Supporting Information for "**Origin of Thermodynamic versus Kinetic Control of Allene Hydroboration with 9-Borabicyclo[3.3.1]nonane and 10-R-9-Borabicyclo[3.3.2]decane**"

Daniel H. Ess*, Jeremy Kister, Ming Chen and William R. Roush*

Department of Chemistry, The Scripps Research Institute, Scripps Florida, Jupiter, Florida 33458

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Cartesian Coordinates and Energies (hartrees)

B3LYP/6-31G(d,p)

9-BBN; Energy = -338.74898410861

C1	3.4200382308	0.0788276694	1.7590358142
H2	4.4135113369	-0.3595150865	1.9148150889
B3	3.4006603826	1.6442897799	1.8873492225
C4	3.0415841597	-0.1752157700	0.2598712242
H5	3.8687901064	0.1924520624	-0.3639217577
H6	2.9884753510	-1.2572563094	0.0754741917
C7	1.9533162803	2.2375674828	1.7443608507
H8	1.9097889945	3.3241057831	1.8890064948
C9	1.5805606685	1.9632487890	0.2475566850
H10	2.2237717299	2.5954781392	-0.3808809044
H11	0.5529789845	2.3041941335	0.0591270669
C12	1.7327769659	0.4961479091	-0.2095530192
H13	1.6900268494	0.4607146210	-1.3055982192
H14	0.8755075184	-0.0880742002	0.1335819694
C15	0.9967330798	1.5824271719	2.7796115303
H16	1.2671749822	1.9717896659	3.7714969138
H17	-0.0351934381	1.9171319469	2.6022780813
C18	2.4502654614	-0.5638569627	2.7891796099
H19	2.9061628952	-0.4546903329	3.7835208660
H20	2.3789261048	-1.6467466667	2.6142098797
C21	1.0307154400	0.0405047371	2.8309193581
H22	0.4322764394	-0.3678908245	2.0120564742
H23	0.5300144812	-0.2943823300	3.7483477922
H24	4.3915362631	2.3163578437	1.9532026579

2a; Energy = -564.67863657662

C1	5.0325351496	2.4637232059	3.4820178672
C2	5.1311782006	2.6678738492	2.1911432440
C3	5.2416314673	2.8555529451	0.8989454840
H4	6.0489383795	3.4498025823	0.4770879684
H5	4.5281435979	2.4274023050	0.1986162402
Si6	5.9056144539	0.9577256245	4.2386747317
C7	4.2343084127	3.4073144170	4.3731176104
H8	3.7930289621	4.2270815588	3.7996801598
H9	3.4237800193	2.8727064828	4.8826029410
H10	4.8709061220	3.8413924981	5.1533839557
C11	7.1585951343	1.5571271220	5.5272394289
H12	6.6792639237	2.1367791164	6.3235510351
H13	7.6670209118	0.7087008018	5.9993265024
H14	7.9252373431	2.1912122991	5.0691960391
C15	4.6126932630	-0.1367049438	5.0873928277
H16	4.0750591216	0.4023432511	5.8749167798

H17	3.8714908757	-0.5036737567	4.3695039435
H18	5.0862260086	-1.0092211425	5.5517320884
C19	6.7913624435	-0.0228767014	2.8906025350
H20	7.5424242899	0.5874042542	2.3792658669
H21	7.3006176918	-0.8932462804	3.3196125139
H22	6.0900232624	-0.3844802823	2.1321576380

TS-Z2; Energy = -903.42010400296

C1	-0.3076628148	-0.0218221776	0.1920400337
C2	0.2585526992	0.0966601966	2.7636536343
C3	1.7683655036	-0.0367258559	2.4254602215
H4	2.2852898264	-0.6280202899	3.1966126484
H5	2.2037344699	0.9705372761	2.4722518896
B6	-0.4016211939	0.9009078847	1.5169953090
C7	-0.4601614523	-1.2591478202	2.9697447866
H8	-1.4670145985	-1.0579598141	3.3639769131
H9	0.0450098071	-1.8459876021	3.7515245077
H10	-0.7784889195	0.4424257532	-0.6880636859
H11	0.1915331626	0.6526003420	3.7108664547
C12	1.2075105503	-0.1465732868	-0.1264526277
H13	1.5621461553	0.8485314325	-0.4286746719
H14	1.3705398589	-0.8030297782	-0.9946230067
C15	2.0892866503	-0.6500440361	1.0411976318
H16	2.0185767116	-1.7400682272	1.1032588593
H17	3.1418358880	-0.4471679321	0.8019978221
C18	-1.0092331704	-1.3838246928	0.4206633690
H19	-2.0955016978	-1.2121014945	0.4539831412
H20	-0.8520550003	-2.0483428794	-0.4421792833
C21	-0.5943522657	-2.1390003500	1.7051421458
H22	-1.3260602462	-2.9341270634	1.9021076641
H23	0.3503069094	-2.6608943039	1.5275454713
C24	-2.1429739987	1.2521976786	1.9581559019
H25	-2.7777767908	0.6508558132	1.3119791120
H26	-2.2715794066	1.0826507905	3.0252178674
C27	-1.7277743033	2.4720373565	1.5297978917
C28	-1.6257545825	3.7147257158	1.1364661934
H29	0.1935180504	1.9591678306	1.3703391700
Si30	-3.2452029063	4.7368298233	1.2622114019
C31	-4.6776813947	3.6677429621	1.8635547749
H32	-5.5902831021	4.2718453985	1.9227002078
H33	-4.8763788454	2.8328559602	1.1844114327
H34	-4.4903081228	3.2520089412	2.8582979753
C35	-2.9372586338	6.1547077282	2.4741327845
H36	-3.8311176816	6.7825197673	2.5621851605
H37	-2.6954673358	5.7780688319	3.4733203177
H38	-2.1134864729	6.7994734046	2.1508289998

C39	-3.6255607479	5.4185378737	-0.4597276710
H40	-3.7766186681	4.6103922426	-1.1828768261
H41	-4.5411620920	6.0203559833	-0.4379322825
H42	-2.8203125309	6.0584436437	-0.8350320638
C43	-0.3922799866	4.4062051084	0.6016420096
H44	0.4802916303	3.7516388129	0.6500476645
H45	-0.5454360291	4.7075020791	-0.4406677026
H46	-0.1824921882	5.3167853951	1.1731077912

TS-E2; Energy = -903.41508667144

C1	-0.0053744181	0.0151398727	0.0070597725
C2	-0.0073682932	-0.0153306211	2.6430988483
C3	1.5459469389	-0.0172441681	2.6334623338
H4	1.9374118013	-0.6209840656	3.4661402279
H5	1.8799523582	1.0119129947	2.8259335228
B6	-0.4623174223	0.8237211167	1.3344074290
C7	-0.6278328331	-1.4345150106	2.6140769917
H8	-1.7075873173	-1.3428483314	2.8015116709
H9	-0.2413351882	-2.0395032377	3.4479200979
H10	-0.3165927560	0.5116974049	-0.9245564144
H11	-0.3197639886	0.4592446195	3.5857837236
C12	1.5478435469	0.0130260738	0.0189247101
H13	1.8819164445	1.0464152159	-0.1492321782
H14	1.9404875143	-0.5713635540	-0.8268997213
C15	2.2015239334	-0.5087608257	1.3208201847
H16	2.2085736755	-1.6026214686	1.3081511895
H17	3.2606634012	-0.2183175688	1.3249896872
C18	-0.6262826717	-1.4040997588	0.0024037700
H19	-1.7057928509	-1.3076406756	-0.1838756846
H20	-0.2390428369	-1.9896583338	-0.8448163124
C21	-0.4241917995	-2.2231406734	1.2990051205
H22	-1.1124060365	-3.0790006738	1.2886191747
H23	0.5764153050	-2.6647834792	1.2944818014
C24	-2.2729287738	1.0163184912	1.3314080984
H25	-2.6611125182	0.6025207069	0.4031964210
H26	-2.6661608254	0.5678790645	2.2411473359
C27	-1.8761821726	2.3148088139	1.3566813790
C28	-1.8132496437	3.6238332931	1.3804217072
H29	0.0427056408	1.9373161049	1.3460651372
Si30	-0.2118365341	4.6810325207	1.4044003332
C31	0.7918611108	4.3759946960	-0.1646784978
H32	1.6844613971	5.0125255149	-0.1705710574
H33	1.1173112872	3.3353979109	-0.2427947741
H34	0.2079291063	4.6157403547	-1.0597678828
C35	-0.7484576195	6.4969795350	1.4374917717
H36	0.1399244358	7.1387736569	1.4519949480

H37	-1.3356679607	6.7751836044	0.5560203557
H38	-1.3401718356	6.7415168423	2.3258882122
C39	0.7835854124	4.3164961244	2.9658943432
H40	1.1076872737	3.2734818459	3.0063714624
H41	1.6764908565	4.9514361519	3.0004091086
H42	0.1952313474	4.5228946241	3.8664023416
C43	-3.1655995118	4.3408375857	1.3913839096
H44	-3.2593533487	4.9683943083	2.2841745678
H45	-3.2562318780	5.0009463172	0.5220195092
H46	-4.0030996973	3.6388620577	1.3769031218

Z-3; Energy = -903.48217179117

C1	0.1015274897	-0.2468083570	2.6618129220
C2	2.6747054319	-0.0672903427	2.2967256150
C3	2.4630758216	-0.2129823299	0.7587171466
H4	3.3036650778	-0.7675118460	0.3178962069
H5	2.5095260454	0.7933210639	0.3176297814
B6	1.3920209645	0.6353531165	2.8863404065
C7	2.8629365837	-1.4171797638	3.0532476154
H8	3.1517146515	-1.1817295731	4.0875716248
H9	3.7135397864	-1.9670285528	2.6259726664
H10	-0.8095730827	0.2149379860	3.0679747286
H11	3.5898882819	0.5187122789	2.4480203611
C12	-0.0973959263	-0.3743449552	1.1198181777
H13	-0.3783484531	0.6172578057	0.7356305700
H14	-0.9557337825	-1.0272516426	0.9072010953
C15	1.1341066685	-0.8747410634	0.3353943385
H16	1.2155887492	-1.9604913578	0.4329873758
H17	0.9714205898	-0.6919863827	-0.7345751060
C18	0.3039480271	-1.6015490534	3.4026730669
H19	0.2683807068	-1.3989596346	4.4831592782
H20	-0.5446324613	-2.2703293419	3.2000065123
C21	1.6235964629	-2.3360168198	3.0844298892
H22	1.7823249183	-3.1210110686	3.8349294542
H23	1.5315663111	-2.8633846992	2.1311426376
C24	1.3317230238	2.0502817081	3.5991558297
H25	0.5840137194	2.6333758335	3.0308973440
H26	0.8522208296	1.9026207823	4.5774685662
C27	2.6108176615	2.8331976934	3.6985641337
C28	3.3119793634	3.1961966842	4.7896714239
H29	3.0182105472	3.1229966774	2.7241633969
Si30	2.7851256640	2.8168871802	6.5770793530
C31	2.6059809026	0.9511706646	6.8781649194
H32	2.3851981183	0.7514902533	7.9332633086
H33	1.8041610880	0.5018689236	6.2841477850
H34	3.5355476782	0.4264140333	6.6309464249

C35	4.1239382481	3.4521213160	7.7602319559
H36	3.8369330226	3.2500247607	8.7984603932
H37	5.0887926842	2.9636104447	7.5862721844
H38	4.2781642228	4.5322226472	7.6669418086
C39	1.1601781940	3.6958458699	7.0096505931
H40	0.3287192704	3.3727961940	6.3755212150
H41	0.8794494771	3.5022055414	8.0514969204
H42	1.2618174227	4.7800678637	6.8898832884
C43	4.6051191097	3.9724649715	4.5964293606
H44	4.5754453829	4.9498138857	5.0948805638
H45	5.4684196002	3.4417475682	5.0176882678
H46	4.8113670747	4.1486517628	3.5344412934

E-3; Energy = -903.48537518106

C1	0.1405823216	-0.1633587554	2.8173046581
C2	2.4617384711	0.2432499715	1.7074253046
C3	1.8690234744	-0.1858401341	0.3355972452
H4	2.6367578554	-0.6995201795	-0.2604318848
H5	1.6265846773	0.7303751688	-0.2222756954
B6	1.3252870767	0.8595296054	2.6124755714
C7	3.0612890286	-0.9265441080	2.5533955562
H8	3.5806710520	-0.4816991914	3.4140488958
H9	3.8373882167	-1.4429392285	1.9710895732
H10	-0.6864691176	0.2551971822	3.4075227943
H11	3.2853639471	0.9402475107	1.5074001578
C12	-0.4371998825	-0.5922709446	1.4397769157
H13	-0.9754322297	0.2714497622	1.0231121915
H14	-1.1967446491	-1.3751158009	1.5770226764
C15	0.6046959692	-1.0672526402	0.4057757421
H16	0.8887108183	-2.1016742158	0.6176212161
H17	0.1347927215	-1.0943675353	-0.5857603202
C18	0.7538465672	-1.3290022712	3.6586724403
H19	0.9826663699	-0.9364052917	4.6600661342
H20	-0.0019889704	-2.1119090143	3.8130212034
C21	2.0356775571	-1.9575973250	3.0713538354
H22	2.5126411884	-2.5763286439	3.8422497321
H23	1.7709622802	-2.6500194336	2.2679380240
C24	1.3518827230	2.2895312147	3.2926035145
H25	0.7997782944	2.9128561759	2.5614311701
H26	0.7265526845	2.3021776760	4.1920776135
C27	2.7102855235	2.8996848954	3.5181563826
C28	3.3574948081	3.1139734188	4.6821247165
H29	3.2274026110	3.1662739101	2.5965422853
C30	2.7619150933	2.7805245931	6.0376211756
H31	3.3823724851	2.0488926896	6.5711851829
H32	2.7151845691	3.6695978470	6.6794027844

H33	1.7514393622	2.3670917830	5.9788962177
Si34	5.0997976641	3.8499238318	4.6707543362
C35	6.3096783604	2.6308390190	5.4782399542
H36	7.3257298629	3.0413716210	5.4979532081
H37	6.0290239298	2.4019219084	6.5121365224
H38	6.3445396888	1.6846815644	4.9270531565
C39	5.1226983528	5.4701042580	5.6577212510
H40	4.4525732840	6.2142170433	5.2135761650
H41	4.8090369458	5.3197649889	6.6964436328
H42	6.1303604253	5.9007149621	5.6794244252
C43	5.6850001731	4.2054627786	2.9047144595
H44	6.6958025670	4.6290655873	2.9245910628
H45	5.7225208608	3.2974470480	2.2937122247
H46	5.0380288181	4.9268003479	2.3942737148

TS-Z3; Energy = -903.45120498032

C1	3.4209242260	0.0638584859	1.7543142383
H2	4.3929540389	-0.4201969409	1.9102538774
B3	3.4589172662	1.6692137492	1.9879779028
C4	3.0289525297	-0.1963889243	0.2745714894
H5	3.8735185129	0.1145744828	-0.3543347579
C6	4.4803156325	2.2037814530	3.4510388839
C7	4.6141204119	2.9653326532	2.2561600664
C8	4.8270372699	2.3540808092	1.0062169238
H9	4.1292724111	3.9427038221	2.2293611874
H10	2.9089882487	-1.2762798221	0.1031942733
H11	4.6423067214	2.9492161279	0.1183622254
H12	5.5193978902	1.5315407133	0.8804526705
Si13	5.9051278043	1.0811848182	4.0753663148
C14	1.9602269941	2.2325933088	1.7582513707
H15	1.8780354278	3.3179807528	1.9172915095
C16	1.5948899784	1.9838350755	0.2693614563
H17	2.2355528445	2.6304897180	-0.3459298076
H18	0.5638871058	2.3113585025	0.0697041081
C19	1.7521234449	0.5248526766	-0.2162481662
H20	1.7392834766	0.5124483174	-1.3139922693
H21	0.8729239129	-0.0510452721	0.0846296548
C22	0.9782417423	1.5688705978	2.7582533638
H23	1.2141286422	1.9405882809	3.7641448498
H24	-0.0513959464	1.8976805162	2.5542372986
C25	2.4357570811	-0.5670361622	2.7736461766
H26	2.8649738291	-0.4492381323	3.7749533302
H27	2.3649746052	-1.6509989316	2.5989208434
C28	1.0129989947	0.0273299346	2.7880698530
H29	0.4365388109	-0.3722324939	1.9491511827
H30	0.4918643899	-0.3253478034	3.6879078071

C31	3.7670551762	2.9268045921	4.5984933074
H32	2.9568112447	3.5642818175	4.2293382214
H33	3.3237133385	2.2164031155	5.3040572929
H34	4.4510324414	3.5640669508	5.1718719363
C35	6.9221750363	2.1552297868	5.2698514942
H36	6.3590735351	2.4279835840	6.1680874200
H37	7.8136025262	1.6075818173	5.5973341077
H38	7.2609427353	3.0819689365	4.7936803754
C39	5.2966347750	-0.4208011849	5.0534811530
H40	4.5312052159	-0.1530793473	5.7895960757
H41	4.8818523256	-1.1996825300	4.4083190716
H42	6.1384730010	-0.8581329098	5.6029884385
C43	7.1087072740	0.4958228242	2.7329729083
H44	7.5309826277	1.3337804712	2.1690571147
H45	7.9439720704	-0.0211186216	3.2207038990
H46	6.6642454588	-0.2055848829	2.0210829544

INT-3; Energy = -903.47598338954

C1	-0.4385901131	0.8249495027	2.3596709889
C2	0.9654719167	2.0371273427	0.5414324827
C3	0.7034565102	0.8544518828	-0.4305468212
H4	1.5711279305	0.7147218303	-1.0911314240
H5	-0.1262528832	1.1406956253	-1.0935084824
B6	-0.2178160348	2.1915159986	1.5873547962
C7	2.2487933371	1.8759848614	1.4215089072
H8	2.4249387900	2.8336924010	1.9303289262
H9	3.1214033364	1.7145917104	0.7727982208
H10	-1.2898167866	0.8437149869	3.0503366952
H11	1.1287898407	2.9281805298	-0.0773650470
C12	-0.6577282668	-0.3709942207	1.3955053062
H13	-1.6662847783	-0.2736617326	0.9707694539
H14	-0.6689083723	-1.3123428142	1.9636908563
C15	0.3547683993	-0.4897215984	0.2382799582
H16	1.2705479857	-0.9675224822	0.5962653268
H17	-0.0483586474	-1.1726525103	-0.5206444359
C18	0.8446310811	0.7023341601	3.2498834128
H19	0.8274316568	1.5179643666	3.9868434788
H20	0.7949535708	-0.2271849310	3.8342853775
C21	2.1824619122	0.7577182780	2.4832898165
H22	2.9989411045	0.9016048909	3.2024758257
H23	2.3766479043	-0.2102175331	2.0144303506
C24	-0.9446577376	3.5509869528	1.9443274635
C25	0.0124686855	4.7174769294	1.8728264383
C26	0.1904609517	5.6844975439	2.7825018936
H27	0.6323249461	4.7592545595	0.9785928542
H28	0.9245061750	6.4680773526	2.6205008839

H29	-0.3674180346	5.7326209519	3.7118895971
C30	-1.7252312969	3.5166010675	3.2786947656
H31	-2.2462863618	4.4584934793	3.4782940204
H32	-2.4737609604	2.7197393644	3.2923866309
H33	-1.0482427604	3.3412000989	4.1231753764
Si34	-2.2537278497	3.8585315087	0.5163564020
C35	-1.4283463947	4.2774606163	-1.1361095694
H36	-0.8201675183	5.1849341886	-1.0690722432
H37	-0.7890153851	3.4703009966	-1.5059178340
H38	-2.2019494113	4.4564846988	-1.8921734381
C39	-3.3425856695	5.3213268767	1.0239036720
H40	-4.0045093341	5.0741444010	1.8594850436
H41	-2.7350227777	6.1830160832	1.3172915094
H42	-3.9733923634	5.6255944828	0.1810611510
C43	-3.3552901240	2.3336895161	0.2718735268
H44	-2.8020525355	1.4878259034	-0.1491563588
H45	-3.8112977074	2.0003051921	1.2099151109
H46	-4.1702918879	2.5694414419	-0.4224696337

TS-E3; Energy = -903.47654073706

C1	3.2795335369	-0.0482122527	1.4672975194
H2	4.2479502652	-0.3741243382	1.8673550461
B3	3.1911552218	1.5137903742	1.2562401775
C4	3.0925230410	-0.7338024582	0.0737285920
H5	4.0881809257	-0.9148176088	-0.3454275846
C6	4.5748849273	2.7013249348	4.0859774080
C7	4.0712234424	3.0779311362	2.8903235212
C8	4.3819219329	2.5259934778	1.5111934680
H9	3.3036141659	3.8514045362	2.8835510228
H10	2.6630560199	-1.7304330130	0.2402992862
H11	4.3723228333	3.3550932340	0.7919482089
H12	5.3654830414	2.0482070229	1.4778941810
C13	1.7503455284	1.9533945418	0.7815224829
H14	1.6383777525	3.0424016992	0.6965152331
C15	1.5108070945	1.3471761796	-0.6406110562
H16	1.7990377288	2.1040431814	-1.3780842698
H17	0.4296475003	1.2099665857	-0.7737540935
C18	2.2521535024	0.0190550617	-1.0115581875
H19	2.9252459528	0.2443054682	-1.8462027835
H20	1.5181209636	-0.6806709454	-1.4243732007
C21	0.6886035435	1.4467002697	1.7972511675
H22	0.8260465857	1.9711599915	2.7538405646
H23	-0.3163036312	1.7158511433	1.4420659493
C24	2.1793755194	-0.4991301746	2.4694231328
H25	2.3998890845	-0.0755209343	3.4595507146
H26	2.2165340861	-1.5915360251	2.5866262837

C27	0.7704825068	-0.0653864488	2.0441469973
H28	0.4782225126	-0.6036849817	1.1325699399
H29	0.0422123748	-0.3579792833	2.8108607244
C30	5.6344038128	1.6274299006	4.2362270370
H31	6.4927491373	1.9957173157	4.8122327492
H32	5.2429629846	0.7616036821	4.7855664654
H33	6.0122233433	1.2607584326	3.2784854240
Si34	3.9676204744	3.5341859119	5.6747242601
C35	5.4195551917	4.3938000846	6.5411517576
H36	5.0919009837	4.8641174679	7.4752885205
H37	6.2203350712	3.6899728288	6.7927273770
H38	5.8521904862	5.1765005725	5.9086485376
C39	2.6261467586	4.8192042594	5.3075017510
H40	2.2887787744	5.2826246742	6.2417126809
H41	2.9915916849	5.6216553446	4.6580745562
H42	1.7484188359	4.3730290847	4.8280269358
C43	3.2543527542	2.2174387613	6.8397809759
H44	2.3984572685	1.7068198163	6.3848325329
H45	3.9975890451	1.4544419120	7.0955608056
H46	2.9114903401	2.6686768653	7.7778315440

Dimethyl allylborane; Energy = -670.02130687495

B1	1.4375648654	0.5649886743	2.8883939651
C2	1.3838841322	2.0084248293	3.5574277199
H3	0.6821167314	2.5652207786	2.9065155484
H4	0.8504343828	1.9385075930	4.5137169607
C5	2.6676663153	2.7798621699	3.6712909427
C6	3.3336540497	3.1644137499	4.7770047987
H7	3.1133140703	3.0344906732	2.7040631963
Si8	2.7393650726	2.8310262500	6.5521551069
C9	2.4848752146	0.9781447368	6.8757620082
H10	2.2272825979	0.8066495316	7.9274676920
H11	1.6842854297	0.5473257576	6.2670541640
H12	3.4008741179	0.4151236090	6.6651350927
C13	4.0640004413	3.4367867800	7.7662191021
H14	3.7389721756	3.2609348225	8.7980231332
H15	5.0152638447	2.9113760583	7.6285773534
H16	4.2600484435	4.5090986251	7.6624384710
C17	1.1339770037	3.7725456091	6.9235014707
H18	0.3113614711	3.4699596835	6.2679811727
H19	0.8148420260	3.6024947585	7.9584150854
H20	1.2768675247	4.8510077553	6.7938632873
C21	4.6411816282	3.9220611946	4.6116281082
H22	4.6028978126	4.9127805627	5.0825665220
H23	5.4828561312	3.3952206234	5.0788196153
H24	4.8882095420	4.0684802931	3.5537837691

C25	2.7238610194	0.0610373602	2.1303115324
H26	3.6434683895	0.2831025771	2.6846085597
H27	2.7090864275	-1.0012344210	1.8673112553
H28	2.8130441244	0.6254138423	1.1882286153
C29	0.1559596949	-0.3504611848	2.9781804015
H30	-0.0352571958	-0.9033470734	2.0503791719
H31	0.3614607104	-1.1228189076	3.7371868191
H32	-0.7623569578	0.1611534868	3.2848517813

Dimethyl allylborane TS; Energy = -669.98965047684

B1	3.3683375389	1.8508819229	2.0561202823
C2	4.5114724492	2.3087325654	3.4213078669
C3	4.6699253133	3.0434418007	2.2089586286
C4	4.7418372283	2.4310044084	0.9480641151
H5	4.2746654077	4.0605004978	2.2035032818
H6	4.5452520344	3.0481766126	0.0774944649
H7	5.3243926012	1.5370652125	0.7682887230
Si8	5.7696815446	1.0011514314	4.0245660772
C9	3.9044736358	3.1029937456	4.5824152308
H10	3.4019973645	2.4383525665	5.2940235889
H11	4.6607308360	3.6629069894	5.1452052209
H12	3.1546754222	3.8193369583	4.2312783137
C13	6.8875826207	1.8713616167	5.2920347894
H14	6.3362874738	2.1993379752	6.1789328950
H15	7.6746700077	1.1875133021	5.6306420826
H16	7.3786273210	2.7507213580	4.8604487419
C17	4.9091703693	-0.4339849869	4.9098446589
H18	4.2347291214	-0.0721625285	5.6935738287
H19	4.3226136484	-1.0518590246	4.2252080529
H20	5.6528429985	-1.0785650818	5.3925631210
C21	6.9266849063	0.3456822626	2.6729576216
H22	7.4147821402	1.1643497150	2.1335706883
H23	7.7172904949	-0.2485335720	3.1462988898
H24	6.4339008644	-0.2967399111	1.9381977019
C25	3.2924103850	0.2544279604	1.8342521025
H26	4.2396675552	-0.2889753987	1.8375100829
H27	2.6551791045	-0.1929778736	2.6071341645
H28	2.8076313238	0.0487903817	0.8719449367
C29	1.9403311539	2.5897354302	1.9960589549
H30	1.2959113820	2.2551097759	2.8203216866
H31	1.9617230094	3.6848669801	2.0368583130
H32	1.4124597859	2.3184147488	1.0723595118

1a; Energy = -786.74957901905

C1	0.1595500927	0.1896771910	-0.3192739465
C2	-0.1823855885	0.2227342735	1.2044151465

C3	2.9300547562	-0.0717628951	1.4088760498
H4	-0.5376314914	0.8575591563	-0.8416540477
C5	-0.0981233369	-1.1806351520	1.8564263340
H6	-0.2554464797	-1.0843581020	2.9385714013
H7	-0.9514451330	-1.7662253986	1.4874562880
H8	3.9986941282	0.0353236282	1.6336216988
H9	-1.2459855123	0.4894853828	1.2627681635
B10	2.1618662301	1.2067482742	1.9435779907
C11	0.6121669193	1.3238270947	1.9563085484
H12	0.3899425596	2.3038980677	1.4942331665
C13	1.1657510789	-2.0138783675	1.6068149619
H14	1.0366986604	-2.9824315886	2.1079365466
H15	1.2330446685	-2.2520992980	0.5383759185
C16	2.4964060883	-1.4102430459	2.0727401352
H17	2.4762534808	-1.2888272481	3.1649175878
H18	3.2818037306	-2.1536991583	1.8757392941
C19	2.7982571563	-0.1058380305	-0.1527399175
H20	3.6875949067	0.3680908379	-0.5844504844
H21	2.7987159137	2.1573539002	2.3194000351
Si22	0.0336585779	1.7490555078	3.7501315223
C23	-1.8412591960	1.5073744741	3.8958292076
H24	-2.1861498671	1.8217676959	4.8875844912
H25	-2.3804070174	2.1069629007	3.1540418570
H26	-2.1391533691	0.4630494796	3.7592311242
C27	0.8958579677	0.7149036443	5.0872903750
H28	0.5637531070	1.0322373218	6.0826936188
H29	0.6818170642	-0.3546470258	4.9963105982
H30	1.9840685759	0.8401764826	5.0521396386
C31	0.4332082201	3.5728676581	4.0711719629
H32	0.1382110336	3.8605692332	5.0867415885
H33	1.5039029468	3.7749518066	3.9659567127
H34	-0.0994132247	4.2300301578	3.3747053040
C35	1.5757233348	0.6211673558	-0.7530898883
H36	1.6844434203	1.6968307968	-0.5538371988
H37	1.6286348212	0.5304892399	-1.8460643535
H38	2.8218835625	-1.1466416203	-0.5018980566
H39	-0.0533096661	-0.8138586883	-0.7110501664

1b; Energy = -155.98470626395

C1	-0.3615810751	0.5715921476	0.0000000000
C2	-0.3245840033	-0.7367636796	0.0000000000
H3	-1.2707329290	-1.2799412048	0.0000000000
C4	-0.3928257101	1.8789329023	0.0000000000
H5	-0.4069451006	2.4487473834	0.9266873198
H6	-0.4069451006	2.4487473834	-0.9266873198
C7	0.9366747259	-1.5665151284	0.0000000000

H8	0.9756395886	-2.2180925559	0.8816368833
H9	0.9756395886	-2.2180925559	-0.8816368833
H10	1.8278769289	-0.9346042257	0.0000000000

2b; Energy = -347.73014105745

C1	2.8728125597	2.5897345054	1.4434856816
H2	3.1408690105	2.0824636311	0.5184551050
H3	1.8748873081	3.0214008613	1.4957040475
C4	3.7056911544	2.6700786444	2.4458675385
C5	4.5436645502	2.7483468845	3.4561047988
H6	4.5212850646	1.9478760773	4.1964780828
C7	5.5259473310	3.8223035291	3.6960691389
C8	6.3517213932	3.7574590926	4.8290009672
C9	7.2913176624	4.7542146531	5.0872600282
C10	7.4224978206	5.8350849170	4.2164943253
C11	6.6055596692	5.9106988951	3.0849224910
C12	5.6678268639	4.9169517242	2.8264022968
H13	6.2541833394	2.9170978749	5.5117532813
H14	7.9211448125	4.6856737955	5.9696590937
H15	8.1538754824	6.6129261506	4.4154394213
H16	6.7012468048	6.7495239341	2.4012480509
H17	5.0349571573	4.9794698747	1.9461931914

TS-Z4; Energy = -942.71302405545

C1	-0.0025910759	-0.0185271401	0.0087673048
C2	0.0092996485	-0.0042758991	1.5679153940
C3	3.0705129272	0.0044808083	1.0484888201
H4	-0.8838612217	0.5458705513	-0.3244781830
C5	0.4370954358	-1.3671010699	2.1844908226
H6	0.6338824229	-1.2312651737	3.2552716456
H7	-0.4318658612	-2.0370498731	2.1257206831
H8	4.1473922271	0.2344132457	1.0483328559
H9	-1.0472260914	0.0950084169	1.8500610221
B10	2.3782281555	1.0860378170	2.0523291981
C11	0.7413751337	1.2534495657	2.1495009794
H12	0.4154861517	2.0847696504	1.5043439140
C13	1.6192602973	-2.1135129521	1.5490381232
H14	1.6941117167	-3.0993506870	2.0275048130
H15	1.3881498748	-2.3231996476	0.4971981922
C16	2.9863951691	-1.4272353381	1.6403570048
H17	3.3021749369	-1.3952186211	2.6921940407
H18	3.7143021122	-2.0705896824	1.1236456384
C19	2.6082833083	0.0357502390	-0.4384946174
H20	3.3120107708	0.6460260060	-1.0222032912
C21	3.0148603968	2.7904536478	1.4206263445
H22	3.4656751768	2.5795756174	0.4552868478

H23	2.1733433752	3.4770097851	1.4223419929
C24	3.6977553543	2.5662574109	2.5579353773
C25	4.5285106595	2.6214490359	3.5735410370
H26	2.8581465721	0.8953825597	3.1590483831
Si27	0.0696763551	1.8040908416	3.8503293553
C28	-1.8332789711	1.8041733582	3.8509786789
H29	-2.2162533810	2.2633338600	4.7699783002
H30	-2.2379781236	2.3734574562	3.0063047243
H31	-2.2492690616	0.7925609230	3.7956017567
C32	0.6407910460	0.7434536702	5.3201620345
H33	0.3359803555	1.2126824283	6.2630361473
H34	0.1997257570	-0.2585173876	5.2985222639
H35	1.7288983015	0.6256349543	5.3446084000
C36	0.6149291927	3.5967745247	4.1805151609
H37	0.2001242135	3.9547154757	5.1297571980
H38	1.7034149367	3.6955569598	4.2405807435
H39	0.2589445386	4.2746730804	3.3956014293
C40	1.2036532639	0.5974770016	-0.7235674200
H41	1.2132951728	1.6739961972	-0.5141841873
H42	1.0146808432	0.5175913787	-1.8029480119
H43	2.6919270381	-0.9716636761	-0.8707763194
H44	-0.1686969135	-1.0446177762	-0.3448337314
H45	4.5178117078	1.8335351932	4.3202380288
C46	5.5140934422	3.7486768562	3.7577846288
H47	5.3363247852	4.2566541280	4.7124109035
H48	6.5378040133	3.3573504109	3.7844439311
H49	5.4444719771	4.4853200108	2.9547247103

TS-E4; Energy = -942.70736759163

C1	-0.1269693190	-0.2537225326	0.1740316193
C2	0.0691173570	-0.1694573667	1.7195159777
C3	3.0250297118	0.1834468147	0.8319605367
H4	-1.1041036855	0.1880651300	-0.0627042374
C5	0.7402322239	-1.4372657608	2.3199042324
H6	1.0701105622	-1.2192301658	3.3437820577
H7	-0.0391666387	-2.2056508284	2.4178636650
H8	4.0550501878	0.5406263251	0.6803531705
H9	-0.9522374939	-0.1942838081	2.1223713542
B10	2.2777762024	1.3376062680	1.7184444600
C11	0.7028972741	1.1951826120	2.1645217597
H12	0.1937694192	1.9492482328	1.5379972344
C13	1.9025917192	-2.0711626295	1.5462498464
H14	2.1544718858	-3.0258495164	2.0277076703
H15	1.5653421584	-2.3384609802	0.5375137834
C16	3.1759858256	-1.2267422418	1.4526006504
H17	3.6127220449	-1.1523670147	2.4584755905

H18	3.9093621713	-1.7924864067	0.8584222503
C19	2.3892597294	0.1011735049	-0.5919615985
H20	2.9341276802	0.7840944205	-1.2562303250
C21	3.4510434304	1.4207742376	3.2952301193
H22	2.8081793494	1.2958646309	4.1592219143
H23	4.2066507276	0.6560340966	3.1462901081
C24	3.5874903130	2.6225165748	2.7134120285
C25	3.9408687439	3.8394625474	2.3715545270
H26	2.4350838459	2.3889584402	1.1232876338
Si27	0.0012607997	1.7742075776	3.8447507389
C28	-1.8956797555	1.8491405555	3.7180264688
H29	-2.3172559131	2.3004763455	4.6238614203
H30	-2.2191844635	2.4586953897	2.8667966543
H31	-2.3508400601	0.8595597599	3.6067265836
C32	0.3753397633	0.6692919612	5.3520005800
H33	-0.0857209609	1.1110710178	6.2434820293
H34	-0.0533603893	-0.3304319393	5.2275872336
H35	1.4400755728	0.5401023427	5.5731747451
C36	0.5702517874	3.5418323620	4.2503174800
H37	0.0381627774	3.9131893038	5.1340090731
H38	1.6420441501	3.6157534220	4.4533567375
H39	0.3482016666	4.2249558130	3.4226666840
C40	0.8986556480	0.4696310414	-0.7201057395
H41	0.7996157128	1.5488534841	-0.5514140246
H42	0.5974494127	0.3132739672	-1.7650413326
H43	2.5533235023	-0.9033809384	-1.0076170019
H44	-0.2084898978	-1.3067752785	-0.1262607849
H45	3.5114907673	4.2943285040	1.4841933312
C46	4.9254520051	4.6561437600	3.1718115569
H47	4.4527314401	5.5778663574	3.5301310425
H48	5.3062614836	4.1044121169	4.0338205876
H49	5.7742682034	4.9497179070	2.5435042340

Z-5; Energy = -942.79205456831

C1	-0.0120072410	0.0382640667	-0.3639575919
C2	-0.3509861237	0.0324378045	1.1603491782
C3	2.7444090725	-0.2281131716	1.3658866918
H4	-0.7143144924	0.7142969339	-0.8686420910
C5	-0.2642142498	-1.3886919390	1.7719036747
H6	-0.4408059349	-1.3277277150	2.8528935894
H7	-1.1066438119	-1.9689639001	1.3706630079
H8	3.8104929828	-0.1140705702	1.6002159644
H9	-1.4166157666	0.2890461819	1.2208227316
B10	1.9861087942	1.0778048187	1.8638703488
C11	0.4210861011	1.1352102951	1.9463753776
H12	0.1389045036	2.1151181464	1.5183829324

C13	1.0121474613	-2.2000146553	1.5211290173
H14	0.8935728248	-3.1784080590	2.0056182395
H15	1.0935437443	-2.4201253140	0.4495844302
C16	2.3248949533	-1.5768409574	2.0098285705
H17	2.2880061671	-1.4635945154	3.1019879027
H18	3.1246460849	-2.3067158787	1.8184860941
C19	2.6257275293	-0.2413231745	-0.1981811297
H20	3.5140054247	0.2466817977	-0.6173156178
C21	5.1079371365	2.0517523025	3.3601722352
H22	5.5751822710	1.9608762758	4.3410914592
C23	3.7816534436	2.2418983735	3.3291423096
C24	2.8768674491	2.3850219120	2.1293205578
H25	3.2756191029	2.2932623481	4.2936411527
Si26	-0.2099672967	1.4182481358	3.7524541333
C27	-2.0777393996	1.0951177234	3.8338670459
H28	-2.4510425465	1.3306762826	4.8372339772
H29	-2.6237476874	1.7267630843	3.1243093062
H30	-2.3385822959	0.0540111712	3.6215496977
C31	0.6600146564	0.3373669140	5.0484187972
H32	0.3175084145	0.6088935002	6.0538412568
H33	0.4574725836	-0.7292025106	4.9106848402
H34	1.7472343550	0.4713688874	5.0262893695
C35	0.0585157684	3.2316134633	4.2408761615
H36	-0.3981337630	3.4239331638	5.2189050935
H37	1.1168170441	3.4976276214	4.3170536443
H38	-0.4057441974	3.9164350483	3.5225785189
C39	1.3999357876	0.4860081317	-0.7923792600
H40	1.4987134208	1.5601629228	-0.5786488426
H41	1.4543229829	0.4123252195	-1.8864919287
H42	2.6587705268	-1.2757787918	-0.5645680056
H43	-0.2209010312	-0.9574436705	-0.7772656517
H44	2.2592727219	3.2847042912	2.2476969397
H45	3.4842310529	2.5396478742	1.2266506699
C46	6.0552396150	1.9599538979	2.1977373368
H47	6.8611359905	2.6989485971	2.2931498400
H48	6.5390495476	0.9752986385	2.1593170234
H49	5.5613396776	2.1231501824	1.2369545645

E-5; Energy = -942.79465570958

C1	-0.7131957562	0.0988615442	0.0360046810
C2	-0.6427075853	-0.0679944723	1.5867887976
C3	2.3955394466	-0.2975067562	0.9575014861
H4	-1.5190156201	0.8069381031	-0.1965264838
C5	-0.4098690542	-1.5416189656	2.0075125967
H6	-0.2875888311	-1.5906448540	3.0966821362
H7	-1.3350474477	-2.0937085631	1.7917769330

H8	3.4876359052	-0.1982549002	0.9012007833
H9	-1.6537336173	0.1595478815	1.9481366717
B10	1.8119744259	0.9329675104	1.7853962075
C11	0.3160060459	0.9630331111	2.2560596419
H12	-0.0500329499	1.9764248738	2.0076393367
C13	0.7434826423	-2.3034576329	1.3454725078
H14	0.7433296514	-3.3290314975	1.7379684365
H15	0.5390745279	-2.4078100133	0.2728715663
C16	2.1455874679	-1.7154112776	1.5383729444
H17	2.3963968949	-1.7210621820	2.6081823963
H18	2.8590029869	-2.4059738887	1.0662184487
C19	1.8723801558	-0.1440976515	-0.5140256830
H20	2.6270310699	0.4011461344	-1.0935947283
C21	4.4633764756	2.5619550323	3.8198695352
H22	3.8707008531	3.3904836063	4.2110607206
C23	4.0338616660	1.9184703186	2.7285971675
C24	2.7618741217	2.2083870180	1.9706641402
H25	4.6470537449	1.1016978190	2.3441378533
Si26	0.1519334823	1.0605091134	4.1839078467
C27	-1.6163417541	0.6018293198	4.7000909661
H28	-1.7276215594	0.7362343919	5.7823435910
H29	-2.3550819253	1.2481750853	4.2130229762
H30	-1.8773259311	-0.4349371070	4.4686123294
C31	1.3845418567	-0.0445792719	5.1086683920
H32	1.2579474556	0.0736376617	6.1913939075
H33	1.2587726398	-1.1069570637	4.8775824050
H34	2.4164203876	0.2338783394	4.8671539660
C35	0.4372561818	2.8461852616	4.7560075411
H36	0.2114960905	2.9343236115	5.8253038181
H37	1.4731574686	3.1658230385	4.6134158813
H38	-0.2102077714	3.5526283216	4.2246876877
C39	0.5420155126	0.6181472899	-0.6923941450
H40	0.7009496428	1.6658665914	-0.3997718386
H41	0.3128058853	0.6583872459	-1.7653373575
H42	1.7997728933	-1.1334750890	-0.9843406096
H43	-1.0272931487	-0.8539878075	-0.4103963826
H44	3.0379842078	2.5043837358	0.9415098075
H45	2.2522624389	3.0725479607	2.4107815347
C46	5.7307130251	2.2475029667	4.5641442698
H47	6.4089442102	3.1105502349	4.5827400150
H48	5.5279078358	1.9883214924	5.6113914669
H49	6.2659968526	1.4086931013	4.1079676967

TS-Z6; Energy = -1134.45674149085

C1	-0.0312812156	-0.0882268377	0.0475992845
C2	0.0225019087	-0.0345806833	1.6052704166

C3	3.0659232827	0.0374562560	0.9982969150
H4	-0.9381122142	0.4412528843	-0.2742638473
C5	0.5062993865	-1.3683436501	2.2448615779
H6	0.7355473786	-1.1960762549	3.3040535057
H7	-0.3462367160	-2.0614510942	2.2357540202
H8	4.1354775746	0.2969304095	0.9651441396
H9	-1.0281383509	0.0429933712	1.9143983791
B10	2.3699026927	1.1116835029	2.0064345354
C11	0.7353479653	1.2566375323	2.1327688412
H12	0.3787656223	2.0601520290	1.4691098750
C13	1.6852311653	-2.1040521036	1.5902060919
H14	1.7993627993	-3.0746823398	2.0915429596
H15	1.4249876392	-2.3473598779	0.5524963204
C16	3.0380690984	-1.3846258791	1.6180392903
H17	3.3911975927	-1.3250957211	2.6566790948
H18	3.7622779264	-2.0201026714	1.0866292082
C19	2.5627486365	0.0280736424	-0.4753545438
H20	3.2336344941	0.6453364208	-1.0896742155
C21	2.9627938535	2.8359543776	1.3440279504
H22	3.3984652707	2.6201298049	0.3717423919
H23	2.1034983727	3.5012441893	1.3525420552
C24	3.6584075522	2.6187430639	2.4716117350
C25	4.5084039378	2.6748768693	3.4802559970
H26	2.8677591879	0.9368494370	3.1046541782
Si27	0.0891056310	1.8459198788	3.8312463390
C28	-1.8110563471	1.7678067914	3.8882527782
H29	-2.1865884902	2.2543341653	4.7962064341
H30	-2.2632894075	2.2793456532	3.0308083338
H31	-2.1849924557	0.7384065649	3.8925508110
C32	0.7447597714	0.8660272055	5.3212021058
H33	0.4275613909	1.3460836570	6.2544010663
H34	0.3640919579	-0.1605813928	5.3376746385
H35	1.8381603719	0.8137452123	5.3310835833
C36	0.5699045672	3.6702813459	4.0747411010
H37	0.1647580758	4.0513398179	5.0191705257
H38	1.6545536890	3.8158379079	4.1032509290
H39	0.1666896503	4.3001358798	3.2726819913
C40	1.1356073238	0.5446946673	-0.7328669328
H41	1.1204818696	1.6264628357	-0.5500484166
H42	0.9189371878	0.4331600645	-1.8042600696
H43	2.6625067962	-0.9853513806	-0.8900514824
H44	-0.1755982181	-1.1271404843	-0.2769319434
H45	4.4998532457	1.8725322309	4.2110374388
C46	5.4840619194	3.7547837929	3.7127310768
C47	6.3050200371	3.6714427820	4.8486695745
C48	7.2462342211	4.6607366456	5.1226779144

C49	7.3826979051	5.7510618342	4.2646656906
C50	6.5710868197	5.8447223021	3.1310445323
C51	5.6304846970	4.8582255450	2.8557435309
H52	6.2004731595	2.8228358336	5.5196969426
H53	7.8720763516	4.5790416326	6.0064723427
H54	8.1157063608	6.5239340302	4.4758120144
H55	6.6728247990	6.6918296017	2.4589940725
H56	5.0036956857	4.9392761469	1.9732666249

TS-E6; Energy = -1134.45141180190

C1	-0.1026768547	0.0782327490	-0.2075345969
C2	-0.1794412858	0.0229754048	1.3490136347
C3	2.9033347494	-0.0798336139	1.0021827108
H4	-0.9381709292	0.6961611945	-0.5627501107
C5	0.1534944610	-1.3855255368	1.9200740298
H6	0.2956430847	-1.3103990419	3.0052231245
H7	-0.7382719698	-2.0119963992	1.7805969698
H8	3.9872900884	0.1015260327	1.0707751367
H9	-1.2445095166	0.1588021663	1.5797423823
B10	2.1957936507	0.9662706959	2.0258359473
C11	0.5717324686	1.2190498550	2.0272953672
H12	0.3149252345	2.0914515723	1.4068515042
C13	1.3367216211	-2.1531400514	1.3126925356
H14	1.3430526971	-3.1634568993	1.7435977091
H15	1.1602509001	-2.3003069386	0.2400719226
C16	2.7226822952	-1.5336403619	1.5185731493
H17	2.9652373493	-1.5681554519	2.5896247915
H18	3.4564594636	-2.1836554609	1.0188846363
C19	2.5318072033	0.0395022815	-0.5049220265
H20	3.2924903179	0.6473073378	-1.0152839244
C21	2.9222691320	2.7535119976	1.4541818899
H22	3.3499536608	2.5772063100	0.4709966531
H23	2.0585581857	3.4092040875	1.4998175597
C24	3.6231159411	2.4902282797	2.5614814952
C25	4.4720823404	2.5087093103	3.5666264787
H26	2.6070418154	0.7583040221	3.1472289352
Si27	-0.1451258676	1.7168450003	3.7273110687
C28	-2.0422919022	1.8326129205	3.6411242705
H29	-2.4431113717	2.2573498457	4.5689634802
H30	-2.3721913626	2.4749289997	2.8165683775
H31	-2.5113171532	0.8523897150	3.5035515465
C32	0.2942772652	0.5496086553	5.1592399058
H33	-0.0381678986	0.9855492045	6.1089028602
H34	-0.1944494996	-0.4255758940	5.0622143909
H35	1.3724956118	0.3780421116	5.2336157723
C36	0.4929142403	3.4513987921	4.1791115610

H37	0.0598480684	3.7811029234	5.1305880420
H38	1.5817054852	3.4752702503	4.2906544329
H39	0.2147458684	4.1949238378	3.4224897602
C40	1.1688931311	0.6714903820	-0.8422476632
H41	1.2090521184	1.7367855666	-0.5851982096
H42	1.0406257561	0.6453963750	-1.9331378923
H43	2.6034599691	-0.9489120693	-0.9809957694
H44	-0.2914312700	-0.9225972968	-0.6176087577
H45	5.0583837089	3.4305373262	3.5983437579
C46	4.7452780360	1.5626583130	4.6666416024
C47	5.0749038031	2.0944480360	5.9243644089
C48	5.3414635575	1.2573019561	7.0044016249
C49	5.3040804746	-0.1277333223	6.8394736895
C50	5.0077160108	-0.6665385181	5.5870298324
C51	4.7325798664	0.1682753445	4.5056494825
H52	5.1045108584	3.1729055007	6.0566776780
H53	5.5796534936	1.6858893219	7.9735694027
H54	5.5152238383	-0.7830613822	7.6795191938
H55	4.9964761703	-1.7434766533	5.4470567806
H56	4.5257727193	-0.2569019612	3.5320995297

Z-7; Energy = -1134.53381770739

C1	0.1667526324	-0.1706483212	-0.3368797177
C2	-0.4036943197	-0.0134871323	1.1085520794
C3	2.5734605788	-0.5601983701	1.8354257786
H4	-0.3695384371	0.5257626894	-0.9944442230
C5	-0.5709545119	-1.3794088313	1.8210080545
H6	-0.9052324143	-1.2103789047	2.8521377476
H7	-1.4003661284	-1.9050780778	1.3279113257
H8	3.5959687125	-0.5302312556	2.2307001481
H9	-1.4306661279	0.3515457320	0.9772779637
B10	1.8970086719	0.8518775841	2.1029308222
C11	0.3551348767	1.0718656301	1.9319789798
H12	0.2481788391	2.0352868005	1.3998603693
C13	0.6306451264	-2.3313761087	1.8367116064
H14	0.3300459014	-3.2492972231	2.3593008400
H15	0.8526672976	-2.6470253656	0.8099102910
C16	1.9123789927	-1.8021738252	2.4903596064
H17	1.7192324516	-1.5956411455	3.5520819657
H18	2.6467868681	-2.6202613521	2.4806252436
C19	2.7007350979	-0.6925628172	0.2768351385
H20	3.6918402393	-0.3296692310	-0.0196329961
C21	4.8133496411	1.6442141976	4.0562464731
H22	5.0347289518	1.5197085247	5.1163628462
C23	3.5467779242	1.9702047984	3.7423891981
C24	2.8861320210	2.0861982930	2.3939847186

H25	2.8775251728	2.1193605142	4.5902064130
Si26	-0.5028848856	1.5637904420	3.5936415355
C27	-2.3858140685	1.4436179126	3.4004967968
H28	-2.8751263415	1.7979003144	4.3151807283
H29	-2.7435431455	2.0677089317	2.5740555063
H30	-2.7288084640	0.4208368389	3.2182475119
C31	0.0303994971	0.5076315992	5.0790209185
H32	-0.4241480727	0.8977569192	5.9972343322
H33	-0.2751342655	-0.5386723444	4.9818231937
H34	1.1167094605	0.5203829870	5.2211176504
C35	-0.1031668265	3.3743118073	3.9975761290
H36	-0.6650545917	3.6897470690	4.8846152484
H37	0.9573613529	3.5405562577	4.2080430544
H38	-0.3871428176	4.0417172220	3.1763263808
C39	1.6693045151	0.0971652539	-0.5586933459
H40	1.8520327288	1.1711537625	-0.4079311441
H41	1.8842328427	-0.0756581408	-1.6214009069
H42	2.6771636775	-1.7525878519	-0.0078474363
H43	-0.0847140626	-1.1724979614	-0.7095474004
H44	2.3684352902	3.0515340460	2.3192148016
H45	3.6432911133	2.0631972233	1.6023236129
C46	5.9649984973	1.3841497650	3.1664127620
C47	6.8560535050	0.3478529846	3.4971845556
C48	7.9651477573	0.0665716380	2.7030401509
C49	8.2214947057	0.8274683156	1.5613694228
C50	7.3619888089	1.8767732523	1.2327853341
C51	6.2501740708	2.1547874372	2.0265107189
H52	6.6655421152	-0.2474539237	4.3867618953
H53	8.6323166914	-0.7458572603	2.9778613619
H54	9.0878877947	0.6134398914	0.9424030772
H55	7.5642595593	2.4915830931	0.3599623652
H56	5.6142388673	2.9979302083	1.7791249287

E-7; Energy = -1134.53957051134

C1	-0.3457545215	0.8098570102	-0.8591450935
C2	-0.6729080617	0.5115144781	0.6375572313
C3	2.3003350261	-0.4056315711	0.6223322558
H4	-0.8995387720	1.7089289314	-1.1588696123
C5	-0.8735725166	-1.0024789567	0.9041215486
H6	-1.0162506791	-1.1638595818	1.9798923673
H7	-1.8238803333	-1.2940655902	0.4359041980
H8	3.3700450727	-0.5739727073	0.8025737698
H9	-1.6641925592	0.9498881744	0.8090774731
B10	1.8261257341	0.8539527498	1.4756292576
C11	0.3080823204	1.2212304503	1.6192829850
H12	0.2502101419	2.3092717370	1.4302871789

C13	0.2020425953	-1.9700043704	0.3983979480
H14	-0.1160372645	-2.9914254877	0.6458153590
H15	0.2318966460	-1.9372861208	-0.6975959219
C16	1.6163762527	-1.7608975367	0.9499625896
H17	1.6066488066	-1.9115427812	2.0383730319
H18	2.2486479199	-2.5653785750	0.5480161979
C19	2.1764206918	-0.0141388800	-0.8921176312
H20	3.1459040915	0.3726145395	-1.2287349114
C21	4.2126919748	1.4876950344	4.2208131540
H22	3.6866123342	2.3472635133	4.6362103409
C23	3.9561510242	1.1481569351	2.9463058562
C24	2.9648802288	1.8309935084	2.0438566230
H25	4.4874219045	0.3036471855	2.5108586166
H26	2.5668057385	2.7287583462	2.5283172490
Si27	-0.2927294328	1.2145374723	3.4626974473
C28	-2.1892109209	1.1521698732	3.5166660340
H29	-2.5261914163	1.2285870798	4.5569958896
H30	-2.6330270521	1.9899859571	2.9672276896
H31	-2.6026508806	0.2273010574	3.1042428403
C32	0.4128643900	-0.2177610042	4.4839927024
H33	0.0576625607	-0.1535478293	5.5192881950
H34	0.1170059598	-1.1978463755	4.0966142005
H35	1.5075898507	-0.1835867385	4.5119641549
C36	0.2106448532	2.8391115180	4.3039358611
H37	-0.2423388406	2.8952819083	5.3007989827
H38	1.2928356782	2.9287094710	4.4325741336
H39	-0.1338440225	3.7122458494	3.7383912263
C40	1.1261431614	1.0618232648	-1.2393951724
H41	1.4407429490	2.0128764702	-0.7862536831
H42	1.1656511594	1.2406058840	-2.3218973452
H43	1.9966732011	-0.9159781443	-1.4918200771
H44	-0.7509099879	-0.0000259142	-1.4803009715
H45	3.5026401982	2.1779991330	1.1417230480
C46	5.1507151700	0.8391541237	5.1524479796
C47	5.3181785790	1.3910664545	6.4347013476
C48	6.1912853579	0.8259163350	7.3618536821
C49	6.9239045150	-0.3128497973	7.0302576980
C50	6.7689872598	-0.8771445559	5.7614253659
C51	5.8959800056	-0.3124033821	4.8371671710
H52	4.7515108081	2.2788742818	6.7036947339
H53	6.2978591774	1.2768213940	8.3446163932
H54	7.6048237890	-0.7578972767	7.7496141671
H55	7.3314213419	-1.7667500581	5.4915162833
H56	5.7900562016	-0.7756319276	3.8612687477

TS-Z7; Energy = -1134.49298866643

C1	-0.1297809261	-0.0961206851	0.0758059348
C2	-0.0610450822	-0.0453036647	1.6319073946
C3	2.9879365530	-0.0756054490	1.0290979940
H4	-0.9846278758	0.5136485393	-0.2458480416
C5	0.2925694158	-1.4263657517	2.2411806806
H6	0.3975844680	-1.3263744586	3.3273160814
H7	-0.5756104883	-2.0827607187	2.0879321140
H8	4.0655465011	0.0914153605	0.9524563712
H9	-1.1011139076	0.1186241881	1.9390998809
B10	2.3331803335	1.1902022211	1.8136851760
C11	0.7528961290	1.1650490847	2.2159959612
H12	0.3122422743	2.0606388880	1.7387265460
C13	1.5215329857	-2.1577295123	1.6928500211
H14	1.6123952233	-3.1151249852	2.2234647610
H15	1.3432129948	-2.4274303832	0.6446948897
C16	2.8574962476	-1.4164940304	1.8065147458
H17	3.0916582459	-1.2507412925	2.8657144498
H18	3.6381058049	-2.0957679087	1.4352288133
C19	2.4665390277	-0.1955658463	-0.4369350188
H20	3.1735550681	0.3179367519	-1.1017362177
C21	3.6393046432	1.7949049854	3.0867116105
H22	3.2609164953	1.8350046608	4.1043306280
C23	3.0589543247	2.7615192681	2.2305755345
C24	2.9993493441	2.6522391217	0.8349238327
H25	2.2976529884	3.3911553868	2.6787002764
Si26	0.2428861210	1.4818954860	4.0502596005
C27	-1.6443446366	1.3387989979	4.2227872586
H28	-1.9494786891	1.6510765878	5.2283140211
H29	-2.1671646370	1.9836696936	3.5071148630
H30	-2.0060745725	0.3166874043	4.0745250198
C31	1.0225336834	0.3260671179	5.3488524681
H32	0.9607697659	0.7891434520	6.3408135792
H33	0.5021362730	-0.6348876753	5.4082429458
H34	2.0772889338	0.1139886353	5.1497201729
C35	0.6494945735	3.2640087105	4.6012879566
H36	0.1233613341	3.4654087890	5.5421815769
H37	1.7127786866	3.4402261242	4.7944301010
H38	0.3072927542	4.0141841331	3.8789528720
C39	1.0797447188	0.3996710628	-0.7348018712
H40	1.1444945631	1.4871693706	-0.6157656989
H41	0.8571903301	0.2385045992	-1.7985690291
H42	2.4942943111	-1.2469894653	-0.7526409494
H43	-0.3801285664	-1.1225387277	-0.2255752035
H44	2.3140885046	3.3107942128	0.3119986353
H45	3.8090235356	2.2518234964	0.2406307235
C46	5.0037314599	1.2176467781	3.0107320594

C47	5.3699388051	0.2278265946	3.9389163005
C48	6.6495610442	-0.3207767362	3.9428628285
C49	7.6021176920	0.1132134976	3.0204133754
C50	7.2612575809	1.1095491984	2.1055378661
C51	5.9798591869	1.6575744136	2.1017103889
H52	4.6384321850	-0.1113057808	4.6680092082
H53	6.9038123238	-1.0873972078	4.6694924050
H54	8.6006878174	-0.3137936559	3.0203667450
H55	7.9992034985	1.4694917073	1.3938908412
H56	5.7434314295	2.4504938622	1.4002551740

INT-7; Energy = -1134.52226639105

C1	-0.6466650528	-0.1302435207	0.5051615146
C2	-0.3408575327	-0.2467458111	2.0306545371
C3	2.5199602539	-0.7964287344	0.9537931187
H4	-1.4123115995	0.6441063077	0.3662871580
C5	-0.1849436951	-1.7193188322	2.4872483306
H6	0.0988022187	-1.7398462926	3.5467155424
H7	-1.1798884835	-2.1834211182	2.4415497837
H8	3.5875676006	-0.7995654997	0.7046323773
H9	-1.2552385354	0.0950155689	2.5306717118
B10	2.2060336535	0.5053175398	1.8147487430
C11	0.8048919025	0.7058831417	2.4966501361
H12	0.5051626655	1.7391132474	2.2385246672
C13	0.7755666046	-2.6165132918	1.6990553097
H14	0.7451078718	-3.6206577307	2.1423497018
H15	0.3961836262	-2.7425163473	0.6776979285
C16	2.2377369767	-2.1604329306	1.6417958474
H17	2.6512988085	-2.1524175705	2.6604451915
H18	2.8022373415	-2.9340713710	1.1019267610
C19	1.7802218112	-0.6489409344	-0.4231764866
H20	2.4830848378	-0.2046564794	-1.1361057540
C21	3.2960286134	1.7138592063	1.8345589511
H22	2.7734007121	2.6154758388	2.1854416064
C23	3.7508395779	2.0257512117	0.4186006604
C24	4.9645391892	1.8447189354	-0.1082926148
H25	2.9707460267	2.4397442604	-0.2223021952
Si26	0.8679798445	0.9198958376	4.4259573674
C27	-0.8885569285	0.7451447524	5.1247119158
H28	-0.8717773128	0.9531887175	6.2009384521
H29	-1.5799334779	1.4597888882	4.6644347219
H30	-1.3058260355	-0.2571839803	4.9905578217
C31	1.9984422924	-0.3112432121	5.3210819384
H32	1.9754365289	-0.1135984561	6.3996217095
H33	1.6911369349	-1.3514233578	5.1733006431
H34	3.0387353763	-0.2176389735	4.9938471540

C35	1.4450389624	2.6740744846	4.8556991478
H36	1.3266909598	2.8449855190	5.9323353400
H37	2.4983713341	2.8398263273	4.6143654915
H38	0.8511584480	3.4351642208	4.3369736442
C39	0.5155202055	0.2328020728	-0.4369855933
H40	0.8130820224	1.2709890085	-0.2304952311
H41	0.1227806744	0.2528698407	-1.4621417886
H42	1.5414637598	-1.6450306714	-0.8184044008
H43	-1.1147300257	-1.0638405207	0.1656424282
H44	5.1662259858	2.1009542145	-1.1441014242
H45	5.7944177225	1.4508068307	0.4701738878
C46	4.4743376961	1.5049970450	2.7859080927
C47	5.0783207499	0.2601101212	3.0173313774
C48	6.1768915989	0.1374658941	3.8725715216
C49	6.6999956001	1.2565287201	4.5173313853
C50	6.1149420935	2.5038740248	4.2949604616
C51	5.0213177707	2.6218040460	3.4396260444
H52	4.6974713596	-0.6272759638	2.5257103183
H53	6.6221735109	-0.8406271057	4.0327390775
H54	7.5523235800	1.1596935402	5.1833412359
H55	6.5113022947	3.3884980223	4.7859660804
H56	4.5837188060	3.6012130470	3.2648245408

TS-E7; Energy = -1134.49000541148

C1	-0.0932558678	-0.0086006425	0.0625598957
C2	-0.0042226047	-0.0487574614	1.6196699833
C3	3.0138476763	0.0151680707	0.9832742616
H4	-0.9975125020	0.5532960580	-0.2064480746
C5	0.4533842565	-1.4248555563	2.1759998721
H6	0.7190428714	-1.3154395929	3.2349648442
H7	-0.4192841520	-2.0921911621	2.1550820833
H8	4.0909691795	0.2186166208	0.9096788763
H9	-1.0477365727	0.0328442682	1.9480511982
B10	2.3827374773	1.1053376085	2.0107052118
C11	0.7413314371	1.2054651711	2.2062422537
H12	0.4173686495	2.0259453130	1.5475114494
C13	1.5942192454	-2.1417069353	1.4472776125
H14	1.6992864607	-3.1464322027	1.8779551772
H15	1.3135308299	-2.3051570558	0.3994907175
C16	2.9529524323	-1.4437132534	1.5183145264
H17	3.3031259070	-1.4638043068	2.5561499385
H18	3.6719720284	-2.0495114441	0.9471813756
C19	2.4908803579	0.1080596615	-0.4836255565
H20	3.1623650279	0.7637924122	-1.0539949457
C21	3.3087148099	1.3517124039	3.6116895109
H22	2.5367281647	1.7324341968	4.2675889449

C23	3.7414378453	2.1955769241	2.5569727997
C24	2.8655547888	2.9323890009	1.7621322390
H25	4.6964576499	1.9409694104	2.1039419652
H26	2.0123309517	3.4501444091	2.1783060421
Si27	-0.1314496673	1.7761079119	3.8199927897
C28	-1.9675260695	2.0887881876	3.4274655306
H29	-2.4597204817	2.5428775199	4.2956744351
H30	-2.0877506597	2.7800407861	2.5854378317
H31	-2.5181652759	1.1742252468	3.1863290098
C32	-0.0679432696	0.5242664574	5.2473097823
H33	-0.4813727642	0.9701796622	6.1596898176
H34	-0.6679644299	-0.3624275329	5.0174727699
H35	0.9450678256	0.1794336668	5.4733781236
C36	0.4901540087	3.4651304221	4.4546096856
H37	-0.1235887219	3.7596993227	5.3142603928
H38	1.5336677963	3.4943012075	4.7805375703
H39	0.3616243739	4.2442491090	3.6936770730
C40	1.0688604315	0.6518951056	-0.6995138151
H41	1.0733813913	1.7222828056	-0.4608136580
H42	0.8403437716	0.5984757068	-1.7726239365
H43	2.5818841528	-0.8785596829	-0.9598517484
H44	-0.2611493278	-1.0239626630	-0.3188657983
H45	3.2328168350	3.3083736248	0.8131473269
C46	4.2429221216	0.4168343697	4.2922633050
C47	3.9723807306	0.0452951802	5.6200815883
C48	4.8146295839	-0.8153764651	6.3210408780
C49	5.9601551826	-1.3265860262	5.7125224866
C50	6.2479092356	-0.9645411560	4.3954529749
C51	5.4026127293	-0.1079574953	3.6936915390
H52	3.0937477115	0.4508351255	6.1145349559
H53	4.5758044710	-1.0809502991	7.3470934648
H54	6.6196687667	-1.9968840046	6.2553378707
H55	7.1355607287	-1.3562214441	3.9065666989
H56	5.6495047911	0.1405497133	2.6663002950

TS for 9-BBN + phenylallene; Energy = -686.51232496607

C1	3.5466935257	0.1418998418	1.6990611548
H2	4.5573633174	-0.2751536913	1.7815168876
B3	3.5124092211	1.7473033521	1.9036443421
C4	3.0326849147	-0.1662785907	0.2677718969
H5	3.7883596947	0.1878940300	-0.4464187857
C6	4.5942827992	2.3000363359	3.2962294664
C7	4.6702954059	3.0485502046	2.0896164109
C8	4.8436962736	2.4522485602	0.8304729351
H9	4.1521898578	4.0046035062	2.0933294904
H10	2.9675033412	-1.2541157135	0.1211776412

H11	4.5989447804	3.0443232746	-0.0449042112
H12	5.5186516571	1.6235650745	0.6615918824
C13	1.9898688662	2.2505611152	1.7911199087
H14	1.8843361186	3.3375284334	1.9252241090
C15	1.4846791529	1.9291297638	0.3581235181
H16	2.0267664285	2.5838877663	-0.3389223830
H17	0.4238719794	2.2007346185	0.2555824115
C18	1.6692149686	0.4641019311	-0.0987252682
H19	1.5370510340	0.4135983184	-1.1874274033
H20	0.8635794587	-0.1487737022	0.3148250371
C21	1.1663495485	1.5845634450	2.9244387107
H22	1.5191115695	1.9986239771	3.8801170555
H23	0.1075868114	1.8721094923	2.8485789686
C24	2.6933092848	-0.5139751679	2.8169615564
H25	3.2352364554	-0.3948487955	3.7624571214
H26	2.6297724281	-1.5980424913	2.6434570717
C27	1.2634334793	0.0453734539	2.9885022227
H28	0.6033353174	-0.3918568570	2.2340858051
H29	0.8628645632	-0.2968066460	3.9518282401
C30	5.5837674682	1.3206279438	3.8161843401
C31	5.3413006960	0.7309506423	5.0691146432
C32	6.2440148586	-0.1665879495	5.6341011638
C33	7.4211795869	-0.4954454613	4.9608099556
C34	7.6847393159	0.0940100150	3.7239406252
C35	6.7804926087	0.9920814308	3.1582085480
H36	4.4322381607	0.9889257278	5.6069308827
H37	6.0281212007	-0.6067106906	6.6036744681
H38	8.1276836790	-1.1943525625	5.3983340973
H39	8.6058081294	-0.1386379824	3.1967384658
H40	7.0240713143	1.4612404266	2.2112131169
H41	4.0597824589	2.8192281600	4.0894952535

TS for 1a + 1,1-dimethylallene; Energy = -982.06027898495

C1	-0.0061059714	0.0052765411	0.0180441045
C2	0.0091932189	-0.0087934148	1.5765617828
C3	3.0590890125	-0.0021788004	1.0951654384
H4	-0.8866485925	0.5766758755	-0.3045752328
C5	0.4069227469	-1.3840348573	2.1801021747
H6	0.5993216781	-1.2593220209	3.2534631752
H7	-0.4711394470	-2.0408920245	2.1092594455
H8	4.1357597932	0.1732835939	1.0537091494
H9	-1.0483548728	0.0888999440	1.8487239041
B10	2.4062167443	1.1240251004	2.0934431454
C11	0.7633557390	1.2271183081	2.1960560280
H12	0.5352009392	2.0613109769	1.5087831235
C13	1.5851003270	-2.1283406570	1.5467014020

H14	1.6543794630	-3.1221647336	2.0090817502
H15	1.3723776553	-2.3173120334	0.4873894726
C16	2.9415486513	-1.4366673423	1.6832742242
H17	3.2176127075	-1.4167620098	2.7457320778
H18	3.6918444709	-2.0712303246	1.1887158432
C19	2.5954642911	0.0525672402	-0.3924478353
H20	3.3124479901	0.6655536773	-0.9548098387
C21	3.5824947275	1.3718470127	3.4584762299
C22	3.1607366599	2.5786172725	2.8068862419
C23	3.2718409429	2.7569463141	1.4318610184
H24	2.4019324855	3.1704288465	3.3071219465
Si25	-0.3132404881	1.8446523234	3.6727511131
C26	-2.0303104002	2.2880775868	2.9724752234
H27	-2.6505512831	2.7181481856	3.7676678474
H28	-1.9558085136	3.0386983651	2.1769120200
H29	-2.5761402747	1.4311652731	2.5667557389
C30	-0.6003529883	0.5748958622	5.0579477175
H31	-1.2247545122	1.0184919230	5.8425097057
H32	-1.1288645188	-0.3074124027	4.6823326756
H33	0.3246065831	0.2285500012	5.5281680967
C34	0.2369861245	3.4895891659	4.4744773440
H35	-0.5805795930	3.8373927539	5.1174142660
H36	1.1301706446	3.4337823507	5.1024035534
H37	0.3999777023	4.2732704595	3.7247888402
C38	1.2043400840	0.6282947764	-0.6946020771
H39	1.2241657033	1.7027157232	-0.4740282094
H40	1.0314507215	0.5601459463	-1.7773544737
H41	2.6761472291	-0.9533134759	-0.8286497774
H42	-0.1731202623	-1.0145140063	-0.3531874013
H43	2.6839519753	3.5371950858	0.9605426856
H44	4.1105519328	2.3841436460	0.8580931731
C45	5.0027948815	0.8589928467	3.2257737823
H46	5.6457606777	1.2291234628	4.0354586820
H47	5.0587989518	-0.2333079102	3.2431979182
H48	5.4402479898	1.2044679749	2.2876432239
C49	3.1471631311	1.1423684788	4.8962164423
H50	3.8459311323	1.6135652685	5.6009317466
H51	2.1527523544	1.5328059983	5.1065885026
H52	3.1374772313	0.0711026781	5.1266718026

TS for 1a + pinacolborane; Energy = -1156.86083921490

C1	-0.0500269441	-0.2005157449	0.1030547416
C2	-0.0430155552	-0.1130880316	1.6587820198
C3	3.0159132621	-0.3577624314	1.1942634262
H4	-0.8560412763	0.4457533008	-0.2694000111
C5	0.1960319743	-1.4955441534	2.3196104584

H6	0.2634083807	-1.3699811490	3.4057445270
H7	-0.7058835335	-2.0997020501	2.1475877757
H8	4.1034212484	-0.2562833496	1.1450898544
H9	-1.0819647821	0.1241708499	1.9165446489
B10	2.4112113303	0.9801023769	1.8976816259
C11	0.8205922996	1.0608360421	2.2474841229
H12	0.4518536321	1.9703494158	1.7366711491
C13	1.3951423813	-2.3223699710	1.8448786968
H14	1.3991275537	-3.2673783939	2.4045508537
H15	1.2421653792	-2.6103306483	0.7974823564
C16	2.7731242195	-1.6691889861	1.9924208173
H17	2.9854611175	-1.4938857931	3.0551345122
H18	3.5157760659	-2.4093753076	1.6586930612
C19	2.5491436048	-0.4704823770	-0.2919818502
H20	3.3171713873	-0.0157540898	-0.9307857195
C21	3.7231596655	1.5124912424	3.2936614095
H22	3.3413469962	1.5839250650	4.3094020718
C23	3.2284515254	2.4970600006	2.4192976269
C24	3.2280603573	2.3458035041	1.0198435955
H25	2.5015354498	3.1983422127	2.8182096149
Si26	0.2519855121	1.4379751216	4.0546926511
C27	-1.6462774255	1.3699073868	4.1504218989
H28	-1.9782227355	1.7218307365	5.1342656645
H29	-2.1173128388	2.0128510277	3.3979171292
H30	-2.0403775994	0.3578187418	4.0162601794
C31	0.9282795997	0.2800749035	5.4064544748
H32	0.8584374718	0.7761533517	6.3818977655
H33	0.3523056920	-0.6481276135	5.4752888208
H34	1.9757028786	0.0057369208	5.2509573098
C35	0.6988761253	3.2157362081	4.5873172728
H36	0.1211853053	3.4635197109	5.4860041267
H37	1.7540967310	3.3482214171	4.8474873661
H38	0.4395536002	3.9608378808	3.8263452356
C39	1.2198460138	0.2105579866	-0.6591400090
H40	1.3491838135	1.2932452313	-0.5477389884
H41	1.0356355556	0.0499650476	-1.7301996865
H42	2.5184329447	-1.5272827389	-0.5892302892
H43	-0.3416157772	-1.2192584912	-0.1870407914
H44	2.6422349636	3.0547379674	0.4431441308
H45	4.0794304333	1.9104920142	0.5105415203
B46	5.0626408687	0.7521876762	3.1728635895
O47	5.4815217769	-0.1272741352	4.1470560094
O48	5.9817426580	0.9053238099	2.1548149296
C49	7.0533053580	-0.0232375818	2.3869491098
H50	6.9939390648	-0.8274952907	1.6444849995
H51	8.0115398467	0.4907064445	2.2669732721

C52	6.8189196364	-0.5383006895	3.8270889625
H53	7.5114863238	-0.0871766672	4.5475610205
H54	6.8955756682	-1.6265734114	3.9080032042

TS for 1a + 10-R = H; Energy = -725.82099334922

C1	-0.1841586843	-0.1608336458	0.1156269555
C2	-0.0406541625	-0.0294268731	1.6593370788
C3	3.0055891396	-0.0554521405	0.8909482108
H4	-1.0802433407	0.3931382559	-0.1935141480
C5	0.3993267446	-1.3470127347	2.3444448018
H6	0.6273845221	-1.1341386220	3.3991857043
H7	-0.4660288403	-2.0240384177	2.3578828550
H8	4.0782775149	0.1174363210	0.7554953600
H9	-1.0553701713	0.1542558242	2.0404878649
B10	2.3730529073	1.1978729997	1.7079367320
C11	0.8025828143	1.1926311361	2.0937628724
H12	0.3224034616	2.0956954537	1.6847586210
C13	1.5685985399	-2.1124673291	1.7145958016
H14	1.6995037630	-3.0515808364	2.2690459065
H15	1.2913390050	-2.4175873267	0.6978801716
C16	2.9216652768	-1.3928142006	1.6799058896
H17	3.2666990685	-1.2289660720	2.7076364122
H18	3.6467185053	-2.0886011169	1.2333769283
C19	2.3932300640	-0.1825245568	-0.5375580888
H20	3.0419754277	0.3545500587	-1.2421252047
C21	3.5605427666	1.7200213841	3.0570273426
H22	3.1047647780	1.6846799202	4.0448301419
C23	3.0347791871	2.7498206705	2.2317238303
C24	3.0589753387	2.7098526133	0.8301889125
H25	2.2312559920	3.3385005326	2.6692065704
C26	0.9720398691	0.3733356653	-0.7523347110
H27	1.0130159906	1.4630631771	-0.6307395055
H28	0.7013694894	0.2109311685	-1.8045383630
H29	2.4297182412	-1.2332168004	-0.8570500218
H30	-0.3903166747	-1.2079412717	-0.1427954147
H31	2.3924668244	3.3792001029	0.2965611117
H32	3.9064846599	2.3442031163	0.2662965120
C33	4.9421058722	1.1754783782	3.0428763872
C34	5.2809794477	0.1826909242	3.9782378905
C35	6.5697163025	-0.3406625469	4.0423586320
C36	7.5590221051	0.1224528767	3.1745701062
C37	7.2448398387	1.1222556508	2.2539864332
C38	5.9545592054	1.6453175050	2.1899814072
H39	4.5201930315	-0.1765968990	4.6667419509
H40	6.8021074376	-1.1095681290	4.7738570293
H41	8.5649377375	-0.2841473314	3.2215005992

H42	8.0106225530	1.5052142327	1.5850909484
H43	5.7410173306	2.4433589860	1.4868944096
H44	0.6900039101	1.2916585518	3.1847831232

TS for 1a + 10-R = SiH_3; Energy = -1016.50993346100

C1	-0.1564737461	-0.1337673266	0.0913675013
C2	-0.0592160190	-0.0524156100	1.6436411727
C3	2.9899782281	-0.0589851906	0.9814952754
H4	-1.0324802304	0.4476178574	-0.2250042972
C5	0.3341559813	-1.4086152306	2.2834886788
H6	0.4849492203	-1.2720495065	3.3627981958
H7	-0.5327312673	-2.0769809574	2.1907172356
H8	4.0652014408	0.1147379519	0.8822708540
H9	-1.0914323519	0.1130277022	1.9828316701
B10	2.3457981905	1.2027764958	1.7794992154
C11	0.7611820189	1.1765535664	2.1617545270
H12	0.3063364917	2.0626899712	1.6845054050
C13	1.5463007131	-2.1425578307	1.7016443256
H14	1.6576201711	-3.0936459220	2.2392461027
H15	1.3329848266	-2.4240371106	0.6630766818
C16	2.8845636654	-1.3991535529	1.7637707874
H17	3.1568794750	-1.2322233871	2.8129371926
H18	3.6512524182	-2.0784526211	1.3647288392
C19	2.4341683174	-0.1825508777	-0.4709708539
H20	3.1157989941	0.3457132624	-1.1504901486
C21	3.5996379939	1.7773331951	3.0775938110
H22	3.1981641356	1.8036215138	4.0885163061
C23	3.0469513659	2.7709718346	2.2296002594
C24	3.0147170875	2.6815081015	0.8313874724
H25	2.2738300655	3.3904379816	2.6777761271
Si26	0.3608344715	1.4788602976	3.9965383838
C27	1.0300339122	0.3885259386	-0.7378124495
H28	1.0773500436	1.4771635467	-0.6152133840
H29	0.7913044870	0.2283817502	-1.7980114226
H30	2.4725746666	-1.2329700300	-0.7894664391
H31	-0.3806852021	-1.1705060002	-0.1933213718
H32	2.3362874230	3.3429781770	0.3030062996
H33	3.8380833958	2.2915008366	0.2482298853
C34	4.9681250194	1.2047812924	3.0289448849
C35	5.3127257753	0.2080032386	3.9572191813
C36	6.5938479860	-0.3363107864	3.9881818229
C37	7.5677281304	0.1095953426	3.0938928797
C38	7.2468732767	1.1131668323	2.1796465512
C39	5.9638804189	1.6567557426	2.1486048916
H40	4.5635617888	-0.1374203405	4.6650504921
H41	6.8330116944	-1.1080895606	4.7144181702

H42	8.5677821667	-0.3134166311	3.1156633546
H43	8.0012992664	1.4825580581	1.4904958281
H44	5.7431412057	2.4566113596	1.4498783770
H45	0.8083318713	2.8392781384	4.4198683204
H46	1.0099250647	0.5177446195	4.9305047322
H47	-1.1094310263	1.4113557425	4.2333093294

TS-Z8; Energy = -956.87049382128

C1	0.6719142029	-0.9772341337	0.9872532919
C2	0.8044993676	-0.5048418963	2.4650882721
C3	3.1984542246	1.0910395136	1.2436493896
H4	-0.3962830256	-1.0916620458	0.7603946058
C5	1.9680339197	-1.2104632351	3.1999479206
H6	2.0586768313	-0.8042054115	4.2128207216
H7	1.6687080585	-2.2587822022	3.3380972258
H8	3.9452274571	1.8206719810	0.9174597248
H9	-0.0979127556	-0.8715282827	2.9725395661
B10	1.9828819492	1.8958289968	1.9603007670
C11	0.7302104836	1.0578508010	2.6065894861
H12	-0.1330663925	1.3306383853	1.9800007171
C13	3.3412700933	-1.2130760294	2.5192171705
H14	4.0358988783	-1.7733518956	3.1593836296
H15	3.2805916619	-1.7917506968	1.5892848961
C16	3.9656101805	0.1551718040	2.2216299309
H17	4.1482744945	0.6846572704	3.1653438007
H18	4.9611912905	-0.0305929139	1.7941431411
C19	2.7338755858	0.3407056873	-0.0431661966
H20	2.9136403041	0.9924356204	-0.9080949212
C21	2.7219012661	3.3569418621	2.9159197681
H22	2.4708716248	3.3464938548	3.9723315737
C23	1.6083850841	3.6200978063	2.0812496651
C24	1.5350565220	3.2299713980	0.7348504491
H25	0.6570976779	3.7280768316	2.5973346478
C26	1.2544771241	-0.0799259642	-0.1211666898
H27	0.6465277585	0.8308096205	-0.1801591565
H28	1.0952864007	-0.5923160865	-1.0795743039
H29	3.3760398477	-0.5351215603	-0.2071466401
H30	1.0941715282	-1.9872414663	0.9034300203
H31	0.5563529918	3.2265819068	0.2662135929
H32	2.3772535718	3.2975887801	0.0588382743
C33	0.3099363746	1.4561597475	4.0182901976
C34	-1.0174913767	1.8429406726	4.2669841549
C35	-1.4527043076	2.2017115259	5.5434691989
C36	-0.5658202510	2.1772863775	6.6180811907
C37	0.7572253014	1.7950609753	6.3977833531
C38	1.1877000752	1.4459522016	5.1177252531

H39	-1.7249151443	1.8581989774	3.4405030763
H40	-2.4864975643	2.5001972206	5.6958344998
H41	-0.8992262633	2.4560835224	7.6134615102
H42	1.4623206132	1.7748508936	7.2244760674
H43	2.2272443519	1.1720488682	4.9703983573
C44	4.1409585725	3.7113856325	2.6625485444
C45	5.1042218101	3.3571392991	3.6224105447
C46	6.4421530582	3.7101088262	3.4664939265
C47	6.8508518964	4.4353391254	2.3470615633
C48	5.9040495277	4.8122026856	1.3949342274
C49	4.5654908468	4.4578786115	1.5512371642
H50	4.7929062875	2.8057555656	4.5059563455
H51	7.1657784905	3.4225921333	4.2239778298
H52	7.8933852251	4.7128963014	2.2235286106
H53	6.2052631954	5.3943285834	0.5284231596
H54	3.8400216046	4.7892697807	0.8163408701

TS-E8; Energy = -956.86762137461

C1	-0.2467433290	0.3755886746	0.1545957970
C2	-0.2839289819	0.2692310921	1.7072118594
C3	2.7714275295	-0.0135382928	1.3075093212
H4	-1.0270336939	1.0824914294	-0.1567260560
C5	-0.1130538621	-1.1864965732	2.1992126745
H6	-0.0860590429	-1.2016102132	3.2939168678
H7	-1.0340193461	-1.7213673018	1.9271888252
H8	3.8685229036	0.0305287819	1.3078198084
H9	-1.3134814568	0.5268101248	1.9894649528
B10	2.2217191354	1.2150300725	2.2062340508
C11	0.5755836161	1.3823065584	2.4232141067
H12	0.2774533439	2.2882427016	1.8842734923
C13	1.0658836728	-1.9897163404	1.6426172860
H14	1.0219481108	-3.0005091062	2.0695426581
H15	0.9319284538	-2.1280315558	0.5625114786
C16	2.4602247020	-1.4148881093	1.9091686396
H17	2.6441712222	-1.3933737111	2.9913380814
H18	3.1890302127	-2.1299042924	1.5016253972
C19	2.3627593183	0.0962457290	-0.1952647748
H20	3.1605392089	0.6253878434	-0.7336276936
C21	3.1327962700	1.6809537647	3.7339622039
H22	2.3699752790	2.2225214880	4.2848880719
C23	3.6322245293	2.3140907061	2.5680314073
C24	2.7722195661	2.9675656061	1.6873134323
H25	4.5714273491	1.9464225125	2.1620163651
H26	1.9572469068	3.5800983489	2.0545508530
C27	1.0571537811	0.8481678196	-0.5112665382
H28	1.2035243963	1.9054559558	-0.2626683787

H29	0.9030272691	0.8269236522	-1.5985712508
H30	2.3311671614	-0.9058492839	-0.6450330672
H31	-0.5482368047	-0.5915950315	-0.2684857882
H32	3.1319816033	3.2018316267	0.6915326073
C33	3.9777468261	0.8127047889	4.5943597308
C34	3.6950614824	0.7546723299	5.9697424654
C35	4.4623745457	-0.0244830580	6.8328441346
C36	5.5360973198	-0.7668669415	6.3423689456
C37	5.8304402119	-0.7203883114	4.9794311442
C38	5.0621888979	0.0576572091	4.1164210922
H39	2.8629524094	1.3319857234	6.3622906627
H40	4.2218932313	-0.0467256650	7.8922523632
H41	6.1363999279	-1.3746900956	7.0128149045
H42	6.6623970404	-1.2960541090	4.5831806750
H43	5.3088945809	0.0654102252	3.0600949628
C44	0.0479561408	1.5936550421	3.8376498651
C45	-0.8109061804	2.6729824736	4.0988458289
C46	-1.3667667852	2.8814807868	5.3619398735
C47	-1.0803506785	2.0031053623	6.4050764752
C48	-0.2249784841	0.9256209614	6.1706846030
C49	0.3359149282	0.7294628878	4.9088723200
H50	-1.0523959270	3.3622721223	3.2924864041
H51	-2.0238338626	3.7310176284	5.5282002468
H52	-1.5116430585	2.1587301809	7.3899265868
H53	0.0153970640	0.2365043710	6.9759104181
H54	1.0278868384	-0.0928879479	4.7640040526

TS-Z9; Energy = -883.05422367950

C1	-0.1928418938	-0.0204218450	0.4308099194
C2	-0.1976618052	-0.0094848890	1.9901544084
C3	2.8332882065	-0.3145351875	1.5461596183
H4	-0.9420516616	0.7047881967	0.0857240255
C5	-0.0344088051	-1.4422589116	2.5605736235
H6	-0.0588207859	-1.4062459038	3.6519608114
H7	-0.9353773582	-2.0020352724	2.2710869459
H8	3.9226716155	-0.2415052073	1.5235690965
H9	-1.2362268020	0.2392513760	2.2239280562
B10	2.2582414918	1.0296215739	2.2719862016
C11	0.6559298429	1.1371776379	2.6569655452
H12	0.3079690670	2.0414288532	2.1274243404
C13	1.1771806700	-2.2691312206	2.1204385000
H14	1.1523449694	-3.2251142733	2.6608097974
H15	1.0669266045	-2.5364032287	1.0625519310
C16	2.5494155126	-1.6237025855	2.3369016969
H17	2.7079015842	-1.4503315454	3.4090193744
H18	3.3070712162	-2.3642464899	2.0436971656

C19	2.3924447545	-0.4284024859	0.0517895541
H20	3.1884633392	-0.0161899554	-0.5821750756
C21	3.6668854732	1.5828160854	3.5216268534
H22	3.3224132122	1.7164835720	4.5425913738
C23	3.1533852173	2.5421726372	2.6233870557
C24	3.0329622933	2.3675043469	1.2364686951
H25	2.4726167456	3.2687837748	3.0486246125
C26	0.2054797332	1.4368545191	4.1698852040
C27	-1.3363724072	1.3906811691	4.3130670603
H28	-1.6242074087	1.7225873570	5.3174176288
H29	-1.8289752366	2.0560836966	3.5939547418
H30	-1.7453101276	0.3861292982	4.1812209370
C31	0.7968019158	0.4796074398	5.2351300256
H32	0.6832907476	0.9167711291	6.2347015748
H33	0.2902778024	-0.4872161635	5.2574200123
H34	1.8596080161	0.2874597048	5.0763463570
C35	0.6015412187	2.8785547094	4.5872221974
H36	0.0751290626	3.1543882811	5.5077382021
H37	1.6657982442	2.9881693239	4.8077456978
H38	0.3246108827	3.6147715571	3.8236924054
C39	1.0974522504	0.2979103897	-0.3439256983
H40	1.2772214844	1.3755955697	-0.2754819060
H41	0.9025480257	0.1068706715	-1.4082303160
H42	2.3281941173	-1.4860197230	-0.2339702413
H43	-0.5745283944	-0.9995190073	0.1106084678
H44	2.4056311238	3.0771489944	0.7076017055
H45	3.7889154027	1.8794481209	0.6364559893
C46	4.9653176325	0.8708164868	3.4516240027
C47	5.2538396041	-0.1067189347	4.4191256714
C48	6.4775253329	-0.7709680068	4.4298145461
C49	7.4492402935	-0.4677227302	3.4756768676
C50	7.1857240134	0.5139022801	2.5202750391
C51	5.9604366876	1.1774705304	2.5089528140
H52	4.5068024280	-0.3437610725	5.1724290358
H53	6.6735214426	-1.5252335822	5.1867189592
H54	8.4044408328	-0.9843626486	3.4820364164
H55	7.9408153224	0.7717424639	1.7828391506
H56	5.7832892797	1.9564676274	1.7750181025

TS-E9; Energy = -883.05411553268

C1	-0.2527702160	0.1323655901	0.3747911863
C2	-0.1658929304	0.0636445823	1.9304131772
C3	2.8211808921	0.1390297261	1.3146360451
H4	-1.1585469534	0.6976848204	0.1174293736
C5	0.3043747785	-1.3220706929	2.4622286042
H6	0.5928705584	-1.2321858429	3.5154944885

H7	-0.5724220250	-1.9842698563	2.4512192492
H8	3.8960066713	0.3562069377	1.2593379424
H9	-1.2091777074	0.1110416458	2.2464834181
B10	2.1855320158	1.2242158286	2.3560256502
C11	0.5152802535	1.3462064649	2.5353087778
H12	0.2333269639	2.1362263604	1.8275933307
C13	1.4305971006	-2.0358578582	1.7125350965
H14	1.5321152276	-3.0496796791	2.1223166650
H15	1.1501959635	-2.1743614507	0.6612032918
C16	2.7823757328	-1.3333830273	1.8064202992
H17	3.1297546723	-1.3789780721	2.8446694309
H18	3.5114366245	-1.9116341851	1.2195683084
C19	2.3247408837	0.2591096522	-0.1597096594
H20	3.0047178156	0.9255747777	-0.7071669343
C21	3.1410478598	1.4749495986	3.9154499194
H22	2.3904531330	1.8681268992	4.5837858278
C23	3.5806282462	2.3093767005	2.8520705780
C24	2.7133220658	3.0300758016	2.0334701375
H25	4.5304957834	2.0354833487	2.3996549310
H26	1.8689027533	3.5805440854	2.4176155238
C27	-0.2216198284	1.8418197874	3.8607652039
C28	-1.7380807445	2.0362647475	3.5789119599
H29	-2.2074482512	2.5597910999	4.4194726860
H30	-1.9023059314	2.6422033949	2.6804741125
H31	-2.2795020944	1.0954679641	3.4553169051
C32	-0.1090379979	0.8666240082	5.0528677937
H33	-0.5470597650	1.3150560300	5.9530137615
H34	-0.6548043087	-0.0606476438	4.8581378541
H35	0.9213595432	0.5912671074	5.2865115124
C36	0.2482838984	3.2545355842	4.2981644826
H37	-0.3272260747	3.5772332282	5.1730037810
H38	1.3006644889	3.3293430522	4.5735021224
H39	0.0602013842	3.9901821796	3.5068501529
C40	0.9057025468	0.8037832987	-0.3825051680
H41	0.9076815981	1.8727395453	-0.1378894811
H42	0.6802471389	0.7562739209	-1.4564884867
H43	2.4237995917	-0.7185432579	-0.6523150190
H44	-0.4209045206	-0.8765596518	-0.0226278837
H45	3.0947975727	3.3633795149	1.0737907087
C46	4.0692249029	0.5279380805	4.5925016891
C47	3.7875649236	0.1476158893	5.9157351095
C48	4.6174362051	-0.7269818687	6.6137047303
C49	5.7621110612	-1.2416460798	6.0070627503
C50	6.0631755376	-0.8689572764	4.6965331751
C51	5.2297086036	0.0017163669	3.9982595526
H52	2.9069293222	0.5521631450	6.4074548487

H53	4.3697896070	-1.0017932069	7.6352389865
H54	6.4118655150	-1.9237643167	6.5473350971
H55	6.9513127495	-1.2629100663	4.2104036173
H56	5.4863115621	0.2576559106	2.9750753131

Acetaldehyde addition TS

Energy = -1288.36467645892

C1	0.0802527523	-0.1345621133	-0.0669669095
C2	0.0170671458	-0.1159483551	1.4899526597
C3	3.0868641128	0.0727107887	1.1639134985
H4	-0.8086405712	0.3848042095	-0.4492167009
C5	0.4545866442	-1.4677588766	2.1168275695
H6	0.5599698441	-1.3454524859	3.2012557960
H7	-0.3720176864	-2.1781152297	1.9757206899
H8	4.1605293252	0.3116548333	1.1759152786
H9	-1.0551053517	-0.0556360287	1.7161933683
B10	2.3190672619	1.1952380940	2.0739097426
C11	0.6786736080	1.1586139051	2.1236154095
H12	0.3286468660	1.9963134263	1.4944038869
C13	1.7219696901	-2.1320714957	1.5691638615
H14	1.8270608832	-3.1164383004	2.0451368257
H15	1.5930066242	-2.3413971719	0.5001422035
C16	3.0221246688	-1.3528696309	1.7802400871
H17	3.2219231647	-1.2956937287	2.8601745617
H18	3.8414990706	-1.9543659007	1.3586295631
C19	2.7075668401	0.0731503785	-0.3471262591
H20	3.4038970298	0.7327600947	-0.8836805821
C21	2.8112789149	2.8983270006	1.5161052943
H22	2.4952466877	2.8890275866	0.4743473899
H23	2.1980254403	3.5549937993	2.1251395240
Si24	-0.1756171804	1.6278469807	3.7780940470
C25	-2.0614960168	1.6840053482	3.5109192748
H26	-2.5523416431	2.1000796546	4.3989452192
H27	-2.3303485793	2.3212601570	2.6601716070
H28	-2.4976816884	0.6955687064	3.3331017378
C29	0.1457980085	0.4574668350	5.2417043804
H30	-0.2760910984	0.8862002576	6.1585690903
H31	-0.3169647937	-0.5245566935	5.1007664352
H32	1.2163561519	0.3055505611	5.4062218595
C33	0.3088970537	3.3754653119	4.3427454014
H34	-0.3108968827	3.6762273874	5.1956236714
H35	1.3531705893	3.4252359174	4.6595726078
H36	0.1547047435	4.1205347347	3.5528917524
C37	1.2908229771	0.5363956614	-0.7364358687
H38	1.2144078869	1.6148960949	-0.5583608327
H39	1.1837992204	0.4201636652	-1.8237117472

H40	2.8899000711	-0.9263692919	-0.7669865061
H41	-0.0173648854	-1.1691350501	-0.4219336246
C42	4.2176301318	2.9201825398	1.7001541713
H43	4.7826179768	2.4255857246	0.9101291372
C44	4.9674568428	3.1741873625	2.8514213823
H45	6.0163354584	2.8918409685	2.7580731001
C46	4.1540065382	1.2514993854	3.7427112433
H47	4.8022359206	0.6588335656	3.0981751179
O48	2.8905710497	1.2818207117	3.4742789006
C49	4.5437337818	1.3686575347	5.1840769463
H50	3.9866879997	2.1640835163	5.6820912516
H51	4.3054159551	0.4176476421	5.6795850310
H52	5.6140715017	1.5496784627	5.2975241320
C53	4.7791538677	4.1898171567	3.9105136596
C54	3.6213784750	4.9633274076	4.1027705463
C55	3.5538025832	5.9116108075	5.1218724928
C56	4.6361948519	6.1187262935	5.9768008887
C57	5.7997284946	5.3713298693	5.7938963838
C58	5.8672288748	4.4257447827	4.7747964752
H59	2.7706738650	4.8429464384	3.4482710785
H60	2.6450322768	6.4935258532	5.2450441575
H61	4.5764812391	6.8571999308	6.7707166975
H62	6.6577086271	5.5261117201	6.4424757078
H63	6.7854089114	3.8601351485	4.6333059946