
C	1.70597914	2.58992588	-0.62974508
H	2.33407386	1.87794045	-1.15533795
C	2.16891642	3.88506976	-0.38871985
H	-1.33155192	2.81236025	0.87254909
C	0.11913545	4.40114350	0.77365822
H	3.15292216	4.17865483	-0.74526610
C	1.37928503	4.79444951	0.31584988
H	-0.50446227	5.10128862	1.32362010
H	1.74269464	5.80006080	0.50985275

ts4concphhh

E [Hartrees] = -925.2312247184

C	-2.70353349	3.11469226	-0.44772996
C	-4.14141042	1.69576563	0.25596058
C	-3.15241006	0.50925511	0.32891219
C	-3.66648704	-0.00740320	-0.81429029
C	-4.72029622	1.10180056	-0.85534126
C	-5.86800919	1.41485502	-1.66304202
C	-3.19041094	-1.02814425	-1.73619324
C	-3.41361521	-0.91591755	-3.12138414
H	-3.99605230	-0.08275191	-3.50138802
C	-2.86288291	-1.84288578	-4.00624853
H	-3.03967802	-1.73654815	-5.07342898
C	-2.08299968	-2.89737606	-3.52749894
H	-1.65667781	-3.62020609	-4.21780758
C	-1.85474451	-3.01856200	-2.15253186
H	-1.24864333	-3.83645753	-1.77182397
C	-2.40291682	-2.09657827	-1.26677486

H	-2.22711739	-2.19304721	-0.19888323
H	-2.30746304	0.27977961	0.96444027
H	-4.57927399	2.31281604	1.03450549
C	-1.62101950	2.53460273	-0.61109281
C	-0.44403962	1.77271211	-0.81084241
H	-3.27287664	4.02095838	-0.53370581
C	1.87180053	0.22249614	-1.20683149
C	1.74793854	1.02220339	-0.06682803
C	0.60733702	1.79441869	0.13306546
C	-0.30402304	0.96558789	-1.96428037
C	0.84035979	0.20063558	-2.15227514
H	2.76330321	-0.38019232	-1.35659390
H	2.54645902	1.04552100	0.67023385
H	0.51050866	2.41649173	1.01794614
H	-1.11541963	0.92550128	-2.68289241
H	0.92092157	-0.42810912	-3.03478768
C	-6.43410062	2.71000946	-1.62157248
C	-6.48005461	0.44748719	-2.49058716
H	-6.07663474	-0.55957148	-2.51851881
C	-7.60704006	0.76673227	-3.24359942
H	-5.97002433	3.46885002	-0.99677086
C	-7.55698166	3.02196996	-2.37797717
H	-8.06642526	0.00545464	-3.86890406
C	-8.15031383	2.05313712	-3.19628638
H	-7.97188781	4.02588022	-2.33670536
H	-9.02666985	2.30018679	-3.78900771

ts4concphhph
E [Hartrees] = -925.2242001120
Gcorr [kcal/mol] = 187.623

C	-3.09086522	2.66294262	0.01483047
C	-4.07973747	1.77550804	0.48477845
C	-2.98329130	0.65125098	0.41758436
C	-4.50295298	0.01407626	-1.61804153
C	-5.09183435	1.03789315	-1.24609023
H	-5.92227769	1.71155160	-1.33988574
C	-3.84878688	-1.15895128	-2.06683400
C	-2.83108314	-1.08829996	-3.04502635
H	-2.54906693	-0.11728029	-3.44044594
C	-2.19819364	-2.24489479	-3.48702687
H	-1.41836782	-2.17385453	-4.24089594
C	-2.55535645	-3.49328750	-2.96664823
H	-2.05543782	-4.39342935	-3.31312935
C	-3.56107872	-3.57499052	-1.99884368

H	-3.84651527	-4.54164298	-1.59195515
C	-4.20713122	-2.42603509	-1.55338180
H	-4.99272127	-2.48890385	-0.80614207
H	-2.96485045	-0.39365628	0.69618592
C	-5.21018795	1.88001897	1.41081829
C	-2.10438327	1.54338382	-0.08140984
H	-1.08916691	1.47077279	-0.45588039
C	-2.95085709	4.06753762	-0.27991793
C	-3.86069562	5.04941055	0.17270871
C	-1.83407200	4.50051225	-1.03127746
C	-6.26637741	2.79444374	1.22971135
C	-5.27819593	0.99959426	2.50626925
H	-4.69906847	4.75508259	0.79143847
C	-3.66823782	6.39279486	-0.12951435
H	-1.11667480	3.76582487	-1.38538792
C	-1.64912788	5.84549762	-1.33497906
H	-6.26686452	3.44563570	0.36079887
C	-7.32339356	2.85442879	2.13425139
H	-4.48747027	0.26867126	2.64938637
C	-6.33346989	1.06620466	3.41436392
C	-7.36020527	1.99578363	3.23652858
H	-8.12722417	3.56809938	1.97279137
H	-6.35644213	0.38475325	4.26091024
C	-2.56707495	6.80054849	-0.88990685
H	-4.37833106	7.13024954	0.23591085
H	-0.78634599	6.15104153	-1.92122081
H	-8.18633687	2.04278047	3.94049607
H	-2.42356404	7.85109978	-1.12695291

ts4concphphh

E [Hartrees] = -925.2361822023

C	-3.06335245	2.37532355	0.13532074
C	-4.08981127	1.59696199	0.61937705
C	-3.08150213	0.38567482	0.62769936
C	-4.64597094	-0.14932207	-1.50233429
C	-5.26182068	0.80029464	-0.99778796
H	-6.14859647	1.40477975	-0.98611131
C	-3.84541811	-1.15758228	-2.08811735
C	-3.05594866	-0.85388958	-3.22259087
H	-3.08191943	0.15303062	-3.62677386
C	-2.24017363	-1.82352613	-3.79376164
H	-1.63484002	-1.57026668	-4.66000271
C	-2.18269721	-3.11145974	-3.24999168
H	-1.53825140	-3.86455027	-3.69504596

C	-2.96150266	-3.42337654	-2.13150036
H	-2.92083174	-4.41995763	-1.70003863
C	-3.79443122	-2.46765174	-1.55733823
H	-4.39174895	-2.71227850	-0.68613426
C	-3.17859865	-0.90611541	1.24151795
C	-4.42508016	-1.32834200	1.76012437
H	-5.28155429	-0.66772741	1.67066459
C	-4.57133298	-2.58281231	2.34232372
H	-5.54142930	-2.88753524	2.72648813
C	-3.47827003	-3.45101164	2.43233204
H	-3.59358914	-4.43225810	2.88426873
C	-2.23427974	-3.04199281	1.94076585
H	-1.37579753	-3.70430618	2.01666959
C	-2.08112665	-1.79002352	1.35573793
H	-1.10698865	-1.47977391	0.99633450
H	-4.93072027	1.83433491	1.26314082
C	-2.14859448	1.20832492	0.02144395
C	-0.84401959	1.05691871	-0.60099081
H	-2.97212821	3.42020380	-0.13957880
C	1.66509652	0.83340996	-1.86254678
C	1.25981362	2.05451711	-1.31677036
C	0.01575590	2.16824301	-0.70088875
C	-0.43008170	-0.16387540	-1.17069549
C	0.81085635	-0.27081051	-1.79224135
H	2.63353519	0.74642491	-2.34774743
H	1.91393636	2.92069530	-1.37414136
H	-0.29600600	3.11997665	-0.27844798
H	-1.10326016	-1.01328111	-1.16284071
H	1.10330786	-1.21795632	-2.23790103

ts4concphphph
E [Hartrees] = -925.2308438252
Gcorr [kcal/mol] = 182.687

C	-3.25680655	2.33658279	0.08704407
C	-4.28552868	1.57156045	0.63674501
C	-3.21600174	0.37984727	0.70747596
C	-4.66923144	-0.25668596	-1.45946071
C	-5.33773463	0.67156716	-0.98066761
H	-6.25785201	1.22623657	-0.98218723
C	-3.82572975	-1.23986574	-2.02372486
C	-2.93185477	-0.88814804	-3.06364026
H	-2.91371767	0.13899269	-3.41510423
C	-2.08901925	-1.84244337	-3.61987207
H	-1.41019521	-1.55785815	-4.41970517

C	-2.10751747	-3.16243572	-3.15369042
H	-1.44405633	-3.90428701	-3.58969213
C	-2.98410933	-3.51981149	-2.12667590
H	-3.00100930	-4.54068688	-1.75469315
C	-3.84294863	-2.57759307	-1.56833940
H	-4.51902952	-2.85670508	-0.76850673
C	-3.21467173	-0.95969816	1.22233763
C	-4.40053300	-1.57168851	1.68724823
H	-5.33223043	-1.01890875	1.64410868
C	-4.38706219	-2.88141923	2.15935442
H	-5.31009315	-3.33128753	2.51598746
C	-3.20079237	-3.62097659	2.16394051
H	-3.19390833	-4.64385020	2.53007369
C	-2.02346112	-3.03594730	1.68440299
H	-1.09834007	-3.60624070	1.67344926
C	-2.02689354	-1.72524921	1.22247846
H	-1.10797534	-1.27676128	0.85545861
C	-5.36106567	2.00449008	1.53259280
C	-2.31314820	1.22733677	0.11361162
H	-1.30206509	1.09504309	-0.25664412
H	-3.19163355	3.37784251	-0.20684674
C	-6.23346348	3.03456814	1.12960352
C	-5.53703143	1.43934485	2.80820361
H	-4.86072266	0.66174179	3.14640239
C	-6.55273961	1.89323322	3.65052121
H	-6.10853032	3.47738743	0.14394097
C	-7.24440977	3.48445077	1.97369027
C	-7.41255502	2.91272537	3.23912165
H	-7.90773184	4.27969680	1.64304519
H	-6.66856941	1.44779928	4.63532091
H	-8.20584359	3.25982233	3.89537716

ts5bcrbhhh_12
E [Hartrees] = -925.2191992727
Gcorr [kcal/mol] = 183.536

C	0.82623845	-0.06641236	0.13019851
C	-0.49205396	0.72034217	0.22176679
C	-1.63561516	-0.27598566	0.56401296
C	-1.65282390	-0.71257036	-0.74615574
C	-0.57230115	0.21005692	-1.14117616
C	2.01518507	0.62022981	0.16836529
C	2.39470731	1.71756585	-0.65094085
H	0.73093795	-1.08843467	0.50006387
H	-0.45717134	1.76558395	0.51966758

C	-2.17773518	-0.63611447	1.85288345
C	-2.34874349	-1.72471389	-1.53597402
H	-0.27109135	0.65381502	-2.07822929
C	-1.94002118	0.20656182	2.96010395
C	-2.92319107	-1.81729753	2.06678898
C	-3.69025413	-2.06761385	-1.28843466
C	-1.68394885	-2.34160549	-2.61115318
C	2.93683122	2.88651342	-0.05114459
C	2.33609606	1.66672940	-2.07140572
H	-1.36088876	1.11499337	2.81922966
C	-2.43673010	-0.10863210	4.22151276
H	-3.08890442	-2.50108030	1.24165308
C	-3.41583708	-2.12725918	3.32940271
H	-4.22839861	-1.56523024	-0.49038711
C	-4.33518053	-3.01992369	-2.07451006
H	-0.65036968	-2.07413475	-2.81512285
C	-2.32956171	-3.29717733	-3.39272084
H	1.97301754	0.76061928	-2.54654514
C	2.78926488	2.73245623	-2.83972642
H	3.02818744	2.91813990	1.03043152
C	3.30936956	3.97542328	-0.82787513
H	-5.37301051	-3.27085101	-1.87181960
C	-3.65680497	-3.64272951	-3.12580057
H	-1.79717892	-3.77296893	-4.21211288
C	3.25299079	3.90115932	-2.22572081
H	2.76203096	2.66387195	-3.92437881
H	3.68230929	4.87651542	-0.34793357
H	-2.24173217	0.55764632	5.05777004
C	-3.18179650	-1.27450706	4.41384896
H	-3.98047120	-3.04504822	3.47246015
H	-4.16142825	-4.38567629	-3.73735213
H	3.58640431	4.73985695	-2.83040031
H	-3.57218069	-1.51976056	5.39761373

ts5bcrbhhph_12
E [Hartrees] = -925.2113993088
Gcorr [kcal/mol] = 184.537

C	0.79376795	-0.12318265	-0.28558862
C	-0.58003637	0.84710263	0.48275223
C	-1.64878938	-0.19820175	0.72920912
C	-1.62411527	-0.61496500	-0.56353968
C	-0.52934800	0.39147822	-0.91661403
C	1.95380993	0.29976310	-0.90419068
C	2.52587311	1.59017395	-1.04766648

H	0.70409918	-1.15044985	0.06929078
C	-0.32866352	2.16209201	1.08139692
C	-2.33852635	-0.67310135	1.92900162
H	-2.05009203	-1.44959625	-1.10809529
H	-0.48432242	1.00376455	-1.81404683
C	2.73941162	2.46473761	0.05280837
C	3.02614086	1.98549011	-2.31844831
C	0.03293109	2.27488247	2.43703979
C	-0.42205907	3.33603623	0.31495539
C	-2.63059743	0.19359971	2.99613802
C	-2.75148627	-2.01528364	2.01957974
H	-2.51705743	-2.69638211	1.20594852
C	-3.43022473	-2.47690616	3.14412584
H	-2.34048554	1.23673181	2.93147224
C	-3.30913810	-0.27141138	4.12219728
H	-0.70262596	3.26456449	-0.73175551
C	-0.13472060	4.57866595	0.87416256
H	0.11904377	1.37264250	3.03600766
C	0.31118178	3.51924469	2.99911901
H	2.37437793	2.17986982	1.03229753
C	3.41524556	3.66484407	-0.11849380
H	2.91478297	1.30025770	-3.15348439
C	3.61576317	3.23057675	-2.49408103
H	-3.73484056	-3.51865903	3.20081356
C	-3.70943625	-1.60656586	4.20206474
H	-3.52977093	0.41295377	4.93723975
H	0.59891809	3.58610021	4.04519139
C	0.23735672	4.67629159	2.21752093
H	-0.19989585	5.47356452	0.26092189
H	3.95039643	3.53544094	-3.48220920
C	3.82986572	4.06922706	-1.39322785
H	3.57996911	4.31152682	0.73911853
H	4.32785121	5.02580695	-1.52616001
H	-4.23482499	-1.96811554	5.08192475
H	0.46358857	5.64557214	2.65354939

ts5bcrbhphh_12
E [Hartrees] = -925.2166931493
Gcorr [kcal/mol] = 183.627

H	-0.20080992	-3.17605809	-1.51682595
C	-2.40108962	-1.14496065	-0.64593325
C	-1.07412390	-1.05562002	-0.99028065
H	-0.35477564	-0.24318010	-0.99089148
C	-0.94060708	-2.48715979	-1.13458536

C	-3.43215142	-0.24703343	-0.19324701
C	-1.72498338	-3.24298552	0.49786351
H	-1.60373635	-2.44736664	1.24887951
C	-1.33955398	-4.55733293	0.68566462
C	-1.21399273	-5.09124649	2.01927240
C	-2.02425364	-4.68067683	3.11028630
H	-2.76090603	-3.89763828	2.94989637
C	-1.90482943	-5.27970883	4.35957341
H	-2.54759171	-4.96544675	5.17825628
C	-0.94200781	-6.27354994	4.57017555
H	-0.84054787	-6.73161074	5.55072802
C	-0.11867289	-6.68667141	3.51601628
H	0.62371892	-7.46355422	3.67979726
C	-0.27447576	-6.12589123	2.25355389
H	0.32752986	-6.46267520	1.41445289
C	-2.35996522	-2.71313747	-0.77769800
C	-3.36313360	-3.47289507	-1.59549416
C	-4.20588700	-2.77595467	-2.47637014
C	-3.46999457	-4.86912397	-1.52577810
H	-2.79241977	-5.40656569	-0.86530576
C	-4.40163470	-5.54823239	-2.31020159
H	-4.14520059	-1.69406699	-2.54047631
C	-5.13191781	-3.45868274	-3.26582494
H	-5.77640241	-2.90020409	-3.93980853
C	-5.23614725	-4.84784944	-3.18396958
H	-4.47201858	-6.63068397	-2.23936512
H	-5.96074857	-5.37966733	-3.79508291
C	-3.22081660	1.14904453	-0.16960234
C	-4.68418301	-0.74817830	0.22138008
H	-4.86010640	-1.81896286	0.19726566
C	-5.68379558	0.11835078	0.65381603
H	-2.26358983	1.54758010	-0.49511787
C	-4.22335900	2.00848646	0.26241658
C	-5.45931411	1.49755156	0.67691273
H	-4.04622818	3.08053135	0.27655132
H	-6.64211977	-0.28258003	0.97229206
H	-6.24179366	2.17216979	1.01307956

ts5bcrbhphph_12
E [Hartrees] = -925.2111552850
Gcorr [kcal/mol] = 183.328

C	0.14716252	-2.97302561	-1.64871789
C	-2.51963029	-1.11202175	-0.49367817
C	-1.19912186	-0.89144181	-0.63145205

H	-0.55590727	-0.02712943	-0.50508567
C	-0.91915992	-2.33271796	-0.90524265
H	-3.38170853	-0.50813177	-0.23087081
C	-1.73465021	-3.20176280	0.59624091
H	-1.75322321	-2.47427800	1.42155135
C	-1.34406612	-4.53473494	0.70039082
C	-1.12509057	-5.07887446	2.02269903
C	-0.62442950	-4.33745026	3.12430690
H	-0.37805507	-3.28745371	2.99192090
C	-0.39670477	-4.94749527	4.35312388
H	0.01631776	-4.36910287	5.17619264
C	-0.71653942	-6.29691957	4.54108379
H	-0.55353941	-6.76551544	5.50810234
C	-1.22553315	-7.04489016	3.47444383
H	-1.46207186	-8.09691740	3.61248734
C	-1.38661779	-6.45534233	2.22466568
H	-1.73216658	-7.03606759	1.37418321
C	-2.35273639	-2.64786202	-0.68403301
C	-3.24440137	-3.43971642	-1.58810607
C	1.31374402	-2.23773621	-1.93540953
C	0.03235889	-4.29234502	-2.13487438
H	1.41076853	-1.22094720	-1.56472768
C	2.33954916	-2.80024269	-2.68995622
H	-0.85014862	-4.86815226	-1.88840972
C	1.06698661	-4.84993191	-2.87918591
H	3.23246050	-2.22012985	-2.90653490
C	2.21938813	-4.10958914	-3.16277832
H	0.97286119	-5.86846333	-3.24582312
H	3.01957239	-4.55103119	-3.75098603
C	-3.40106310	-3.01835480	-2.91634237
C	-3.95320094	-4.56059768	-1.14438363
H	-3.81386826	-4.90786629	-0.12552762
C	-4.80684180	-5.24531949	-2.01042829
H	-2.84726815	-2.15078926	-3.26659713
C	-4.24989822	-3.70433670	-3.78356372
H	-4.35506501	-3.37029342	-4.81245740
C	-4.95860291	-4.82016115	-3.33159597
H	-5.34920398	-6.11657546	-1.65264408
H	-5.61903197	-5.35806221	-4.00654526

ts5bhh_12
E [Hartrees] = -925.2349003613
Gcorr [kcal/mol] = 182.230

C	0.93312396	-0.52030517	1.51622417

C	-0.38698490	0.03344628	0.96424778
C	-1.56961338	-0.98237683	1.19548681
C	-1.72230524	-1.10334092	-0.20811378
C	-0.67105968	-0.21783923	-0.47814263
C	2.14476862	-0.13518206	1.29632586
C	3.44390333	0.25475452	1.09962495
H	0.73912113	-1.48888978	2.00698947
H	-0.60425113	1.03060915	1.36764789
C	-2.18309148	-1.44414962	2.39170856
C	-2.63816569	-1.81733687	-1.10969640
H	-0.21256702	0.15264038	-1.38756153
C	4.11293061	1.12323820	2.02564712
C	4.17877918	-0.18235786	-0.05293575
C	-1.88144535	-0.80997141	3.62815730
C	-3.08908049	-2.53979475	2.41959342
C	-4.00534206	-1.94373856	-0.81450592
C	-2.15577051	-2.34364098	-2.31888645
H	-1.17864755	0.01866950	3.63730913
C	-2.46993090	-1.23174583	4.81173270
H	-3.31009921	-3.06895727	1.49906049
C	-3.66405517	-2.95687078	3.61201015
H	-1.09855004	-2.24888184	-2.55248936
C	-3.01438971	-2.99536806	-3.20264696
H	-4.39280553	-1.51684486	0.10551539
C	-4.86369746	-2.59235215	-1.70093083
H	3.57413602	1.46007392	2.90581517
C	5.41612935	1.52609968	1.79584623
H	3.69033088	-0.84401063	-0.76160414
C	5.48499253	0.22859003	-0.25197964
H	-2.62466025	-3.40493311	-4.13078069
H	-4.34794330	-3.80202259	3.60700532
H	5.90322110	2.18801355	2.50744178
C	-3.36857550	-2.30616247	4.81663702
H	-2.22739931	-0.72327351	5.74147673
C	6.11703802	1.08586498	0.66184911
H	6.02505986	-0.11660362	-1.13001019
C	-4.37097032	-3.12346813	-2.89545444
H	-5.92009887	-2.67879446	-1.46105726
H	-5.04065018	-3.63174357	-3.58390467
H	7.14168090	1.40407002	0.49469557
H	-3.82574948	-2.63540459	5.74524544

ts5bhphh_12
E [Hartrees] = -925.2322684600

Gcorr [kcal/mol] = 181.470

C	2.31570267	0.23250218	1.53370264
C	1.11463971	0.55510990	0.64107547
C	-0.14924920	-0.29686590	0.99910278
C	-0.09702367	-0.98173506	-0.19015675
C	1.05467310	-0.25241980	-0.67979582
C	3.46931424	0.00908165	0.94620469
C	4.75365396	-0.02188009	0.46881222
H	2.13181308	0.24442875	2.62226897
C	0.89077046	2.04957057	0.39027601
C	-1.07123487	-0.21212001	2.10999857
H	-0.73987744	-1.72634038	-0.64868673
H	1.55528521	-0.37457654	-1.70009449
C	-0.30456169	2.67537205	0.77093303
C	1.87897974	2.83247915	-0.22301628
C	5.64186139	0.98841944	1.04430875
C	5.34314470	-1.02310449	-0.37354843
C	-0.88227771	0.74712632	3.12859316
C	-2.17192006	-1.09421864	2.21016968
H	-2.32756113	-1.84125499	1.43644384
C	-3.04288337	-1.02321379	3.29160885
H	-0.05093342	1.44297041	3.05684131
C	-1.76456734	0.82100415	4.20320427
H	2.80485525	2.36395292	-0.53391863
C	1.67799159	4.19445205	-0.45189664
H	-1.07363335	2.09934104	1.26770925
C	-0.50699038	4.03399646	0.54389614
H	4.70403124	-1.80977285	-0.76584980
C	6.69036679	-1.01220903	-0.63350410
H	5.19788280	1.86455304	1.50126026
C	7.01783397	1.02288256	0.64947483
H	7.64416905	1.84402193	0.99047636
C	7.54022682	0.02601367	-0.14042420
H	7.12657829	-1.79879399	-1.24093879
C	-2.84392492	-0.06429962	4.29284184
H	-1.60518346	1.56670003	4.97749190
H	-3.88097583	-1.71389462	3.35832169
C	0.48411654	4.80128856	-0.07231595
H	2.45421400	4.77453525	-0.93608649
H	-1.44136767	4.49588215	0.85106560
H	-3.52724720	-0.00911076	5.13610789
H	0.32243791	5.86120456	-0.25730401
H	8.59232676	0.03001821	-0.42109519

ts5bhphph_12
E [Hartrees] = -925.2058347111
Gcorr [kcal/mol] = 181.161

C	0.76818627	-0.17845756	-0.72098159
C	-0.53788889	0.61654512	-0.72653006
C	-1.27915058	0.17959670	0.63394488
C	-2.38703990	-0.26169072	-0.13821896
C	-1.80688481	0.05569115	-1.34515820
C	1.63755044	-0.01899980	0.25596945
C	2.64115767	0.11688263	1.29538004
H	1.06586954	-0.73441812	-1.62719723
C	-0.38101981	2.13911842	-0.70756321
C	-0.69110872	0.10505785	2.02486508
H	-3.33769613	-0.71414552	0.13156006
H	-2.12961826	-0.02207499	-2.37781992
C	-1.46182936	2.94542544	-0.31165792
C	0.80455916	2.77065781	-1.10444704
C	3.75179807	-0.75017031	1.32144302
C	2.51579253	1.07442786	2.31962564
C	0.12786386	-1.08711896	2.32545855
C	-0.94242062	1.05725289	3.04841176
H	-1.56143377	1.91622875	2.80260853
C	-0.43104680	0.89882803	4.31228581
H	0.30616391	-1.86406431	1.63139462
C	0.60758915	-1.20522343	3.69040473
H	1.64777475	2.16687331	-1.42180776
C	0.92256326	4.16329953	-1.07726922
H	-2.39791540	2.47995542	-0.02066401
C	-1.34495297	4.33342765	-0.27982120
H	1.66086833	1.74037057	2.31950838
C	3.46141846	1.15606024	3.33495667
H	3.86647715	-1.48679333	0.53172252
C	4.69824587	-0.66558546	2.34184816
H	5.54835398	-1.34272008	2.34579250
C	4.55693588	0.28874973	3.35163464
H	3.33729976	1.89521667	4.12153264
C	0.36073194	-0.24181432	4.62918935
H	1.21866753	-2.07160511	3.93225546
H	-0.62846522	1.63714614	5.08438536
C	-0.14981328	4.95072728	-0.66107355
H	1.85590895	4.62845871	-1.38364148
H	-2.19090001	4.93531255	0.04243542
H	0.77061464	-0.33430473	5.63113155
H	-0.05929983	6.03363559	-0.63554463

H	5.29457267	0.35773919	4.14601320

ts6crbhhh_124

E [Hartrees] = -925.2212408168

H	-0.20635914	-3.49360233	-0.63561447
C	-2.38270831	-1.54024353	-0.16765282
C	-1.04124832	-1.46064058	0.10769855
C	-0.04608811	-0.47772018	0.49718934
C	1.30404645	-0.87022138	0.58119317
H	1.57649964	-1.89450213	0.34223561
C	2.28736073	0.03161136	0.98017832
H	3.32289345	-0.29251164	1.03821648
C	1.94379229	1.34435774	1.30950538
H	2.71034142	2.04913338	1.61948714
C	0.60474402	1.74286532	1.24890547
H	0.32635240	2.75710563	1.52267168
C	-0.38066114	0.84511991	0.85019562
H	-1.41920749	1.15709887	0.83573897
C	-0.89384031	-2.97813887	0.01934636
C	-3.49364865	-0.63876126	-0.41844031
C	-3.30965936	0.64947724	-0.95863639
H	-2.30745100	0.98207827	-1.20970890
C	-4.40074636	1.47922940	-1.20066345
H	-4.24081762	2.46828436	-1.62162343
C	-5.69769332	1.04102903	-0.91630988
H	-6.54731305	1.69114796	-1.10570354
C	-5.89618165	-0.24210497	-0.40026829
H	-6.90187542	-0.59355778	-0.18584900
C	-4.80741138	-1.07745475	-0.16315738
H	-4.96384408	-2.07686057	0.23447300
C	-1.90675098	-3.53202236	1.27207290
H	-2.11196293	-2.87259613	2.13012647
C	-0.95227483	-4.54151929	1.26119893
C	-0.15317448	-4.69251781	2.47361666
C	1.25121799	-4.78981927	2.39491692
H	1.72394107	-4.73665532	1.41744193
C	2.02404535	-4.94187818	3.54228164
H	3.10718032	-4.99051932	3.45958586
C	1.41322925	-5.06094899	4.79519128
H	2.01664581	-5.20557952	5.68727046
C	0.02099062	-5.00591056	4.88778886
H	-0.46389996	-5.10476191	5.85614250
C	-0.75341499	-4.80203138	3.74615681
H	-1.83657134	-4.74834936	3.83039137

C	-2.39336641	-3.06958613	-0.09240080
H	-2.91220951	-3.74383173	-0.76753902

ts6crbhhph_123

E [Hartrees] = -925.2119428788

C	0.07681628	-3.73823904	-0.94114848
C	-2.32663148	-1.60923732	-0.07322621
C	-0.99046217	-1.54591489	0.13246690
C	-0.02956540	-0.51840726	0.51037398
C	1.12795589	-0.87479309	1.22622488
H	1.30184708	-1.91911034	1.47372011
C	2.03323072	0.10332052	1.63326591
H	2.91953003	-0.18424114	2.19208512
C	1.80251759	1.44616555	1.32558965
H	2.51220598	2.20709990	1.63844079
C	0.65663180	1.80853656	0.61061018
H	0.47566070	2.85152418	0.36496279
C	-0.25359219	0.83568755	0.20628173
H	-1.13949041	1.11518157	-0.35795640
C	-0.85373233	-3.07753427	0.01996002
H	-3.11441942	-0.86246950	-0.08416857
C	-1.86264255	-3.54629291	1.39300831
H	-1.99512583	-2.81483893	2.20568706
C	-1.01855936	-4.64502159	1.45407832
C	-0.17462304	-4.75487221	2.63657183
C	1.20728901	-4.99650190	2.48019315
H	1.60654227	-5.09758180	1.47475057
C	2.04385611	-5.09096725	3.58908440
H	3.10967917	-5.25278996	3.44721975
C	1.51516219	-5.01350310	4.88207255
H	2.16561301	-5.11686917	5.74648308
C	0.14311625	-4.81573036	5.05442617
H	-0.27654637	-4.76192684	6.05620386
C	-0.69035650	-4.66175601	3.94731670
H	-1.75487859	-4.49056155	4.09035233
C	-2.36455796	-3.12866725	0.01729415
H	-2.93980057	-3.81190931	-0.60236338
C	1.12476802	-2.98997466	-1.49845272
C	-0.12137833	-5.05628014	-1.39181776
H	-0.89550648	-5.64930943	-0.91918132
C	0.69838606	-5.59915514	-2.37330549
H	1.29886790	-1.97024315	-1.17836610
C	1.95603941	-3.54546290	-2.47636167
C	1.74675940	-4.84795043	-2.91965454

H	0.52833781	-6.61931622	-2.70725869
H	2.76601670	-2.94911845	-2.88805138
H	2.39401158	-5.28127934	-3.67749513

ts6crbhhph_124
E [Hartrees] = -925.2142671970
Gcorr [kcal/mol] = 182.580

C	0.60780449	-2.93280182	-1.62458923
C	-1.89423593	-1.47178314	0.22012109
C	-0.64263820	-1.08058275	-0.12082712
C	0.09750274	0.16912235	-0.11755663
C	1.49147802	0.16846946	-0.30713961
H	2.00584476	-0.77274170	-0.47351286
C	2.20777806	1.36388941	-0.28666131
H	3.28444119	1.34836062	-0.43204079
C	1.54574288	2.57642568	-0.08437085
H	2.10482637	3.50803158	-0.07259830
C	0.15825387	2.58961209	0.09773739
H	-0.36141991	3.53156135	0.25103206
C	-0.56007742	1.39906619	0.07889891
H	-1.63881584	1.41075517	0.21116415
C	-0.18255355	-2.53063707	-0.42500479
H	-2.75286805	-0.98310823	0.66554389
C	-0.28592007	-3.33019654	0.86546747
H	-0.11052603	-2.78667717	1.80779791
C	-0.91061030	-4.56610488	0.77590375
C	-1.38879721	-5.15213573	2.02301171
C	-0.55382121	-5.24739680	3.15754345
H	0.45708098	-4.84844926	3.11057464
C	-0.99660387	-5.87412278	4.32177867
H	-0.32997322	-5.95313499	5.17732405
C	-2.29561800	-6.38062155	4.39920417
H	-2.64440845	-6.85728069	5.31134767
C	-3.13960431	-6.28254409	3.28769589
H	-4.15003084	-6.68116913	3.33665267
C	-2.68372863	-5.70342244	2.10709577
H	-3.32633668	-5.66138560	1.23165284
C	-1.62858323	-2.91334903	-0.14724143
H	-2.22857398	-3.52337612	-0.80763933
C	0.63252156	-2.09042290	-2.74717615
C	1.33245182	-4.13262663	-1.66656954
H	0.08515855	-1.15245417	-2.72586270
C	1.36287545	-2.43841474	-3.88335819
H	1.29768850	-4.80189028	-0.81428752

C	2.06286753	-4.47811075	-2.80288321
H	1.37094688	-1.77168525	-4.74174418
C	2.08263595	-3.63378530	-3.91544346
H	2.61787492	-5.41249172	-2.81819159
H	2.65384023	-3.90547944	-4.79913571

ts6crbhphph_12
E [Hartrees] = -925.2040537681
Gcorr [kcal/mol] = 183.173

C	-0.05520287	-3.46251173	-1.23043772
C	-2.48852828	-1.18704832	-0.57896694
C	-1.19211989	-1.29541316	-0.24719699
H	-0.42103680	-0.61640983	0.09749157
C	-1.16635095	-2.78289685	-0.54332806
H	-3.19831621	-0.36639093	-0.60167333
C	-2.46625309	-3.34919667	0.62839347
H	-2.75799847	-2.74631266	1.50266202
C	-1.70306911	-4.49491565	0.67077768
C	-1.03036336	-4.85790974	1.90374347
C	-0.36094535	-3.91804141	2.72093781
H	-0.36328089	-2.86969630	2.43089976
C	0.31558586	-4.31957929	3.87016557
H	0.83909394	-3.58245909	4.47462234
C	0.30923954	-5.66270789	4.25696111
H	0.82934619	-5.97427678	5.15886556
C	-0.35476191	-6.60609558	3.46575311
H	-0.35369235	-7.65404274	3.75521272
C	-0.98610225	-6.21562196	2.28843097
H	-1.46522521	-6.94968808	1.64673129
C	-2.66812007	-2.71080143	-0.75301198
C	-3.48753408	-3.32920515	-1.84139788
C	1.23488699	-3.34926845	-0.68460900
C	-0.22805651	-4.14163987	-2.44753899
H	1.37166298	-2.82924978	0.25984722
C	2.32651530	-3.92865931	-1.32777905
H	-1.21816889	-4.22793536	-2.87831897
C	0.87012093	-4.70232425	-3.09349283
H	3.31638283	-3.84868712	-0.88650207
C	2.14904757	-4.60499661	-2.53645701
H	0.72674787	-5.22037664	-4.03811010
H	3.00070666	-5.05085550	-3.04295778
C	-4.04596331	-2.51308830	-2.83500953
C	-3.71048323	-4.71455961	-1.90191922
H	-3.25242119	-5.34817749	-1.14942639

C	-4.47467515	-5.26098680	-2.93107047
H	-3.87832380	-1.43991021	-2.80750658
C	-4.81145913	-3.06315536	-3.86495619
H	-5.23572827	-2.41304887	-4.62566181
C	-5.02998087	-4.43969616	-3.91634558
H	-4.63499990	-6.33553758	-2.96469412
H	-5.62460224	-4.87021582	-4.71766448

ts7hh_124
E [Hartrees] = -925.3002838300
Gcorr [kcal/mol] = 185.211

C	-2.79390889	2.29989504	0.21538514
C	-4.22063626	1.99416495	0.03795807
C	-3.17801302	0.19264571	0.22623086
C	-3.91169711	-0.04526402	-1.01797971
C	-4.74669602	1.06081205	-0.97148959
C	-5.96638646	1.35144546	-1.74334898
C	-3.52408983	-0.96096618	-2.08353499
C	-3.79682677	-0.69259939	-3.44034600
H	-4.31803702	0.22128227	-3.70578896
C	-3.38742611	-1.57566870	-4.43336665
H	-3.60343091	-1.34968741	-5.47440697
C	-2.68503388	-2.74008617	-4.10202651
H	-2.36330261	-3.42491923	-4.88194968
C	-2.40122435	-3.01540367	-2.76367455
H	-1.85847313	-3.91796832	-2.49503023
C	-2.82388546	-2.13960638	-1.76523579
H	-2.62853092	-2.36786659	-0.72082462
H	-3.71805253	0.12764423	1.17121190
H	-4.94597188	2.63827877	0.54342392
C	-2.05658362	1.14987034	0.13525381
C	-0.66123513	0.89494845	-0.18530354
H	-2.42989497	3.31718638	0.36676666
C	2.03983585	0.38185539	-0.79316160
C	1.50430614	1.65938229	-0.98861627
C	0.16746917	1.91197990	-0.69814276
C	-0.10699788	-0.38213486	0.01465581
C	1.22672455	-0.63846514	-0.29560498
H	3.08177125	0.18450126	-1.03005941
H	2.12909475	2.45567480	-1.38480446
H	-0.25488664	2.89470242	-0.88853953
H	-0.73289464	-1.16880502	0.42669462
H	1.63477739	-1.63369654	-0.13984958
C	-6.35052876	2.67703521	-2.00812090

C	-6.79032565	0.30998867	-2.20867800
H	-6.50829260	-0.71706690	-1.99628478
C	-7.95146693	0.58645642	-2.92454530
H	-5.71287797	3.49157289	-1.67443860
C	-7.52133428	2.95392893	-2.71396309
H	-8.57444511	-0.23143975	-3.27720042
C	-8.32479454	1.91048030	-3.17717301
H	-7.80041656	3.98572738	-2.91153543
H	-9.23463846	2.12548188	-3.73113829

ts7hph_123
E [Hartrees] = -925.3014291499
E [Hartrees] = -925.3014291499
Gcorr [kcal/mol] = 184.655

C	-2.84604922	1.99894996	0.46838028
C	-4.22431729	1.50606447	0.40646475
C	-2.87871467	-0.17358918	0.27096852
C	-3.75600773	-0.34451048	-0.92842367
C	-4.69004279	0.61229261	-0.65705086
H	-5.65046255	0.75147151	-1.15541612
C	-3.52250834	-1.20852786	-2.06934758
C	-4.20411831	-1.02337934	-3.29007555
H	-4.88124335	-0.18025410	-3.39609202
C	-3.99745404	-1.89093414	-4.35660834
H	-4.53204262	-1.73342139	-5.28990481
C	-3.09081019	-2.95141663	-4.24091283
H	-2.92450644	-3.62139658	-5.08001129
C	-2.40014394	-3.14002646	-3.04250545
H	-1.69605189	-3.96199139	-2.94266155
C	-2.61976103	-2.28495521	-1.96431056
H	-2.10774628	-2.45569549	-1.02164575
C	-3.02867934	-0.95391396	1.47916745
C	-3.93282722	-2.04135637	1.52877166
H	-4.54961725	-2.25299498	0.66129829
C	-4.02794008	-2.82900168	2.66944237
H	-4.73093321	-3.65752997	2.69299958
C	-3.21242356	-2.57219780	3.77749173
H	-3.27815814	-3.20086531	4.66120910
C	-2.29017632	-1.52051522	3.72973340
H	-1.63956275	-1.32985443	4.57918809
C	-2.18706724	-0.72696927	2.59393410
H	-1.45766953	0.07524357	2.54778518
H	-4.97166406	1.98291926	1.04328796
C	-1.96271324	1.00407836	0.16551579

C	-0.58177675	1.00406686	-0.27695644
H	-2.60934190	3.03829021	0.70057908
C	2.12322613	0.97428023	-1.06580258
C	1.40123589	2.17377086	-1.06606783
C	0.06364672	2.18898362	-0.68750102
C	0.15951259	-0.19396482	-0.27309979
C	1.49432603	-0.20851332	-0.67301315
H	3.16568059	0.96461410	-1.37206798
H	1.88264760	3.09681684	-1.37890818
H	-0.50294289	3.11538078	-0.72411932
H	-0.31651588	-1.10966743	0.06577749
H	2.04752314	-1.14408560	-0.66731563

ts7phh_124
E [Hartrees] = -925.2968141438
Gcorr [kcal/mol] = 184.082

H	0.97958828	-4.29738757	-1.14295644
C	0.09536424	-3.75900933	-0.79907644
C	-1.20138419	-4.01565960	-1.15565177
C	-1.80357032	-4.70904935	-2.27625386
C	-1.04346913	-5.12570762	-3.38901614
H	0.01316308	-4.87620420	-3.43197069
C	-1.63882427	-5.82592492	-4.43211633
H	-1.03741880	-6.14070000	-5.28115988
C	-3.00992236	-6.10797814	-4.40429373
H	-3.47324299	-6.64660857	-5.22634477
C	-3.77775863	-5.68990345	-3.31560890
H	-4.84240115	-5.90666162	-3.28442298
C	-3.18113381	-5.00697065	-2.25757168
H	-3.77384523	-4.71274453	-1.39492626
C	-1.90092086	-3.19362544	-0.12291538
C	-1.90531006	-1.75279845	-0.44194311
H	-2.59856987	-1.21900920	-1.08527954
C	-0.63238014	-1.40288985	-0.08438938
C	-0.07904942	-0.04300086	0.02439147
C	1.29741285	0.19626315	-0.12395344
H	1.96273932	-0.63671175	-0.33432380
C	1.80983010	1.48959432	-0.03440070
H	2.87725278	1.65593605	-0.15467594
C	0.95523942	2.57001353	0.19666334
H	1.35500153	3.57822393	0.26529685
C	-0.41637412	2.34613739	0.34478261
H	-1.08698723	3.18053791	0.53357511
C	-0.92589612	1.05198268	0.26997039

H	-1.98700360	0.87103019	0.42050449
C	0.18904817	-2.61684359	0.10211002
H	1.02443111	-2.57187934	0.80236162
C	-2.29102392	-3.73682125	1.16561584
C	-2.22286684	-5.12889965	1.40214726
H	-1.84271062	-5.77820718	0.62025862
C	-2.63692808	-5.66075295	2.61865926
H	-2.57301167	-6.73265076	2.78620677
C	-3.14898627	-4.82613634	3.61667270
H	-3.48599998	-5.24621321	4.56039244
C	-3.25403291	-3.44923578	3.38251038
H	-3.66897194	-2.79876540	4.14797317
C	-2.84501357	-2.91038359	2.17005726
H	-2.93795093	-1.84602347	1.97929058

ts7phph_124
E [Hartrees] = -925.3023984815
Gcorr [kcal/mol] = 183.716

H	-2.77733508	-3.77419659	-0.67054409
C	-2.45402094	-2.89848899	-0.10620231
C	-2.68465257	-1.61569446	-0.46668822
H	-2.95943815	-1.23607392	-1.44708543
C	-2.16563189	-0.84114429	0.68529658
C	-0.67706322	-0.85072713	0.71969403
C	-0.41232609	-2.12171389	1.15570568
H	0.56992090	-2.47674205	1.47042171
C	-1.54292091	-3.04650564	1.05522708
C	-1.65996729	-4.18121132	1.95289641
C	-2.67692657	-5.15399290	1.79000664
H	-3.41040701	-5.03527530	0.99967871
C	-2.76713801	-6.25355658	2.63582023
H	-3.55617729	-6.98512542	2.48168361
C	-1.86219306	-6.41311860	3.68954148
H	-1.94102220	-7.26749245	4.35617090
C	-0.87229957	-5.44709390	3.89331633
H	-0.17960058	-5.54581540	4.72517230
C	-0.77881577	-4.34604585	3.05013631
H	-0.02969172	-3.58786950	3.25168068
C	0.19730087	0.19632902	0.22513055
C	-0.30280137	1.50475453	0.06642783
H	-1.34017630	1.70630407	0.32196554
C	0.51983930	2.53440494	-0.38597704
H	0.11355323	3.53559944	-0.50461574
C	1.86422317	2.28623967	-0.66955400

H	2.50876896	3.09027426	-1.01409421
C	2.37661947	0.99299832	-0.50971693
H	3.41989244	0.79104012	-0.73890407
C	1.55381453	-0.04211739	-0.08017495
H	1.94686622	-1.05142842	0.00378758
C	-2.94912617	-0.55891369	1.85765811
C	-4.35071410	-0.77650324	1.88150301
H	-4.82798043	-1.20363496	1.00552076
C	-5.09652186	-0.46414613	3.00822480
H	-6.16776902	-0.64779524	3.01260803
C	-4.47948787	0.09657587	4.13480544
H	-5.07077570	0.35369481	5.00928575
C	-3.10351417	0.35101692	4.11619747
H	-2.62365507	0.80375854	4.97989643
C	-2.34723306	0.04245537	2.99324579
H	-1.28365690	0.25612604	2.97164241

ts8hh_124
E [Hartrees] = -925.3021835549
Gcorr [kcal/mol] = 181.351

C	-2.21319944	1.58907306	-1.90778418
C	-3.60433358	1.83673375	-2.10688233
C	-2.93582943	-0.22230937	-0.56584762
C	-3.99769787	-0.26079914	-1.53946328
C	-4.64884648	1.03520851	-1.58513565
C	-6.06570424	1.35775111	-1.54961272
C	-4.08008140	-1.27664964	-2.56302524
C	-4.94732600	-1.14989891	-3.67469157
H	-5.56390353	-0.26166973	-3.76441962
C	-4.98875967	-2.13881866	-4.64512243
H	-5.65379496	-2.03461029	-5.49786489
C	-4.16814475	-3.27150791	-4.53192649
H	-4.20852433	-4.04590390	-5.29352926
C	-3.30988113	-3.41258989	-3.43844396
H	-2.68119310	-4.29425997	-3.35021194
C	-3.27581089	-2.43190557	-2.45203347
H	-2.64627246	-2.53326991	-1.57366022
H	-3.27776228	0.01145358	0.45228535
H	-3.88451086	2.66324088	-2.76211001
C	-1.83557432	0.63147261	-0.95637744
C	-0.57390152	0.66245307	-0.20723832
H	-1.49050678	2.24125399	-2.38987855
C	1.85436822	0.64374723	1.22591570
C	1.45660105	1.78878002	0.52927240

C	0.25242668	1.80280314	-0.16930164
C	-0.15750984	-0.48186396	0.49878573
C	1.03753199	-0.48977074	1.21348922
H	2.79085017	0.63763623	1.77740010
H	2.08000895	2.67911768	0.54592544
H	-0.06831345	2.71087893	-0.67053019
H	-0.78814881	-1.36594836	0.46424558
H	1.33855942	-1.38393146	1.75333906
C	-6.53398175	2.67799833	-1.71878898
C	-7.02300556	0.34486573	-1.32588758
H	-6.68481683	-0.67631274	-1.17071567
C	-8.38413376	0.63435500	-1.30515318
H	-5.81957378	3.48701610	-1.84348103
C	-7.89649715	2.96098778	-1.70875942
H	-9.09915969	-0.16593290	-1.13137275
C	-8.83273779	1.94280731	-1.50444442
H	-8.23085388	3.98611801	-1.84763643
H	-9.89521626	2.16880351	-1.48664912

ts8hph_123
E [Hartrees] = -925.3064004932
Gcorr [kcal/mol] = 185.426

C	-2.58261530	1.63140923	1.22096965
C	-3.82739129	1.52134401	0.61096421
C	-2.38584051	-0.56684834	0.48824012
C	-3.15614942	-0.39561826	-0.78426859
C	-4.06703187	0.59741123	-0.49908767
H	-4.92419484	0.78696040	-1.14535681
C	-3.02694296	-1.21338098	-1.97720066
C	-3.69294049	-0.91302920	-3.18427406
H	-4.28974684	-0.00810919	-3.25568302
C	-3.57439178	-1.75053881	-4.28751279
H	-4.09563353	-1.50257950	-5.20855798
C	-2.77642118	-2.89967873	-4.22570780
H	-2.67935079	-3.54605163	-5.09348768
C	-2.10267462	-3.20430315	-3.04233586
H	-1.48177911	-4.09421035	-2.97913719
C	-2.23012258	-2.37602969	-1.93029725
H	-1.72855305	-2.63139744	-1.00224774
C	-2.79051066	-1.49599040	1.49543995
C	-3.71559291	-2.54342917	1.22469582
H	-4.26623804	-2.53081882	0.28982015
C	-3.88588096	-3.58385620	2.12423749
H	-4.57588852	-4.39051931	1.89099243

C	-3.15480233	-3.61701802	3.32151587
H	-3.26820446	-4.45413223	4.00499220
C	-2.24654321	-2.59214749	3.61230305
H	-1.65948259	-2.62956575	4.52620424
C	-2.05124371	-1.55653349	2.70962762
H	-1.28871416	-0.80443222	2.88651277
H	-4.59442587	2.26638933	0.81630998
C	-1.63870444	0.63601354	0.79836511
C	-0.33100131	0.87428624	0.24544908
H	-2.30035675	2.54778058	1.73995446
C	2.29124242	1.18583286	-0.75157336
C	1.52862490	2.30827392	-0.39748263
C	0.23229908	2.16222424	0.07754992
C	0.46447510	-0.24793550	-0.09391292
C	1.74567125	-0.09186730	-0.60915594
H	3.30369397	1.30862117	-1.12534290
H	1.94933690	3.30377249	-0.51340057
H	-0.36789937	3.03904713	0.30247735
H	0.06526347	-1.24111990	0.08977848
H	2.33050442	-0.97026984	-0.86930522

ts8hph_124
E [Hartrees] = -925.2926616814
Gcorr [kcal/mol] = 184.682

C	-1.22464034	1.90580013	-0.79515426
C	-0.86121915	0.88240256	-1.79596460
C	-0.27623986	-0.29546804	-1.30246224
C	0.04465177	2.30968871	-0.45169517
C	1.07241220	0.06469247	-1.08562032
C	1.20108294	1.50069671	-0.91759209
H	-0.49383637	1.29357442	-2.74004645
H	-0.77603730	-1.04293690	-0.68704886
C	2.11537452	-0.93011271	-0.75154934
C	-2.51803093	2.23972122	-0.22387322
H	0.23431721	3.21773791	0.11865904
C	2.52308614	2.15877684	-1.02459428
C	3.10977319	-0.70525023	0.21877212
C	2.07845575	-2.18380205	-1.38590311
C	2.92628712	3.19980434	-0.16569688
C	3.42771102	1.73859351	-2.01871201
C	-3.69437490	1.80962801	-0.86651723
C	-2.64076250	2.99532707	0.95958327
H	-1.74500277	3.30590722	1.48991440
C	-3.89450434	3.32120878	1.46613023

H	-3.60859874	1.23558999	-1.78619577
C	-4.94836292	2.12187817	-0.34657454
H	2.26112584	3.54394629	0.62037371
C	4.18937265	3.77561989	-0.28105424
H	3.12863443	0.94450307	-2.69565062
C	4.68532477	2.32256193	-2.14241277
H	3.14530945	0.24761777	0.73622030
C	4.03850109	-1.69473602	0.52865196
H	1.31807943	-2.36094737	-2.14204713
C	3.00322036	-3.17851330	-1.06932407
C	-5.05534870	2.88467743	0.81825878
H	-3.96966993	3.90563171	2.37952119
H	-5.84406653	1.77692160	-0.85653427
H	4.79768455	-1.50117429	1.28213088
C	3.99110386	-2.93599306	-0.11381151
H	2.95643329	-4.13970925	-1.57482877
C	5.07450349	3.34278346	-1.27151582
H	4.48325967	4.56640398	0.40418276
H	5.36246778	1.98120603	-2.92078219
H	-6.03289088	3.13468066	1.22128817
H	6.05601239	3.79941250	-1.36551325
H	4.71743833	-3.70641857	0.13118968

ts8phph_124
E [Hartrees] = -925.2983997061
Gcorr [kcal/mol] = 185.146

H	-2.93755926	-3.82178611	-0.39888999
C	-2.57523647	-2.95983415	0.16185578
C	-2.85894363	-1.68796135	-0.20263648
H	-3.24393521	-1.35052365	-1.16072574
C	-2.29350163	-0.85670230	0.89089878
C	-0.81079989	-0.90334666	0.92977228
C	-0.52495774	-2.17439121	1.37068556
H	0.47890343	-2.48228736	1.66463429
C	-1.56621091	-3.16845069	1.23081040
C	-1.51346768	-4.42220276	1.96327267
C	-2.42614271	-5.47857489	1.71275344
H	-3.22715946	-5.34007098	0.99514109
C	-2.33058951	-6.69479155	2.37924437
H	-3.04474900	-7.48348488	2.15610715
C	-1.33588679	-6.90386196	3.33882464
H	-1.26824210	-7.85225514	3.86446578
C	-0.44720485	-5.86508258	3.63312607
H	0.31428363	-6.00138172	4.39693153

C	-0.54062349	-4.64700719	2.97141277
H	0.13353915	-3.84490945	3.25167341
C	0.06567374	0.11206053	0.38173518
C	-0.42947954	1.41252542	0.13787224
H	-1.46993427	1.63285016	0.36014886
C	0.40108275	2.41436949	-0.36026228
H	-0.00514420	3.40557947	-0.54560540
C	1.75084585	2.15488479	-0.60338627
H	2.40119135	2.93838727	-0.98239591
C	2.25950572	0.87244281	-0.35901307
H	3.30674973	0.65818667	-0.55745784
C	1.43013734	-0.13831205	0.11007560
H	1.82454224	-1.14034869	0.25159618
C	-3.07801923	-0.27693016	1.91994656
C	-4.50061150	-0.34803446	1.89929119
H	-4.98130609	-0.90187155	1.09926296
C	-5.25079018	0.27254745	2.88273758
H	-6.33519020	0.20841173	2.85769604
C	-4.61739888	0.99324353	3.90805796
H	-5.21306155	1.49422795	4.66611929
C	-3.22008866	1.08933156	3.93851315
H	-2.73324758	1.65883015	4.72544287
C	-2.45547631	0.47397026	2.95915801
H	-1.37441968	0.56263707	2.96159790

tstrmr

E [Hartrees] = -925.1349444598

C	2.16495047	0.23682889	1.75399428
C	4.32185333	0.28286757	1.05211593
C	4.46625492	0.61386817	-0.13347928
C	2.76199286	1.07098204	-1.63476576
C	1.66466728	0.67771810	-1.22220588
C	1.16481441	0.14754813	1.02914278
C	-0.23219097	-0.08540684	0.77333911
C	4.88553528	-0.15237731	2.30991065
C	3.62122140	1.67445711	-2.62477872
C	4.39461827	0.87639871	-3.48786656
C	5.21070575	1.46730421	-4.45159570
C	5.27761827	2.85783808	-4.56266187
C	4.52129379	3.65665940	-3.70086126
C	3.70257480	3.07419141	-2.73552949
C	-2.47245337	0.74802053	0.33017691
C	-1.11915681	0.98763315	0.56196890
C	-0.73133710	-1.40060104	0.72105977

C	-2.08504858	-1.63089701	0.48543720
C	-2.96141301	-0.55996851	0.29058422
C	5.81301567	-1.91546720	3.69879894
C	5.99081921	-1.00983202	4.74799954
C	5.61027279	0.32339176	4.58036651
C	5.05568104	0.75111730	3.37468909
C	5.26087453	-1.49557131	2.49028553
H	2.56989265	0.26129117	2.74506430
H	5.10556321	0.83008226	-0.96376531
H	0.62577562	0.46763148	-1.36177267
H	4.33887560	-0.20474557	-3.40026813
H	5.79495021	0.83830523	-5.11806972
H	5.91614540	3.31591872	-5.31291999
H	4.57096466	4.73956127	-3.77873918
H	3.11748801	3.69190915	-2.06123523
H	-3.14698649	1.58668925	0.17892696
H	-0.73513989	2.00302089	0.58912644
H	-0.04742314	-2.23043362	0.87048544
H	-2.45691123	-2.65163637	0.45230717
H	-4.01620322	-0.74364965	0.10589641
H	6.10354676	-2.95545413	3.82250935
H	6.41989674	-1.34146663	5.68946837
H	5.74532040	1.03491253	5.39074274
H	4.75990996	1.78782102	3.24143963
H	5.11694665	-2.19749617	1.67472129

Methylacetylene Stationary Points

123me3ph
E [Hartrees] = -350.2139504572
Gcorr [kcal/mol] = 96.218

C	1.25143891	0.05389368	0.01902023
C	1.24099056	-1.35754773	0.02981038
C	0.02094897	-2.04105831	0.04596556
C	-1.18552503	-1.34509295	0.05142453
C	-1.17363258	0.04685061	0.04054819
C	0.03161108	0.76084742	0.02433722
C	-0.01090109	2.27463944	0.01288284
C	2.58341302	0.77229128	0.00179047
H	-2.11319981	0.59465713	0.04455768
C	2.53748077	-2.13425522	0.02392086
H	0.02067220	-3.12869728	0.05430974
H	-2.12919033	-1.88425935	0.06406345
H	3.19101295	0.50605685	0.87666833
H	2.47828960	1.85825849	-0.00335811

H	3.17382201	0.49595692	-0.88172638
H	3.15918335	-1.89484619	0.89660024
H	3.14348703	-1.90772573	-0.86312372
H	2.35261059	-3.21277797	0.03348817
H	0.49221790	2.70581477	0.88743323
H	-1.04433567	2.63473875	0.01882646
H	0.47732974	2.69201066	-0.87665334

124me3ph
E [Hartrees] = -350.2162015906
Gcorr [kcal/mol] = 95.582

C	1.23951598	0.03651457	0.01962561
C	1.24530317	-1.37474885	0.03537579
C	0.02082860	-2.04774683	0.03424716
C	-1.19166532	-1.35668282	0.01896107
C	-1.21201214	0.03977994	0.00629110
C	0.01696968	0.71244970	0.00435188
H	0.02069392	1.80142969	-0.01118449
C	2.53819217	0.80787111	0.01524094
C	-2.51230139	0.80955205	0.01933704
C	2.54642247	-2.14111857	0.04792480
H	0.01480499	-3.13575548	0.04174092
H	-2.12795486	-1.91049045	0.01576782
H	-2.75277951	1.16789005	1.02933030
H	-3.35000970	0.18836494	-0.31505501
H	-2.46414362	1.69018578	-0.63157637
H	3.14533381	0.58111746	0.90153977
H	2.36090871	1.88768606	-0.00026360
H	3.15432066	0.55713967	-0.85828990
H	3.15643487	-1.89027509	0.92578512
H	3.15954993	-1.91365376	-0.83416440
H	2.37142633	-3.22141331	0.06186943

135me3ph
E [Hartrees] = -350.2159746401
Gcorr [kcal/mol] = 94.781

C	1.22452376	0.02177673	-0.03429909
C	1.23437323	-1.37781715	0.01768103
C	0.01155437	-2.05321724	0.06468755
C	-1.20593164	-1.36085450	0.06733955
C	-1.18048594	0.03563301	0.01448863
C	0.02733359	0.74311337	-0.03345597
C	0.03050179	2.25437459	-0.06531241
H	2.17039854	0.55886048	-0.08338420

H	-2.12012413	0.58576129	0.00340468
C	2.54170699	-2.13622680	0.04172220
H	0.00454449	-3.14165544	0.09305852
C	-2.51639223	-2.11010763	0.14611141
H	2.94586448	-2.19583409	1.06127954
H	3.30127223	-1.64682257	-0.57828572
H	2.41863822	-3.16243892	-0.32060736
H	-0.09185448	2.67186465	0.94316434
H	-0.79058735	2.64450221	-0.67738009
H	0.96977069	2.64668735	-0.46941008
H	-2.78538017	-2.32809374	1.18850591
H	-2.46317286	-3.06926241	-0.38104344
H	-3.33827387	-1.53032776	-0.28769787

int1b_14eee
E [Hartrees] = -233.2753689635
Gcorr [kcal/mol] = 53.540

H	-2.23662154	-2.59846875	-2.36197152
C	-1.81225518	-2.56652277	-1.34917441
C	-1.29426086	-1.42882507	-0.91009670
C	-1.07963643	-0.05290567	-1.38442483
H	-0.01383625	0.21190733	-1.39319666
H	-1.46264315	0.07363457	-2.41178404
H	-1.59147341	0.68075506	-0.74733998
C	-1.87193736	-3.81438634	-0.58891664
H	-1.44759385	-3.78229735	0.42388548
C	-2.39008327	-4.95218207	-1.02757633
C	-2.60483577	-6.32762728	-0.55180552
H	-2.22057238	-6.45300560	0.47519616
H	-3.67074586	-6.59187672	-0.54136404
H	-2.09410709	-7.06222307	-1.18870121

int1b_14eez
E [Hartrees] = -233.2753506503
Gcorr [kcal/mol] = 53.295

H	-2.24202574	-2.59252203	-2.38245055
C	-1.81628153	-2.55481705	-1.37036704
C	-1.30166147	-1.42077754	-0.93371164
C	-1.07267479	-0.03674120	-1.37405678
H	-0.00468902	0.21874235	-1.36846227
H	-1.44691566	0.11934127	-2.40061086
H	-1.58254919	0.68525032	-0.72240619
C	-1.87169301	-3.81303763	-0.59544090
H	-1.44722114	-3.76851246	0.40773594

C	-2.38991388	-4.94813360	-1.03783649
C	-3.04340996	-5.48708570	-2.24087371
H	-2.47690240	-6.32474895	-2.66860754
H	-4.05485559	-5.85399259	-2.02202553
H	-3.13404218	-4.71455046	-3.02469398

int1b_14eze
E [Hartrees] = -233.2712169964
Gcorr [kcal/mol] = 53.057

H	-1.68678457	-3.25261630	-2.61801370
C	-1.62585855	-2.89431135	-1.58052811
C	-1.06529807	-1.71341093	-1.35992016
C	-0.44045565	-0.62773500	-2.13023254
H	0.60011587	-0.45776554	-1.82251155
H	-0.43459559	-0.86299130	-3.20882509
H	-0.97596046	0.32250886	-2.00122857
C	-2.18370869	-3.78788981	-0.55921011
H	-2.61100978	-4.73142869	-0.92747676
C	-2.21445402	-3.55601840	0.74567136
C	-2.68065523	-4.21838456	1.97305247
H	-3.14052223	-5.19525900	1.74290615
H	-1.85634280	-4.39761410	2.67642899
H	-3.43146660	-3.61474718	2.50055647

int1b_14zez
E [Hartrees] = -233.2789053585
Gcorr [kcal/mol] = 53.582

H	-2.25197026	-2.62858921	-2.37437735
C	-1.82156284	-2.55960880	-1.37501015
C	-1.30612971	-1.42863745	-0.93915982
C	-0.65116390	-0.87325188	0.25410294
H	-1.22116246	-0.03477540	0.67509008
H	-0.55269898	-1.63739356	1.04539638
H	0.35701628	-0.50315102	0.02655879
C	-1.86335021	-3.82079516	-0.56123145
H	-1.43356225	-3.75178278	0.43840484
C	-2.37806478	-4.95188729	-0.99756387
C	-3.03205440	-5.50735902	-2.19133730
H	-3.12871396	-4.74362290	-2.98317634
H	-2.46228951	-6.34658028	-2.61112720
H	-4.04086606	-5.87637655	-1.96489147

int1c
E [Hartrees] = -233.2506146903

Gcorr [kcal/mol] = 53.516

C	-1.86835927	1.40143619	-0.36292935
C	-0.80216043	0.83135135	0.03636751
C	0.02463091	3.08263498	-0.83169664
C	-0.78774874	2.40510330	0.13297686
C	0.13544128	-0.26285788	0.33861039
C	0.56280994	4.38408978	-0.33806339
H	-2.86495792	1.42346430	-0.77215724
H	-0.94963524	2.80995778	1.14789091
H	0.43768982	-0.23247824	1.39249245
H	1.04102536	-0.14690516	-0.26874681
H	-0.31367483	-1.23916996	0.12820048
H	0.50818878	4.59346707	0.74813826
H	-0.04764277	5.15028478	-0.84929288
H	1.58570547	4.56329624	-0.69481941

int2_12

E [Hartrees] = -233.3317296429

Gcorr [kcal/mol] = 55.906

H	-0.00001463	1.54592294	-2.09195726
C	-0.00002880	0.78356704	-1.32021012
C	-0.00004714	-0.78356579	-1.32021108
H	-0.00004596	-1.54591106	-2.09196900
C	-0.00002799	-0.79879285	0.01683076
C	-0.00002547	0.79879214	0.01683199
C	0.00001149	1.81672084	1.09549038
H	0.88093339	1.71360116	1.74603940
H	0.00016108	2.83081731	0.68028324
H	-0.88104987	1.71385976	1.74590469
C	0.00002248	-1.81673370	1.09547614
H	0.88091123	-1.71356353	1.74606288
H	0.00023283	-2.83082553	0.68026891
H	-0.88103263	-1.71388872	1.74590791

int2_13

E [Hartrees] = -233.3323853491

C	0.83769220	0.46390251	-0.11848317
C	-0.83621065	-0.46742659	0.67741608
C	-0.69721571	0.74410086	0.12664239
C	0.69868252	-0.74764406	0.43226628
C	1.56661550	-1.91296587	0.72353241
C	-1.56534973	1.90921348	-0.16490658
H	-1.65924981	-1.02496969	1.11103677
H	1.66062835	1.02119877	-0.55250483

H	1.57407718	-2.14133135	1.79944296
H	2.59804986	-1.73314034	0.40129431
H	1.19767167	-2.81708670	0.21725503
H	-1.57307831	2.13725281	-1.24090020
H	-1.19663653	2.81354900	0.34111978
H	-2.59667877	1.72918670	0.15743418

int3bhh_12
E [Hartrees] = -350.0114949258
Gcorr [kcal/mol] = 90.224

C	1.28678596	-0.29630031	0.10642370
C	-0.08552374	0.29704693	-0.15741346
C	-1.26485069	-0.46548835	0.47914666
C	-1.79052478	-0.78692931	-0.77921338
C	-0.76868516	-0.11615774	-1.47008268
C	2.32669382	0.35843323	0.57925976
C	2.71372727	1.71306293	1.01033284
H	1.36717259	-1.36308271	-0.11715471
H	-0.08515468	1.37762607	0.04044614
C	-1.61394877	-0.74764615	1.89315225
C	-3.00398882	-1.55108753	-1.20843770
H	-0.50919382	0.02494225	-2.51311115
H	3.55004527	2.10135209	0.41428695
H	3.03001551	1.72613560	2.06162044
H	1.87620889	2.42443262	0.90774732
H	-3.78039753	-0.87734501	-1.59301224
H	-3.43520695	-2.11308149	-0.37281764
H	-2.76342491	-2.26013946	-2.00910067
H	-0.75540267	-1.16915628	2.43526467
H	-2.44717873	-1.45627761	1.96734343
H	-1.90512847	0.16632805	2.43433423

int3bhh_13
E [Hartrees] = -349.9715688798
Gcorr [kcal/mol] = 89.194

C	1.15627704	-0.17215406	0.14503515
C	-0.16710929	0.62685648	0.01546682
C	-1.33209701	-0.28454061	0.58135247
C	-1.82073755	-0.46002610	-0.68712767
C	-0.84680162	0.41744018	-1.27686125
C	2.31363092	0.29091074	0.55708647
C	2.89796548	1.64691826	0.59054773
H	0.94924639	-1.24401067	0.02147319
H	-0.06110480	1.65104284	0.38951145

C	-1.64628261	-0.75109724	1.94890856
H	-2.62968375	-1.06082561	-1.09551893
C	-0.50336896	0.82146389	-2.65790941
H	3.65827911	1.74679123	-0.19764959
H	3.40130229	1.86322043	1.54142780
H	2.15294701	2.45049125	0.40728756
H	-2.04247781	0.07521078	2.56079218
H	-0.74208523	-1.10722707	2.45851572
H	-2.39214935	-1.55319931	1.94340242
H	0.07797717	1.75100489	-2.66808727
H	-1.40447875	0.95675492	-3.26919600
H	0.10784113	0.05495595	-3.16375028

int3bhme_12
E [Hartrees] = -349.9597177441
Gcorr [kcal/mol] = 88.996

C	1.00226191	-0.24773485	0.32652751
C	-0.20943214	0.63090246	-0.01066529
C	-1.46690364	-0.04656673	0.56476483
C	-1.85833946	-0.46429394	-0.71367804
C	-0.78377184	0.16151681	-1.35021040
C	2.18283101	0.10157276	0.80628495
C	3.02640760	1.22041502	1.24418469
H	0.78812146	-1.30340252	0.12420980
C	-0.04928625	2.12388996	0.21885189
C	-1.94332769	-0.24167277	1.95334025
H	-2.68128866	-1.08070790	-1.06721951
H	-0.38345537	0.16801033	-2.35723165
H	0.16326382	2.33614066	1.27328045
H	-0.96758011	2.65019957	-0.06212517
H	0.77573642	2.52520889	-0.38026315
H	-1.18948678	-0.75446937	2.56720755
H	-2.86521781	-0.83233153	1.98127239
H	-2.13919451	0.72205275	2.44940639
H	3.37326824	1.07053265	2.27647691
H	2.52568734	2.20615163	1.21368187
H	3.92646050	1.29927579	0.61821881

int3bmeh_12
E [Hartrees] = -350.0056556312

C	1.25114417	-0.22304507	-0.27566614
C	-0.17751845	0.25689378	-0.03001978
C	-1.18697336	-0.76016999	0.52863746
C	-1.97303775	-0.68341241	-0.63326792

C	-1.12368719	0.24351475	-1.24954132
C	2.28036101	0.50297636	0.11116804
H	2.41705285	1.44850943	0.62361136
C	1.41278599	-1.54722369	-0.99216380
H	-0.16156703	1.21472561	0.50670954
H	-1.24319129	-1.31051255	1.46085278
C	-3.25319685	-1.32972218	-1.06208609
C	-1.06670784	0.94395915	-2.55585851
H	2.46735302	-1.80318149	-1.12079093
H	0.93643610	-1.51480229	-1.98030709
H	0.91945950	-2.35030351	-0.43107074
H	-4.08830144	-1.01722610	-0.42289685
H	-3.18565846	-2.42229295	-0.99605738
H	-3.50417602	-1.06701408	-2.09535559
H	-1.13325616	2.03612313	-2.43703591
H	-1.88353447	0.62863498	-3.21534266
H	-0.11585803	0.74738951	-3.07313867

int3bmeme_12
E [Hartrees] = -350.0001699868
Gcorr [kcal/mol] = 90.795

C	1.21060936	-0.26092209	-0.10133485
C	-0.09624791	0.53239893	-0.26331124
C	-1.26754975	-0.01984736	0.59385115
C	-1.98248370	-0.37391270	-0.55292133
C	-0.99345759	0.07705638	-1.43421706
C	2.36479929	0.32223113	0.14963746
H	2.74404167	1.32637183	0.28510880
C	1.11112888	-1.77011806	-0.22529645
C	0.08591420	2.04850483	-0.15805174
C	-1.44799184	-0.10462074	2.06302675
H	-2.96016232	-0.82747000	-0.69894546
H	-0.87513780	0.11995884	-2.51051045
H	2.08673132	-2.24079279	-0.08065253
H	0.72606042	-2.05336212	-1.21215067
H	0.41205935	-2.17842116	0.51501381
H	0.49976900	2.32890262	0.81810101
H	-0.87876967	2.55134761	-0.28033923
H	0.76799322	2.41816650	-0.93237801
H	-1.41114517	0.89001641	2.53251623
H	-0.64505355	-0.69507140	2.52962252
H	-2.40653337	-0.56630568	2.32413908

int4crbhhh_12

E [Hartrees] = -349.9745794653

C	0.90732819	-0.23979883	-0.18642048
C	-0.28592320	0.67659798	0.31061507
C	-1.50748803	-0.20846600	0.54279636
C	-1.51844328	-0.61512310	-0.74466481
C	-0.26658118	0.19259050	-1.10212120
C	2.14116956	0.47206384	0.03498869
C	2.34862891	1.70886508	-0.76691162
H	0.85049151	-1.26134222	0.19274933
H	-0.10817488	1.68661223	0.66479309
C	-2.23926931	-0.57298103	1.78734151
C	-2.29347683	-1.61547627	-1.52984170
H	-0.10817657	0.79766062	-1.98856625
H	-1.63314283	-2.40468517	-1.91536502
H	-2.77973502	-1.15552008	-2.40047065
H	-3.07131550	-2.08579537	-0.91822912
H	2.95851256	2.45169650	-0.23910432
H	1.49071827	2.20993531	-1.24975766
H	2.99329653	1.33613193	-1.58622984
H	-2.73582153	0.29760268	2.23644292
H	-1.55175213	-0.97381989	2.54473178
H	-3.00541800	-1.33003848	1.58653847

int4crbhhme_12

E [Hartrees] = -349.9671586449

C	0.90957045	-0.20811443	-0.04429200
C	-0.27728481	0.70739355	0.41743238
C	-1.52178024	-0.19742843	0.57235245
C	-1.49021650	-0.57859839	-0.71687178
C	-0.26695981	0.27502901	-1.00769882
C	2.19158411	0.16096873	-0.58489977
C	2.46105697	1.58743147	-0.91449931
H	0.80754849	-1.24909401	0.26798896
C	-0.15886958	2.05252037	1.08209539
C	-2.30833712	-0.55541752	1.78314519
H	-2.01271538	-1.32927315	-1.30113680
H	-0.04551755	0.86240223	-1.89199500
H	2.99131638	1.94896940	-0.01206506
H	1.62917109	2.28990530	-1.09426163
H	3.18877033	1.68288564	-1.72977707
H	-0.15563195	1.92965495	2.17251994
H	-1.01773565	2.68513047	0.82288406
H	0.75131973	2.58899617	0.81190567
H	-2.75609634	0.33476706	2.24507823

H	-1.66274817	-1.01513141	2.54437755
H	-3.11340372	-1.25778936	1.54315007

int4crbhmeh_12
E [Hartrees] = -349.9692196252
Gcorr [kcal/mol] = 91.923

C	0.96150302	-0.22805418	-0.17636755
C	-0.19760844	0.68839858	0.32355348
C	-1.43474843	-0.16277605	0.56546803
C	-1.45365403	-0.64641302	-0.69116079
C	-0.25688899	0.22603772	-1.10045615
C	2.23877670	0.16987347	-0.71045409
C	2.59118968	1.60987465	-0.61895747
H	0.87590347	-1.27523192	0.11769371
H	-0.01772002	1.70266300	0.66351387
H	-1.97738057	-0.41738716	1.47219345
C	-2.19598184	-1.69512977	-1.44247466
C	-0.17449257	0.98526964	-2.39543088
H	3.27389484	1.60490878	0.25336798
H	1.81550774	2.36566133	-0.40305262
H	3.21362538	1.94385720	-1.45838244
H	-0.03582052	0.30276951	-3.24233232
H	0.64051528	1.71259558	-2.41229858
H	-1.11655241	1.52557502	-2.55234978
H	-2.97795869	-2.14630476	-0.82243680
H	-1.51930015	-2.49353118	-1.77683532
H	-2.67058311	-1.28388299	-2.34367913

int4crbhmeme_12
E [Hartrees] = -349.9594504730
Gcorr [kcal/mol] = 91.897

C	0.91186027	-0.16518888	-0.10800742
C	-0.29857903	0.74649324	0.36155383
C	-1.49757362	-0.18640089	0.55298914
C	-1.46329157	-0.62406113	-0.71546275
C	-0.29233059	0.29515860	-1.06627867
C	2.22513643	0.15146091	-0.59792023
C	2.70107539	1.55098577	-0.70601462
H	0.78923546	-1.20607393	0.19361430
C	-0.20298221	2.12066348	0.97058630
H	-2.05405240	-0.47714371	1.44023139
H	-1.95582561	-1.41485073	-1.27263668
C	-0.17289266	1.06968877	-2.34808873
H	3.31016221	1.64377701	0.21484850

H	2.00245619	2.40265972	-0.70603939
H	3.41850227	1.67367785	-1.52723230
H	0.11161167	2.06201282	2.01983403
H	-1.18590921	2.60725372	0.94554196
H	0.50296608	2.77108436	0.45175288
H	0.04920065	0.40530368	-3.19121588
H	0.60082704	1.83942548	-2.30995213
H	-1.13145862	1.56195212	-2.55341554

int5crbhhh_12

E [Hartrees] = -349.9791225422

C	0.84706876	-0.17047541	0.36867817
C	-0.40428943	0.70230239	0.62606080
C	-1.65642294	-0.19024825	0.61982719
C	-1.42579607	-0.61679145	-0.63704585
C	-0.17238430	0.25473636	-0.76718154
C	2.08358776	0.53126093	0.15738862
C	3.27881534	-0.33170945	0.34392854
H	0.78283510	-1.22571737	0.67553823
H	-0.29074205	1.71035872	1.00829950
C	-2.61360560	-0.54408330	1.70420133
C	-2.00411023	-1.65052087	-1.53966356
H	0.16060360	0.85726666	-1.60321757
H	-1.25663170	-2.41505045	-1.79276175
H	-2.34633521	-1.21442175	-2.48767134
H	-2.85954366	-2.14997708	-1.07131744
H	4.12136091	-0.04204663	-0.29604840
H	3.14106689	-1.42934577	0.31936813
H	3.60146544	-0.07255759	1.37144066
H	-3.18340681	0.33218919	2.04111063
H	-2.08248538	-0.93403107	2.58369407
H	-3.32949089	-1.30317959	1.36981938

int5crbhhme_12

E [Hartrees] = -349.9768035864

C	0.86689269	-0.33879039	-0.02811769
C	-0.26740216	0.61608225	0.44211710
C	-1.56465515	-0.21659479	0.55792248
C	-1.53578511	-0.55788000	-0.74193876
C	-0.26305357	0.24050990	-0.99491938
C	2.11150239	0.24459511	-0.43294371
C	3.19473808	-0.75717170	-0.60978924
H	0.74527369	-1.40608164	0.21028833
C	-0.01223203	1.95698431	1.07121559

C	-2.38911717	-0.56466891	1.74635657
H	-2.09739058	-1.25269447	-1.35867734
H	0.00014472	0.86786261	-1.83763239
H	3.77855294	-0.65181304	0.32509487
H	3.89646102	-0.48937950	-1.40934013
H	2.91082319	-1.82307069	-0.69447936
H	0.08755586	1.86902066	2.16086208
H	-0.84260309	2.64310104	0.86344064
H	0.91073537	2.38294840	0.67067006
H	-2.79554481	0.33596527	2.22562099
H	-1.78161673	-1.07787589	2.50483335
H	-3.22673260	-1.21593842	1.47531362

int5crbhmeme_12
E [Hartrees] = -349.9730527746
Gcorr [kcal/mol] = 91.834

C	0.86872313	-0.35468692	-0.26409397
C	-0.22232922	0.60883551	0.35449053
C	-1.49687802	-0.22804575	0.52824218
C	-1.57399792	-0.50036478	-0.78247139
C	-0.31168592	0.31016341	-1.09886024
C	2.17050672	0.20707440	-0.48100788
C	3.30135945	-0.74505506	-0.34053811
H	0.72524119	-1.42161480	-0.04314646
C	0.10828968	1.89705014	1.05325964
H	-2.02599823	-0.57058997	1.41304056
H	-2.18969359	-1.15434086	-1.39339558
C	-0.09171951	1.20610645	-2.28401885
H	3.69130625	-0.57120850	0.67951678
H	4.13757306	-0.50338553	-1.00889211
H	3.06245884	-1.82198731	-0.41402785
H	0.31621593	1.72714300	2.11740450
H	-0.73909392	2.59037060	0.98396912
H	0.98838157	2.36140921	0.60251158
H	0.81984588	1.79406715	-2.15562864
H	-0.94500219	1.88572019	-2.40131834
H	0.00203496	0.62320020	-3.20898971

int6hh_124
E [Hartrees] = -350.0966135498
Gcorr [kcal/mol] = 93.856

C	-1.30234622	1.24772937	-0.26580002
C	-1.29603871	-0.09285709	-0.35482002
C	-0.00283479	-0.26365844	0.44356765

C	-0.00746078	1.30028393	0.55921968
C	1.31964078	-0.09076648	-0.31293089
C	1.31594106	1.25159305	-0.21130794
H	-1.93064105	-0.80525622	-0.87682025
H	-0.01511481	-0.89502311	1.33781602
C	2.18919104	-1.09204274	-0.99333861
C	-2.15352221	2.34418410	-0.81001699
H	-0.03189577	1.79794211	1.53468348
C	2.18612957	2.34757414	-0.72758177
H	1.62331228	-1.64167306	-1.75905589
H	2.57344107	-1.83957792	-0.28609770
H	3.04752950	-0.61684136	-1.48225986
H	2.56096924	2.98184828	0.08716914
H	1.62881217	3.00493212	-1.40977941
H	3.05115799	1.95178250	-1.27224315
H	-1.56894031	3.00012678	-1.47022546
H	-2.54993809	2.97872292	-0.00588482
H	-3.00050172	1.95118954	-1.38322106

int6hme_123

E [Hartrees] = -350.0930048154

C	-1.29710096	1.25330344	-0.21160151
C	-1.29731678	-0.08693951	-0.28067248
C	0.02200698	-0.23217552	0.50109191
C	0.02524737	1.34096902	0.55308077
C	1.31175127	-0.09074263	-0.32920805
C	1.31792511	1.24949265	-0.26032758
C	-2.16649820	-1.12436715	-0.90575929
C	0.04393879	-1.09788498	1.74688075
C	2.15402261	-1.13059286	-0.98627718
H	-1.95433834	2.01808154	-0.61865216
H	0.04392655	1.86563187	1.51353731
H	1.96169810	2.01236545	-0.69173241
H	-2.50802771	-1.85762564	-0.16248135
H	-1.61546987	-1.68651695	-1.67282926
H	-3.04977513	-0.68090735	-1.37823032
H	0.94491777	-0.90663782	2.34164355
H	0.03695905	-2.16432831	1.48460586
H	-0.83318403	-0.90348347	2.37539930
H	1.57164798	-1.69444750	-1.72850336
H	2.52528609	-1.86222852	-0.25570272
H	3.01758521	-0.68913355	-1.49564795

int6hme_124

E [Hartrees] = -350.0930198970

C	-1.28951780	1.26058914	-0.20073476
C	-1.29993597	-0.07982561	-0.26837000
C	0.01611903	-0.23631610	0.51982451
C	0.03202211	1.33745098	0.56329409
C	1.30322506	-0.10357509	-0.30262727
C	1.32425969	1.23803379	-0.26161806
C	-2.16777013	-1.11152622	-0.90204847
C	0.01352625	-1.09001565	1.77422249
H	1.92807450	-0.84389749	-0.79794195
H	-1.93851382	2.03074706	-0.61083661
H	0.06387605	1.87200154	1.51856548
C	2.17947828	2.30682464	-0.85013754
H	-2.53126183	-1.83646732	-0.16097898
H	-1.60309463	-1.68346756	-1.65212767
H	-3.03662678	-0.66379708	-1.39675169
H	0.91205632	-0.90678667	2.37459409
H	-0.00645777	-2.15831030	1.52115521
H	-0.86703045	-0.87680142	2.39217691
H	3.01856607	1.88881327	-1.41707822
H	2.58643666	2.96685754	-0.07229376
H	1.59038461	2.94234201	-1.52657659

int6meme_124

E [Hartrees] = -350.0887174514

Gcorr [kcal/mol] = 94.308

C	-1.32522931	1.20284713	-0.17487051
C	-1.29437278	-0.13515204	-0.21944881
C	0.04449819	-0.25162566	0.52064359
C	0.00764599	1.33315624	0.57794108
C	1.30442997	-0.07158943	-0.34596820
C	1.27189584	1.26782134	-0.28654774
H	-1.94365178	-0.88756595	-0.66128358
C	0.13387030	-1.11169677	1.76744537
C	2.15495974	-1.09017026	-1.02360636
H	-2.00869956	1.95166848	-0.56865341
C	0.04073004	2.09850443	1.88793798
H	1.88043862	2.04810534	-0.73893627
H	1.04733029	-0.89018146	2.33222302
H	0.15238820	-2.17801791	1.50709815
H	-0.72734656	-0.94422115	2.42442276
H	1.55978525	-1.67861848	-1.73641623
H	2.57638263	-1.80272230	-0.30154748
H	2.98390125	-0.62774884	-1.57037066

H	0.95955663	1.88171766	2.44512362
H	-0.81734027	1.83804551	2.51868822
H	0.00680531	3.18089063	1.70868027

int7hh_124
E [Hartrees] = -350.0516012745
Gcorr [kcal/mol] = 93.731

C	-1.33722745	1.44681564	-0.25689534
C	-1.16985911	0.02752440	-0.71547212
C	-0.19432946	-0.56218394	0.02102366
C	-0.07700790	1.97551121	-0.26018573
C	1.15820467	-0.19174674	-0.51292084
C	1.17548763	1.18285628	-0.53404837
H	-1.06449340	-0.04247708	-1.80694179
H	-0.26589125	-0.42530573	1.10878147
C	2.30471774	-1.13909028	-0.69518798
C	-2.61158618	2.22122418	-0.12650314
H	0.05444825	3.05333611	-0.14178477
C	2.41451058	2.01844883	-0.75715908
H	2.06164446	-1.89039147	-1.45763890
H	2.49178924	-1.69262552	0.23600577
H	3.23541977	-0.64765050	-0.99192988
H	2.62222060	2.64856283	0.11847593
H	2.27425188	2.69910986	-1.60770030
H	3.30442442	1.41727967	-0.95413737
H	-2.42743967	3.28589323	0.05556266
H	-3.22550880	1.83185940	0.69599811
H	-3.21596931	2.12364719	-1.03920652

int7hme_123
E [Hartrees] = -350.0485123808
Gcorr [kcal/mol] = 93.591

C	-1.07747896	1.08949310	-0.83625678
C	-1.34293897	-0.16246955	-0.06239665
C	-0.11322984	-0.76693254	0.02574610
C	-0.21963528	1.91491679	-0.16924253
C	1.14238894	0.02103083	-0.32138303
C	1.13652401	1.39602993	-0.42080584
C	-2.68241717	-0.67078429	0.37220929
C	0.07752549	-2.19051800	0.50003790
C	2.44914704	-0.73173903	-0.39341861
H	-0.76061018	0.86627628	-1.86284874
H	-0.43405866	2.19820429	0.86896233
H	2.07071969	1.95881106	-0.39240939

H	-3.20364103	0.09899209	0.95576109
H	-2.62475566	-1.57543427	0.98386260
H	-3.31924725	-0.88387611	-0.49791708
H	0.69161203	-2.23710101	1.40943334
H	0.58648454	-2.80086428	-0.25664387
H	-0.87531881	-2.67641584	0.72008499
H	2.42437866	-1.48808207	-1.18939512
H	2.67175645	-1.26499788	0.53883830
H	3.28125414	-0.05344940	-0.60382380

int7hme_124
E [Hartrees] = -350.0513473386
Gcorr [kcal/mol] = 92.345

C	-1.06735792	1.10403159	-0.15284108
C	-1.04804797	-0.24783764	-0.33649065
C	0.26379312	-0.78680734	0.14784887
C	0.10437057	1.88643839	0.35290654
C	1.28863052	0.01240215	-0.37684182
C	1.34392490	1.32510061	0.34169934
C	-2.24455110	-1.08428507	-0.68155468
C	0.30359339	-1.32516139	1.55892631
H	1.21615017	0.16836128	-1.46332599
H	-1.99931827	1.65347291	-0.29500779
C	-0.16179467	3.29020241	0.83278297
H	2.23367703	1.86803096	0.65598071
H	-2.44975903	-1.80886274	0.11903782
H	-2.06709930	-1.66927581	-1.59328869
H	-3.14255424	-0.47520179	-0.83258047
H	1.32373974	-1.30843876	1.95469954
H	-0.04222757	-2.36845606	1.57955399
H	-0.34992906	-0.75956541	2.23837386
H	-0.89884346	3.29701433	1.64751858
H	-0.57503560	3.91328449	0.02794362
H	0.75239297	3.76925514	1.19696781

int7meme_124
E [Hartrees] = -350.0513312807
Gcorr [kcal/mol] = 92.250

C	-1.06838740	1.10324729	-0.14445435
C	-1.05907852	-0.24789462	-0.33677316
C	0.25087726	-0.78594650	0.15575853
C	0.11236346	1.87906464	0.35562049
C	1.27388947	-0.00249200	-0.37973703
C	1.34936341	1.31109659	0.33677341

C	-2.25831760	-1.07570677	-0.69057068
C	0.30118538	-1.31632681	1.56857273
H	1.18286715	0.15973122	-1.46396649
H	-1.99736211	1.65957914	-0.28045391
C	-0.14269198	3.28581337	0.83293784
H	2.24475877	1.85228995	0.63802104
H	-2.47093487	-1.80199076	0.10665119
H	-2.07897875	-1.65871432	-1.60322439
H	-3.15211740	-0.46122676	-0.84484743
H	1.27622197	-1.11427065	2.02483710
H	0.16290337	-2.40754866	1.56974197
H	-0.48737946	-0.89341198	2.20524721
H	-0.86981729	3.29829871	1.65648050
H	-0.56323763	3.90773214	0.03101276
H	0.77762696	3.76237903	1.18468146

proprgyl
E [Hartrees] = -116.6545140176
Gcorr [kcal/mol] = 20.084

H	-1.12546150	-0.00000278	0.00017423
C	-0.05923979	0.00000275	0.00007809
C	1.14788250	0.00000113	-0.00002367
C	2.60835984	-0.00000005	-0.00004056
H	3.00459121	-0.00000062	1.02260168
H	3.00463308	-0.88561724	-0.51134515
H	3.00463465	0.88561681	-0.51134462

ts1b_14zez
E [Hartrees] = -233.2646319663
Gcorr [kcal/mol] = 51.887

H	-2.26885628	-2.63550461	-2.41233503
C	-1.81285084	-2.41536352	-1.45950230
C	-1.28679230	-1.41450212	-0.90173523
C	-0.63384940	-0.82962129	0.26653155
H	-1.20852690	0.01035414	0.67612681
H	-0.52814054	-1.58184791	1.07052713
H	0.37123073	-0.45986956	0.02846704
C	-1.87085562	-3.96580560	-0.47722206
H	-1.41457826	-3.74583162	0.47551394
C	-2.39728112	-4.96655700	-1.03489254
C	-3.05066469	-5.55099875	-2.20315842
H	-3.15507679	-4.79894680	-3.00750353
H	-2.47703769	-6.39192798	-2.61227810
H	-4.05632423	-5.91925847	-1.96522239

ts1c
E [Hartrees] = -233.2337390267
Gcorr [kcal/mol] = 52.862

C	-1.84404367	1.41714980	-0.29106545
C	-1.02747514	0.51041964	0.04694576
C	0.10607294	3.00273941	-0.63352919
C	-0.91125696	2.60541163	0.13279901
C	0.21266266	-0.20000105	0.28978680
C	0.71730819	4.35599940	-0.45733666
H	-2.85472001	1.51360208	-0.66722556
H	-1.17588648	2.93391855	1.14457157
H	0.43660819	-0.28627355	1.35981544
H	1.01636754	0.36103792	-0.21470128
H	0.17515727	-1.21238190	-0.13454059
H	0.41557097	4.92122479	0.44479077
H	0.43699000	4.96728030	-1.32873757
H	1.81390201	4.30129347	-0.48665568

ts2b_14eee_eze
E [Hartrees] = -233.2639493271
Gcorr [kcal/mol] = 53.237

H	-2.57929405	-2.55970275	-2.13485692
C	-1.76339461	-2.62897680	-1.39948452
C	-0.74148026	-1.80983129	-1.50405259
C	-0.26900897	-0.70828008	-2.35977098
H	0.69418408	-0.94667983	-2.82924458
H	-0.99100356	-0.49574923	-3.16708630
H	-0.13154782	0.21659517	-1.78490492
C	-1.91252879	-3.69874834	-0.35719427
H	-1.43169609	-4.66172352	-0.58692050
C	-2.58056680	-3.57328232	0.76719093
C	-2.93835478	-4.36696435	1.95498062
H	-2.51826374	-5.38571793	1.89250715
H	-2.55754277	-3.90648200	2.87567234
H	-4.02649823	-4.46212007	2.06383336

ts2b_14eez_eee
E [Hartrees] = -233.2665478795
Gcorr [kcal/mol] = 53.103

H	-2.25524855	-2.60275786	-2.36155545
C	-1.81952404	-2.56844444	-1.35415175
C	-1.29766829	-1.43357998	-0.91951239
C	-1.08034054	-0.05295019	-1.37829948

H	-0.01337571	0.20691157	-1.39206170
H	-1.47069287	0.08975222	-2.40083246
H	-1.58330154	0.67483217	-0.72754176
C	-1.87065941	-3.82952059	-0.58428331
H	-1.42742032	-3.76374297	0.41895342
C	-2.38571534	-4.96071422	-1.00629734
C	-2.96829484	-6.19342210	-1.50569478
H	-2.96792303	-7.00560317	-0.75698862
H	-4.01472855	-6.05081648	-1.81543036
H	-2.41917122	-6.57027528	-2.38112973

ts2b_14zez_eez
E [Hartrees] = -233.2698790833
Gcorr [kcal/mol] = 53.061

H	-2.23890419	-2.62459371	-2.34679457
C	-1.80421855	-2.55360106	-1.34003335
C	-1.29177814	-1.44065835	-0.89874829
C	-0.73482078	-0.17282082	-0.46270399
H	0.33171138	-0.26648910	-0.21117883
H	-0.81265362	0.61497595	-1.23300387
H	-1.24904923	0.20649440	0.43237488
C	-1.86467905	-3.84102392	-0.55481856
H	-1.44127328	-3.79844107	0.44663265
C	-2.38899245	-4.95717296	-1.02483554
C	-3.03598992	-5.43529255	-2.25600713
H	-2.47742492	-6.26257126	-2.71317879
H	-4.05602085	-5.79399303	-2.06558178
H	-3.10385652	-4.62644598	-3.00658163

ts2c_12
E [Hartrees] = -233.2479038800

C	-1.97033456	1.30463068	-0.28549507
C	-0.75080141	0.97182786	-0.06239850
C	-0.14662030	2.99114615	-0.84330808
C	-1.15734025	2.54451673	0.04060782
C	0.37327306	0.08236245	0.27919019
C	0.78483819	3.98685309	-0.20969121
H	-2.99942737	1.01577689	-0.42842142
H	-1.33608031	2.97911397	1.04134673
H	0.71502339	0.28118593	1.30275973
H	1.21686396	0.25195495	-0.39742197
H	0.06488565	-0.96705182	0.21276315
H	0.53307994	4.37641793	0.79635266
H	0.89219000	4.83656324	-0.89979101

H 1.79190410 3.54537585 -0.16296846

ts2c_13
E [Hartrees] = -233.2463994817
C 0.82355501 0.93046953 0.11080559
C -0.40640491 1.23456402 -0.11134826
C -0.99771786 -0.76063399 0.68521961
C 0.00627355 -0.30994696 -0.21447910
H -1.21793392 1.89652541 -0.36401855
C -1.93463748 -1.75689397 0.05909784
C 2.23778274 1.29205394 0.33469715
H 0.18735278 -0.75085326 -1.21176752
H -1.79264239 -2.02229383 -1.00627718
H -1.82904952 -2.67639972 0.65760954
H -2.97839977 -1.45032679 0.21020707
H 2.86793194 0.87092636 -0.45839750
H 2.37703267 2.37713355 0.35663322
H 2.58818970 0.86892441 1.28456660

ts3b_14eze
E [Hartrees] = -233.2686878936
Gcorr [kcal/mol] = 52.051
H -1.68958932 -3.29865503 -2.80358512
C -1.68166269 -3.04237038 -1.73769597
C -1.17063607 -1.90664283 -1.27234484
C -0.51088000 -0.68207011 -1.74446939
H 0.49062156 -0.56381540 -1.30880431
H -0.39659026 -0.70023628 -2.84223930
H -1.08613982 0.21737101 -1.48591334
C -2.23757906 -3.93370844 -0.71909617
H -2.68796481 -4.90031942 -0.97344267
C -2.15395275 -3.48259086 0.52873793
C -2.50134667 -3.87263376 1.90167457
H -2.99323118 -4.86077814 1.91264803
H -1.61326196 -3.93722181 2.54501706
H -3.18939808 -3.15465695 2.36844287

ts4bcrbhh_12
E [Hartrees] = -349.9684759147
Gcorr [kcal/mol] = 90.582
C 0.97296774 -0.13889964 0.13485302
C -0.30033468 0.69230525 0.28674909
C -1.51803486 -0.22527746 0.52443307
C -1.50883093 -0.63890701 -0.77543350

C	-0.36213500	0.23096216	-1.11594047
C	2.23686704	0.42345098	0.03189548
C	2.54120097	1.70645472	-0.65396523
H	0.86046427	-1.18538405	0.41903240
H	-0.22603443	1.72578982	0.62071951
C	-2.23139976	-0.62745388	1.76633268
C	-2.23828339	-1.69035319	-1.54336989
H	0.00151643	0.68876666	-2.02692272
H	-1.54565006	-2.45982211	-1.90951963
H	-2.74501915	-1.27062995	-2.42203623
H	-2.99457636	-2.18121274	-0.92118345
H	3.31675834	2.27778967	-0.12765233
H	1.67473690	2.37031076	-0.82206136
H	2.95946439	1.47539515	-1.64709501
H	-2.77206402	0.21735841	2.21553118
H	-1.52964802	-0.99372781	2.52860249
H	-2.95951526	-1.42110518	1.56405377

ts4bhh_12
E [Hartrees] = -349.9676328141
Gcorr [kcal/mol] = 87.053

C	1.33596122	-0.23491403	0.05066253
C	-0.58265835	0.70575053	-0.21129782
C	-1.47450049	-0.31951249	0.47787614
C	-1.95173036	-0.74206180	-0.75898163
C	-1.16217448	0.28379727	-1.45149599
C	2.26066298	0.43893760	0.52732260
C	3.03490250	1.56109069	1.04837693
H	1.01018537	-1.20261955	-0.28458872
H	-0.29806082	1.70194000	0.11191280
C	-1.63624284	-0.73826977	1.89209822
C	-2.87691260	-1.82061630	-1.20772437
H	-1.06232540	0.60207995	-2.48236798
H	3.91803197	1.75849905	0.42741554
H	3.38761255	1.36791546	2.06948355
H	2.43701534	2.48569344	1.07350624
H	-3.74659502	-1.40964921	-1.73898848
H	-3.24808563	-2.40262568	-0.35698017
H	-2.38082177	-2.51286651	-1.90211145
H	-0.66294361	-0.98244119	2.34093408
H	-2.28623304	-1.61661333	1.97726780
H	-2.07304791	0.06315369	2.50669494

ts4bhme_12

E [Hartrees] = -349.9669509023
Gcorr [kcal/mol] = 87.168

C	1.12536341	-0.48993977	-0.77364710
C	-0.62053972	0.73739954	-0.52688806
C	-1.23575115	0.02618970	0.66852604
C	-2.16243205	-0.59036336	-0.17723805
C	-1.65139399	0.10827174	-1.33485166
C	2.23905131	0.04367842	-0.88962042
C	3.34982287	0.98000845	-1.02954253
H	0.59295391	-1.42181143	-0.70208160
C	-0.08028499	2.13118138	-0.60276775
C	-0.87488705	-0.02246109	2.10688594
H	-2.93858291	-1.33373521	-0.02306424
H	-1.92120106	0.15769800	-2.38280824
H	0.73349868	2.27546470	0.11608275
H	-0.86377719	2.87059533	-0.38236436
H	0.31039780	2.34252614	-1.60445539
H	0.17544605	-0.32143664	2.23519776
H	-1.50498480	-0.73153777	2.65469943
H	-0.98028085	0.96251209	2.58588610
H	3.97096195	0.73132201	-1.90006862
H	4.00125973	0.96127360	-0.14648200
H	2.99976728	2.01424184	-1.16192411

ts4bmeh_12
E [Hartrees] = -349.9632159238
Gcorr [kcal/mol] = 87.301

C	1.48119467	-0.37331361	-0.08758226
C	-0.40228816	0.68549842	-0.21201763
C	-1.35769430	-0.14609498	0.61371374
C	-2.02437215	-0.55621616	-0.53551553
C	-1.15974557	0.28781526	-1.37499828
C	2.29174364	0.23818782	0.63620410
H	2.58670496	1.06771047	1.24644613
C	1.23960397	-1.58395765	-0.90498823
H	0.00288258	1.66695887	0.00920217
H	-1.42788533	-0.38910445	1.66722796
C	-3.14852137	-1.48760282	-0.83504388
C	-1.08958913	0.59541931	-2.82677612
H	2.04124963	-2.31355854	-0.74979831
H	1.19934544	-1.33334224	-1.97143814
H	0.28353590	-2.04891816	-0.64158848
H	-3.54151463	-1.94305805	0.07976805
H	-2.82960690	-2.29576897	-1.50830344

H	-3.97630724	-0.96851735	-1.33779190
H	-0.37890050	1.40575542	-3.02173419
H	-2.06861427	0.89712999	-3.22555196
H	-0.76796456	-0.27603903	-3.41929169

ts4bmeme_12
E [Hartrees] = -349.9536069908

C	1.27176581	-0.36137380	-0.08487938
C	-0.27455465	0.71437273	-0.34875740
C	-1.30436558	-0.04396560	0.62153847
C	-1.96213059	-0.51549163	-0.46248506
C	-1.07696351	0.22732286	-1.39378496
C	1.93922996	-0.07473962	0.95203345
H	2.10823470	0.63996490	1.73756979
C	1.32219981	-1.42691896	-1.12841235
C	0.14935485	2.14835227	-0.19325848
C	-1.36706424	-0.19569795	2.09239784
H	-2.79441684	-1.20000531	-0.59842959
H	-1.08094160	0.40297702	-2.46464877
H	2.11188474	-2.15070201	-0.90247887
H	1.51531471	-0.98546246	-2.11339107
H	0.35867927	-1.94732854	-1.18657746
H	0.80869752	2.27231838	0.67445567
H	-0.72821238	2.79404221	-0.05888734
H	0.69392205	2.49279187	-1.08051365
H	-0.48633047	-0.73639651	2.46547146
H	-2.26712638	-0.73931927	2.39976557
H	-1.36676629	0.78522000	2.59014919

ts4concmehh_12
E [Hartrees] = -349.9733603275

C	1.64463934	0.34386460	-0.24694595
C	-0.36777772	0.72202132	-1.13669243
C	-0.93797961	0.79743600	0.33116261
C	-1.55825784	-0.39448979	0.11557329
C	-1.03417789	-0.46441419	-1.28698611
C	1.35173655	0.36611390	0.95129108
C	1.31321631	0.34915505	2.41567444
H	2.28988085	0.26360528	-1.09788867
H	-0.03150911	1.47921803	-1.83626211
H	-1.04785687	1.59526679	1.05584542
C	-2.37759573	-1.32618742	0.94011459
C	-1.13667866	-1.49000797	-2.36026208
H	-0.65598442	-2.43437672	-2.06386923

H	-0.65829880	-1.14484078	-3.28337783
H	-2.18447890	-1.72930081	-2.58952363
H	-1.86742698	-2.28957899	1.08300760
H	-3.33935422	-1.54809123	0.45746005
H	-2.58452984	-0.90219977	1.92883421
H	2.31263820	0.18568628	2.84440486
H	0.65173286	-0.44416741	2.78354387
H	0.93384843	1.29835591	2.81348537

ts4concmehme_12
E [Hartrees] = -349.9718301792

C	1.74188040	0.06896902	-0.23601326
C	-0.38719522	0.95738810	-0.82172885
C	-0.86671536	0.33420276	0.55940534
C	-1.53380310	-0.62135204	-0.16905091
C	-1.08802500	-0.02311650	-1.45420865
C	1.25623192	-0.40970987	0.79120940
H	1.22026630	-0.91219109	1.73580342
C	2.61705083	0.50400830	-1.32870774
H	0.01094177	1.92303860	-1.10991499
C	-1.09371459	0.94568754	1.90056836
C	-2.34543771	-1.81822764	0.18381504
H	-1.21485321	-0.30801548	-2.49482661
H	-0.17858080	1.38072573	2.31812603
H	-1.47367245	0.20035991	2.61000363
H	-1.84098937	1.75195815	1.83488124
H	-1.86585967	-2.74783663	-0.15614278
H	-3.33799785	-1.78418445	-0.28661514
H	-2.48920585	-1.89126018	1.26765493
H	2.63078231	1.59761011	-1.41336755
H	2.27135946	0.10824210	-2.29092873
H	3.65251385	0.16961363	-1.17266066

ts4concmemeh_12
E [Hartrees] = -349.9728062000
Gcorr [kcal/mol] = 89.033

C	1.78356573	0.03047504	-0.20627433
C	-0.40620343	1.00067582	-0.83076661
C	-0.84416008	0.31774393	0.53546286
C	-1.49700426	-0.62471124	-0.21395914
C	-1.04169851	-0.01191437	-1.49093890
C	1.24298446	-0.31215894	0.84835711
H	1.22476055	-0.74100308	1.83028727
C	2.63433248	0.32622208	-1.35805738

C	0.02577010	2.38204395	-1.16708175
H	-1.00348873	0.71193864	1.53335085
H	-2.06006278	-1.52152706	0.02533383
C	-1.20408321	-0.38025500	-2.92570877
H	2.59214741	1.38859700	-1.62688434
H	2.31623034	-0.24600682	-2.23795413
H	3.68665413	0.07917102	-1.15581618
H	0.87834726	2.70616645	-0.55855156
H	-0.79000340	3.09956650	-0.98431494
H	0.30403330	2.46326234	-2.22495048
H	-0.73152817	0.36118277	-3.57973436
H	-2.26466035	-0.44876237	-3.20435343
H	-0.75572506	-1.35994480	-3.14384112

ts4concmememe_12
E [Hartrees] = -349.9716120305
Gcorr [kcal/mol] = 89.263

C	1.77483709	0.03098843	-0.23246207
C	-0.38523395	1.01376755	-0.82532377
C	-0.84744232	0.34243791	0.55792304
C	-1.48030959	-0.61137335	-0.20163191
C	-1.02981322	-0.00218264	-1.46865157
C	1.24420187	-0.34843887	0.81426391
H	1.21481062	-0.78496279	1.79255105
C	2.64502893	0.35102010	-1.36427864
C	0.05046479	2.39318236	-1.16894009
C	-1.12172840	0.93016990	1.90320885
H	-2.05338710	-1.50016922	0.04360257
H	-1.13787927	-0.27284651	-2.51493450
H	-0.24013530	1.42359236	2.32825457
H	-1.45070117	0.15293902	2.60392433
H	-1.92426219	1.68067550	1.84418426
H	2.63311461	1.42418361	-1.58946675
H	2.31997932	-0.17605255	-2.26937694
H	3.68788481	0.06817539	-1.16163471
H	0.88311173	2.73008723	-0.54020711
H	-0.77325686	3.10907955	-1.02327700
H	0.35915389	2.45842534	-2.21930751

ts5bcrbhhh_12
E [Hartrees] = -349.9609597898
Gcorr [kcal/mol] = 90.477

C	0.97690010	-0.11549828	0.06908857
C	-0.31679766	0.71475390	0.14984823

C	-1.50532519	-0.24130173	0.50371143
C	-1.60348802	-0.63409654	-0.79571476
C	-0.52937079	0.28262164	-1.22073800
C	2.22923900	0.43662475	0.05021436
C	2.52157777	1.68326089	-0.70933327
H	0.79963516	-1.16000480	0.33949560
H	-0.23993803	1.74531607	0.49441296
C	-2.11960076	-0.63204447	1.79783919
C	-2.38892847	-1.67737265	-1.51785433
H	-0.16235882	0.66140632	-2.16544519
H	-1.72378949	-2.42110442	-1.97564322
H	-2.98952551	-1.24113913	-2.32634348
H	-3.06916163	-2.20036690	-0.83719213
H	3.07950938	2.39343187	-0.08395619
H	1.67664789	2.21177152	-1.18877105
H	3.22654935	1.40863616	-1.51046620
H	-2.68102872	0.20118558	2.24493268
H	-1.35591032	-0.92576261	2.53027005
H	-2.81321010	-1.47048758	1.66850030

ts5bcrbhhme_12
E [Hartrees] = -349.9591204964
Gcorr [kcal/mol] = 93.209

C	1.00155436	-0.25842590	-0.26527310
C	-0.49489934	0.81740708	0.40812341
C	-1.57813676	-0.19423310	0.60465410
C	-1.44793374	-0.65965470	-0.65833285
C	-0.26819232	0.30807265	-0.93731275
C	2.27990998	0.15954653	-0.58665932
C	2.57993321	1.57693435	-0.93035096
H	0.82387623	-1.24088340	0.17717758
C	-0.17757033	2.07711184	1.13337024
C	-2.37647638	-0.57073536	1.80616199
H	-1.85017068	-1.50421965	-1.20751321
H	-0.15092375	0.90107138	-1.84303798
H	3.02266472	2.02050663	-0.02120888
H	1.74451521	2.23758102	-1.22976368
H	3.36680051	1.64510952	-1.69228192
H	-0.01020824	1.89717318	2.20241705
H	-1.02425704	2.77667378	1.05238557
H	0.70564300	2.57383924	0.72929168
H	-2.95342456	0.28187640	2.18738616
H	-1.71983872	-0.90275835	2.62128691
H	-3.07605683	-1.38110754	1.57762626

ts5bcrbhmeh_12
E [Hartrees] = -349.9581034803
Gcorr [kcal/mol] = 89.309

C	1.05059443	-0.23577867	-0.36568135
C	-0.45268863	0.88370360	0.33487531
C	-1.51581666	-0.09697289	0.58654727
C	-1.40123077	-0.65095605	-0.64706543
C	-0.23283684	0.34923556	-1.00294158
C	2.33210790	0.18381689	-0.59718713
C	2.69980843	1.62049567	-0.71030422
H	0.84737805	-1.22459538	0.05805329
H	-0.10202046	1.78607351	0.81783423
H	-2.09205007	-0.35455658	1.47051228
C	-2.00440598	-1.77548445	-1.40464318
C	-0.20111583	1.09721259	-2.31315450
H	3.59320330	1.81530893	-0.09920555
H	1.93967986	2.37892595	-0.44811571
H	3.03650708	1.80356357	-1.74316772
H	0.06503728	0.42346953	-3.13599897
H	0.52178017	1.91764847	-2.29978909
H	-1.19106679	1.52086666	-2.51852911
H	-2.52123604	-1.41492831	-2.30604354
H	-2.73302541	-2.31823707	-0.79283263
H	-1.23989303	-2.48640383	-1.74520487

ts5bcrbhmeme_12
E [Hartrees] = -349.9544022430
Gcorr [kcal/mol] = 90.946

C	1.00167208	-0.22157480	-0.32016136
C	-0.42672341	0.84116199	0.37375342
C	-1.50284944	-0.15822506	0.61555914
C	-1.42011511	-0.66286768	-0.63321895
C	-0.28038749	0.33733827	-0.99465751
C	2.29868873	0.16730271	-0.60727361
C	2.73047001	1.58128518	-0.69206034
H	0.81740843	-1.22757920	0.06588584
C	-0.09806395	2.14550582	1.02596284
H	-2.05050509	-0.44110357	1.51055039
H	-1.83023960	-1.52054717	-1.15476574
C	-0.26291589	1.12533783	-2.27869114
H	3.20330070	1.78201549	0.28665412
H	1.97019425	2.37234065	-0.82714274
H	3.53024988	1.72018472	-1.43027257

H	0.72132909	2.06866540	1.75085547
H	-0.97731739	2.51182416	1.56975804
H	0.18665571	2.90741948	0.28997342
H	0.03739513	0.49192893	-3.12082468
H	0.42463812	1.97474572	-2.23315900
H	-1.26863876	1.51223626	-2.47936248

ts5bhhh_12
E [Hartrees] = -350.0058022285
Gcorr [kcal/mol] = 87.691

C	-2.44986448	0.26551827	0.42161560
C	0.60070380	-1.63605642	-0.92519174
C	1.53773796	-0.59648966	-0.88188370
C	0.82820298	0.11477652	0.09820977
C	-0.26222183	-0.96606003	0.15953346
C	-1.67664949	-0.57265777	-0.23227722
H	-2.05878368	-1.01922891	-1.16279860
H	-0.27692841	-1.52703988	1.10632573
H	0.94516666	1.06927011	0.59766501
C	2.82468324	-0.35732065	-1.60846231
C	0.44874528	-2.90432449	-1.68136463
C	-3.79354991	0.86114769	0.32821797
H	-4.41057821	0.61013975	1.20109442
H	-4.32419547	0.49913812	-0.56960249
H	-3.74795148	1.95645039	0.26614550
H	2.84081876	0.63817412	-2.06801327
H	2.97801003	-1.09889821	-2.40002940
H	3.68212161	-0.41346345	-0.92604245
H	0.48172569	-3.78328464	-1.01891838
H	1.24247634	-3.02035295	-2.42860929
H	-0.51667870	-2.95080979	-2.20781659

ts5bhhme_12
E [Hartrees] = -350.0075085535
Gcorr [kcal/mol] = 88.954

C	-2.47899785	-0.37743099	-0.39309615
C	0.51222439	-1.43510563	-0.77979023
C	1.66402442	-0.64979154	-0.93624783
C	1.24709831	0.30060316	0.00497819
C	-0.04765112	-0.47723329	0.28541710
C	-1.36324256	0.21302416	-0.02422733
H	-1.35819245	1.30914793	0.07257092
H	-0.08541884	-0.91918468	1.29356010
H	1.66715224	1.21478040	0.40961172

C	2.88837169	-0.80227042	-1.78423712
C	-0.05973230	-2.64954752	-1.40542478
C	-3.86679277	-0.02882014	-0.74449672
H	-4.11959033	-0.34546706	-1.76471739
H	-4.02636808	1.06185140	-0.68542773
H	-4.58808147	-0.50525134	-0.06751886
H	3.25745070	0.17077244	-2.12694596
H	2.68529878	-1.42114978	-2.66550303
H	3.70139678	-1.28297840	-1.22464363
H	-0.10504491	-3.49647403	-0.70287674
H	0.52377376	-2.96947581	-2.27685249
H	-1.09463344	-2.45866951	-1.72787780

ts5bhhpre_12
E [Hartrees] = -349.9575453588
Gcorr [kcal/mol] = 87.858

C	1.19792082	-0.21121853	0.07894970
C	-0.17383443	0.44767247	-0.08749596
C	-1.27648609	-0.42779897	0.51878845
C	-1.75717205	-0.75339842	-0.75890637
C	-0.82825098	0.06847965	-1.41460172
C	2.27069051	0.35520078	0.54484463
C	3.47287285	0.98343659	1.04146007
H	1.17310840	-1.26817475	-0.23820763
H	-0.15210810	1.50619921	0.19225923
C	-1.58895215	-0.83071509	1.91000285
C	-2.85380443	-1.65882890	-1.22773796
H	-0.53270289	0.21819512	-2.44618021
H	4.37013278	0.33861183	0.95069593
H	3.38571371	1.24170453	2.10738453
H	3.71134219	1.91048261	0.49467638
H	-3.65359409	-1.08967538	-1.71772461
H	-3.29811191	-2.21036016	-0.39212203
H	-2.48069161	-2.38770416	-1.95729660
H	-0.69192688	-1.18184395	2.43988276
H	-2.33367558	-1.63522982	1.93510848
H	-1.98831413	0.00796946	2.50479125

ts5bhmeh_12
E [Hartrees] = -350.0019977022
Gcorr [kcal/mol] = 89.890

C	-2.51395557	-0.34330472	-0.33502180
C	0.51383670	-1.45068032	-0.77307329
C	1.65157434	-0.65276023	-0.92381552

C	1.23176576	0.30133552	0.00746094
C	-0.06918206	-0.48955912	0.28264353
C	-1.35085697	0.23069042	-0.12175264
H	-1.27589412	1.32268328	-0.23376519
C	-0.17666082	-1.06678069	1.70171801
C	1.75580657	1.56772530	0.57566383
H	2.54636033	-0.73763646	-1.53643103
H	0.13751940	-2.36220539	-1.22135974
C	-3.89171808	0.00710478	-0.71741795
H	-1.01023377	-1.77597957	1.75974765
H	-0.36633675	-0.27072058	2.43271988
H	0.74832327	-1.58415603	1.98097188
H	1.87735391	1.50250279	1.66782217
H	1.07012719	2.40974906	0.39241158
H	2.72830830	1.82840157	0.14342590
H	-4.19275709	-0.49047852	-1.64862289
H	-3.99286448	1.09515174	-0.87412131
H	-4.61401937	-0.28471757	0.05618775

ts5bhmeme_12
E [Hartrees] = -350.0036494086
Gcorr [kcal/mol] = 89.441

C	-2.47271785	-0.36363766	-0.40695834
C	0.48335418	-1.44944563	-0.77427881
C	1.61242160	-0.64917209	-0.97320583
C	1.23263475	0.30359908	-0.02384159
C	-0.04976326	-0.48617876	0.31011205
C	-1.35352377	0.21899403	-0.03692383
H	-1.33632207	1.31544107	0.05527430
C	-0.10363930	-1.07911610	1.72655900
H	1.66354852	1.21696700	0.37008319
H	2.47364967	-0.74452603	-1.63057979
C	-0.09550355	-2.68702577	-1.34428777
C	-3.85450666	-0.01010961	-0.77452099
H	-4.09823798	-0.33452738	-1.79443503
H	-4.00933505	1.08179514	-0.72644344
H	-4.58469013	-0.47737215	-0.10074426
H	-0.16489864	-3.48958564	-0.59384930
H	0.49653193	-3.06221456	-2.18650710
H	-1.12350480	-2.50161557	-1.69262676
H	-0.29358379	-0.29714007	2.47192961
H	0.84238574	-1.57338230	1.97571528
H	-0.91657458	-1.81129479	1.79865613

ts6crbhhh_124
E [Hartrees] = -349.9706987375

C	0.99052699	-0.42217023	-0.42045665
C	-0.12850197	0.64974473	0.33155387
C	-1.33024155	-0.25253302	0.63183861
C	-1.49310793	-0.56543530	-0.67119672
C	-0.22439366	0.18514614	-1.09971568
C	1.84885655	0.48702651	0.18211956
C	2.74204987	-0.09372964	1.24203322
H	0.95800840	-1.50554208	-0.20101220
H	-0.04962468	1.68243070	0.64294702
C	-1.98182665	-0.62930921	1.91582063
C	-2.42734805	-1.43235104	-1.44064712
H	-0.11722891	0.84495989	-1.95632455
H	-1.88443111	-2.24952132	-1.93645757
H	-2.94038549	-0.86875635	-2.23110179
H	-3.19031765	-1.87296622	-0.78959044
H	3.76662632	-0.07999171	0.84142436
H	2.52376185	-1.13203361	1.56275642
H	2.77152047	0.54598625	2.13296969
H	-2.36752888	0.25154144	2.44604301
H	-1.26631328	-1.11912843	2.59019307
H	-2.81875836	-1.31606044	1.74803647

ts6crbhhme_123
E [Hartrees] = -349.9661692650

C	0.72115280	-0.48062873	-0.89627137
C	-0.09689416	0.60227843	0.20478457
C	-1.32078443	-0.25008174	0.60095078
C	-1.75036409	-0.31017990	-0.67226854
C	-0.49687754	0.36983964	-1.22723359
C	1.82481361	0.19721701	-0.40241807
C	2.79917938	-0.65291561	0.36084097
H	0.55889429	-1.57173229	-0.82009483
C	0.18298880	1.90707659	0.90778675
C	-1.75910130	-0.75929526	1.92752230
H	-2.60092396	-0.78255879	-1.15503719
H	-0.45677237	1.13171934	-2.00123964
H	3.03106965	-0.19752011	1.33305393
H	3.75012762	-0.64373808	-0.19190981
H	2.51624412	-1.71146799	0.52914857
H	0.68405078	1.74006732	1.86807582
H	-0.78283971	2.39645472	1.11391444
H	0.81026522	2.55730583	0.30063945

H	-1.87844482	0.06095782	2.64788159
H	-1.01139516	-1.44517538	2.34839064
H	-2.71251458	-1.29270027	1.85380169

ts6crbhmeh_124
E [Hartrees] = -349.9683803982
Gcorr [kcal/mol] = 90.613

C	0.99183917	-0.42953835	-0.41307036
C	-0.13234346	0.65459203	0.33351043
C	-1.32835898	-0.24654866	0.62398478
C	-1.48368820	-0.57501469	-0.67256304
C	-0.21823565	0.19562358	-1.10283257
C	1.85016050	0.47969953	0.18327185
C	2.74474369	-0.08265539	1.25052784
H	0.95741684	-1.51182706	-0.19164889
H	-0.05047081	1.68573125	0.65043413
H	-1.82114003	-0.53165593	1.54756598
C	-2.41120759	-1.43342258	-1.45732367
C	-0.09949811	1.08329064	-2.31403185
H	-1.86773605	-2.26658961	-1.92532921
H	-2.88165999	-0.86819075	-2.27273450
H	-3.20360288	-1.84955957	-0.82663768
H	3.77000746	-0.07101738	0.85176863
H	2.52769323	-1.11651785	1.58426935
H	2.77042059	0.56887431	2.13291129
H	-0.07677991	0.49171357	-3.23784634
H	0.82464976	1.66432189	-2.24811854
H	-0.94751262	1.77575350	-2.37636894

ts6crbhmeme_124
E [Hartrees] = -349.9628474975
Gcorr [kcal/mol] = 91.254

C	0.99865990	-0.42334504	-0.40944802
C	-0.13857902	0.70243762	0.31768786
C	-1.31112034	-0.24123877	0.61674795
C	-1.46073886	-0.56513668	-0.67716188
C	-0.20571373	0.20868104	-1.10964084
C	1.90026500	0.46890614	0.14307149
C	2.78736121	-0.09239482	1.21545661
H	0.94075405	-1.50096146	-0.17201391
C	-0.13760401	2.12313756	0.82517407
H	-1.79886272	-0.52106674	1.54467570
H	-2.13944773	-1.21581217	-1.22120199
C	-0.06962840	1.06649494	-2.34032885

H	3.82626246	-0.02275852	0.86118937
H	2.60116376	-1.14201814	1.51783947
H	2.75076262	0.53803417	2.11428282
H	-0.04474157	0.45104994	-3.24793685
H	0.86083895	1.63852101	-2.28315183
H	-0.90992112	1.76514346	-2.42757786
H	0.20596324	2.17180888	1.86436710
H	-1.17295155	2.49792427	0.79735866
H	0.50727272	2.75943450	0.22091711

ts7hh_124
E [Hartrees] = -350.0439052669
Gcorr [kcal/mol] = 91.176

C	-1.27528490	1.24025287	-0.27515702
C	-1.20821214	-0.12511974	-0.38671153
C	0.00298141	-0.36876262	0.38222445
C	-0.00217457	1.76438226	0.23929253
C	1.28715968	-0.11871380	-0.27355731
C	1.31919382	1.24745134	-0.15891680
H	-1.71818386	-0.77414857	-1.09138760
H	-0.05044611	-0.10621299	1.44120510
C	2.09621267	-1.05596962	-1.11244630
C	-2.40946714	2.15253855	-0.66330805
H	-0.02511443	2.73331081	0.75083212
C	2.45246881	2.18557545	-0.48584342
H	1.45379978	-1.59512394	-1.82361101
H	2.60302055	-1.81766257	-0.50541505
H	2.85834451	-0.52171678	-1.68903741
H	2.69486130	2.81943652	0.37800369
H	2.19615000	2.85802923	-1.31522911
H	3.36142418	1.63857617	-0.75725166
H	-2.07854747	2.93751980	-1.35540219
H	-2.82966307	2.65598893	0.21835176
H	-3.22071630	1.59096625	-1.13849974

ts7hhme_123
E [Hartrees] = -350.0422181463

C	-1.23261095	1.32495527	-0.39831807
C	-1.28292460	-0.01790610	-0.15249027
C	0.01922211	-0.49458399	0.37107993
C	0.02030188	1.64986879	0.27083353
C	1.30222956	-0.02141679	-0.20088066
C	1.24649958	1.32155806	-0.44472910
C	-2.43487302	-0.95764700	-0.39809798

C	0.03370373	-1.72928314	1.24491300
C	2.44164725	-0.96435107	-0.48906501
H	-1.78736377	1.90371290	-1.13076193
H	0.04042703	1.51882266	1.35455453
H	1.77543143	1.89908023	-1.19698068
H	-2.87277672	-1.31420201	0.54454491
H	-2.12469012	-1.84624116	-0.96336168
H	-3.23026578	-0.45265844	-0.95604142
H	0.93322466	-1.78363000	1.86672427
H	0.01831662	-2.63913350	0.62388631
H	-0.83990133	-1.77862704	1.90310000
H	2.10832116	-1.85172405	-1.04299502
H	2.91279336	-1.32269471	0.43670225
H	3.21755142	-0.46147069	-1.07569526

ts7hhme_124
E [Hartrees] = -350.0376370151

C	-1.34617572	1.10093996	0.07146675
C	-1.30717534	-0.24435368	-0.18197784
C	0.02664744	-0.52496839	0.37598645
C	-0.03627060	1.67144717	0.38594095
C	1.15454650	-0.16277624	-0.47168288
C	1.19755062	1.19500787	-0.22522512
C	-2.14475702	-1.08273656	-1.09676247
C	0.20699724	-0.77955690	1.84469229
H	1.54167956	-0.68019940	-1.34606054
H	-2.22096317	1.74150527	-0.06404214
H	-0.00819785	2.62099298	0.92693273
C	2.30907914	2.14090178	-0.60272212
H	-2.53276235	-1.97957315	-0.59559100
H	-1.56331678	-1.42916443	-1.96337497
H	-2.99583495	-0.50907142	-1.47823196
H	1.15642862	-0.38298504	2.21769288
H	0.24340349	-1.87542768	1.97654537
H	-0.63962780	-0.41621566	2.43588065
H	3.01904548	1.65635735	-1.28192016
H	2.87483313	2.46137420	0.28321547
H	1.92336237	3.04653899	-1.08750145

ts7meme_124
E [Hartrees] = -350.0395749898
Gcorr [kcal/mol] = 91.712

C	-1.24850292	1.08562328	0.00281776
C	-1.19435397	-0.25767877	-0.22940025

C	0.12892705	-0.51337324	0.37153216
C	0.04955437	1.67884111	0.37009948
C	1.26504581	-0.15321970	-0.46860123
C	1.28720655	1.20036754	-0.22842248
C	-2.02182352	-1.13333203	-1.11722740
C	0.28258530	-0.71631144	1.85278097
H	1.66791030	-0.68667570	-1.32638589
H	-2.12175234	1.72853159	-0.14202733
C	0.06129654	2.91820337	1.21791803
H	2.08069592	1.90273381	-0.49906319
H	-2.41912208	-2.00516807	-0.58057340
H	-1.42761298	-1.52107201	-1.95703953
H	-2.86542815	-0.57611844	-1.53775152
H	1.21888029	-0.29049590	2.22884420
H	0.32792237	-1.80335299	2.03800441
H	-0.57763821	-0.33438106	2.41375858
H	0.12642277	2.66415721	2.28777683
H	-0.85820020	3.50529317	1.09006758
H	0.92723334	3.55363525	0.99064074

ts8hh_124
E [Hartrees] = -350.0482528036
Gcorr [kcal/mol] = 92.606

C	-1.32548508	1.49927336	-0.40757487
C	-1.09779576	0.24183337	-1.07422975
C	-0.30547399	-0.72402225	-0.38410419
C	-0.06757865	2.09520559	-0.51750517
C	0.99654443	-0.21295797	-0.47601909
C	1.06939429	1.22034325	-0.72656023
H	-0.63547938	0.43961054	-2.04663601
H	-0.60783543	-1.45928091	0.35930284
C	2.22023849	-1.00695034	-0.07545713
C	-2.42743305	1.90688620	0.51932278
H	0.12813619	3.12508012	-0.20751366
C	2.41152864	1.86556120	-0.96910665
H	2.88955564	-1.17878250	-0.92902201
H	1.91959318	-1.99015376	0.30093403
H	2.81421995	-0.51310352	0.70458413
H	2.38008743	2.94272857	-0.77398016
H	2.71798873	1.73580305	-2.01679951
H	3.20563392	1.42589241	-0.35585445
H	-2.19126006	2.84539062	1.03112941
H	-2.59849230	1.13596898	1.28462233
H	-3.37742957	2.03518693	-0.01501623

ts8hme_123
E [Hartrees] = -350.0481580592
Gcorr [kcal/mol] = 93.106

C	-1.08981526	1.06882401	-0.84992475
C	-1.33238094	-0.19890223	-0.09669377
C	-0.11097888	-0.81241144	-0.01098355
C	-0.21387243	1.94905832	-0.19144840
C	1.12436903	-0.00755837	-0.32582923
C	1.10927186	1.38204388	-0.33839417
C	-2.66668329	-0.67113945	0.39174757
C	0.08463576	-2.22616798	0.49010695
C	2.44159733	-0.73755931	-0.41616466
H	-0.73132489	0.83870664	-1.86209162
H	-0.47117210	2.48744441	0.72493933
H	2.04329864	1.93255512	-0.21319962
H	-3.15598931	0.12226634	0.97211759
H	-2.60181993	-1.56087462	1.02450643
H	-3.33737302	-0.89738537	-0.44898852
H	0.67769560	-2.25729277	1.41424921
H	0.61543520	-2.84117321	-0.24770692
H	-0.86960979	-2.71775329	0.69253913
H	2.43723191	-1.45210136	-1.25071052
H	2.65653964	-1.31833162	0.48929824
H	3.26940404	-0.04115760	-0.57897419

ts8hme_124
E [Hartrees] = -350.0475888375
Gcorr [kcal/mol] = 95.339

C	-1.05258468	1.17189815	-0.68525079
C	-1.35053325	-0.02203875	0.03500128
C	-0.16594649	-0.76965214	-0.10405732
C	-0.14450236	2.11782724	-0.09513983
C	0.99705901	0.02471672	-0.41522762
C	1.09225624	1.45880180	-0.24164970
H	-2.06966439	-0.18674617	0.83449765
C	-0.02932059	-2.21859924	0.29960438
H	1.93718232	-0.51329531	-0.55554493
H	-0.67798172	0.89343566	-1.67524811
C	-0.46980850	3.26744308	0.80828503
C	2.43559943	2.09327089	0.03956539
H	0.96145458	-2.44114560	0.71269466
H	-0.19170974	-2.89029178	-0.55422283
H	-0.77994596	-2.47908037	1.05560820

H	0.34962990	3.50942695	1.49256559
H	-1.36251433	3.03770370	1.40576236
H	-0.70278622	4.17642030	0.23639299
H	2.35673293	2.86966794	0.80968077
H	2.84515841	2.57879927	-0.85655162
H	3.17027265	1.35702161	0.38454627

ts8meme_124
E [Hartrees] = -350.0512902276
Gcorr [kcal/mol] = 92.326

C	-1.04757420	1.16825123	-0.17347682
C	-1.02041564	-0.19065551	-0.28265196
C	0.28996955	-0.71464703	0.21044019
C	0.11878545	1.98121555	0.28802084
C	1.32735731	0.07282353	-0.33899629
C	1.35954587	1.42599633	0.29842501
C	-2.21545924	-1.04900825	-0.57706014
C	0.35750526	-1.25377646	1.61818606
H	1.28958141	0.15780690	-1.43540163
H	-1.98258170	1.70336585	-0.34575127
C	-0.15358840	3.40543849	0.69838905
H	2.24739950	1.99106406	0.57711757
H	-2.41106470	-1.73259655	0.26122303
H	-2.04115797	-1.67928183	-1.45864183
H	-3.11761569	-0.45279258	-0.75250900
H	1.27131988	-0.91277149	2.11891455
H	0.39034133	-2.35345567	1.60887088
H	-0.51062760	-0.96235673	2.22334876
H	-0.88672375	3.44897326	1.51550849
H	-0.57495308	3.98446630	-0.13469699
H	0.75929697	3.90787673	1.03308983

tstrim_mestln
E [Hartrees] = -349.8895580413
Gcorr [kcal/mol] = 86.467

H	0.52002003	-0.64117114	-2.50132371
C	0.63596825	-0.78276466	-1.44913806
C	1.13767747	-1.39764968	-0.50556119
C	0.47028260	-0.58550644	1.59827895
H	1.09975022	-1.36607823	1.96584580
C	-0.29372082	0.35782413	1.81400692
C	-1.10507442	1.36935945	-0.14883455
H	-1.61681511	2.00951703	0.53594461
C	-0.84424897	1.03996720	-1.30796010

C	-0.96372978	1.17925073	-2.77122365
H	-1.36867278	0.27027505	-3.23341300
H	-1.63718339	2.00870810	-3.01791308
H	0.00686970	1.38545918	-3.23950520
C	-1.03565052	1.26959560	2.70454344
H	-0.74201608	2.31541540	2.54992226
H	-0.83706837	1.01796309	3.75318636
H	-2.11879285	1.20175149	2.54314316
C	1.99741886	-2.45050567	0.06647268
H	1.42389414	-3.14914900	0.68844417
H	2.47115581	-3.02848265	-0.73597434
H	2.79485277	-2.02835058	0.69076704

[1] K. Yamaguchi, F. Jensen, A. Dorigo and K. N. Houk, *Chem. Phys. Lett.*, 1988, **149**, 537–542.