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Supplementary Materials for

Gas-phase preparation of silylacetylene (SiH_3CCH) through a counterintuitive ethynyl radical (C_2H) insertion

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Data S1
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Other Supplementary Material for this manuscript includes the following:

Data S2

Supplementary Text

The quantum chemistry method employed in the AIMD simulation must accurately represent the potential energies of this reaction. The AIMD simulation involves millions of energy gradient calculations, hence finding a quantum chemistry method with of good accuracy/cost ratio is of utmost importance. In this study, the potential energy surface computed at the CCSD(T)-F12/cc-pVTZ-F12//B2PLYP-D3/cc-pV(T+d)Z+ZPE(B2PLYP-D3/cc-pV(T+d)Z) level of theory served as the benchmark to evaluate a series of affordable methods such as MP2 and DFT combined with different basis sets. The accuracy of the method (*A*) was determined by possessing a maximum overlap with the benchmark PES, e.g., smallest RMSD as computed with the following equation:

$$RMSD(A,ref) = \sqrt{\frac{1}{K}\sum_{i=1}^{K}\left(E_i^A - E_i^{ref} - \Delta E(A,ref)\right)^2} \quad \textbf{(S1)}$$

$$\Delta E(A,ref) = arg\ min_{\Delta E}\left(\frac{1}{K}\sum_{i=1}^{K}\left(E_i^A - E_i^{ref} - \Delta E\right)^2\right) = \overline{E_A} - \overline{E_{ref}} \quad \textbf{(S2)}$$

K is the number of stationary points including products and $K = 8$ in the present study. The index *i* indicates the i^{th} structure. $\overline{E_A}$ and $\overline{E_{ref}}$ are the mean relative energies of the candidate method and benchmark method after shifting the energies to the separated reactants to zero. $\Delta E(A,ref)$ is the optimum shift in energy between the PES profile by candidate method E_A and benchmark method E_{ref}.

Same convergence criteria such as maximum and RMSD in an energy gradient of $< 1.5 \times 10^{-5}$ and $< 1.0 \times 10^{-5}$ Hartree/Bohr respectively and maximum and RMSD in coordinates $< 6.0 \times 10^{-5}$ and $< 4.0 \times 10^{-5}$ Bohr respectively was applied to all candidate methods being surveyed. The RMSD values of 21 different quantum chemical methods are summarized in Table S1. The purpose of Table S1 is to assess the performance of these method on this specific system and should not be taken as their general performance. As shown, B3LYP has an overall better accuracy compared to MP2 and PBE0. Considering the wall time for the gradient calculation for B3LYP/def2-TZVP and B3LYP/def2-TZVPP being twice as long compared to B3LYP/cc-pVDZ and B3LYP/def2-SVP, these two methods are employed to test their stability in AIMD simulations. It turns out that they are less unstable (e.g., large energy jump, self-consistent field convergence failure, etc.) than B3LYP/cc-pVDZ trajectories, thus the latter was chosen to run AIMD simulations.

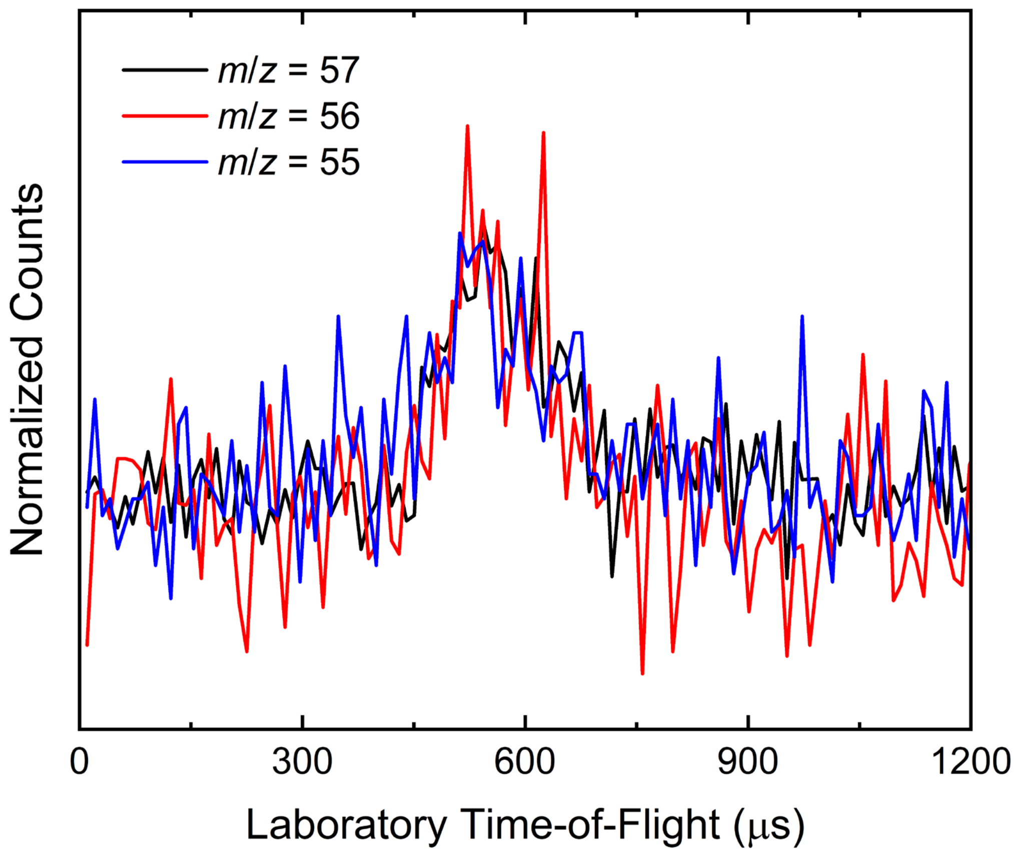

Fig. S1. Time-of-flight (TOF) overlay. TOF spectra for the reaction of D1-ethynyl radicals (C_2D) with silane (SiH_4) taken at *m*/*z* = 57 (black), 56 (red), and 55 (blue).

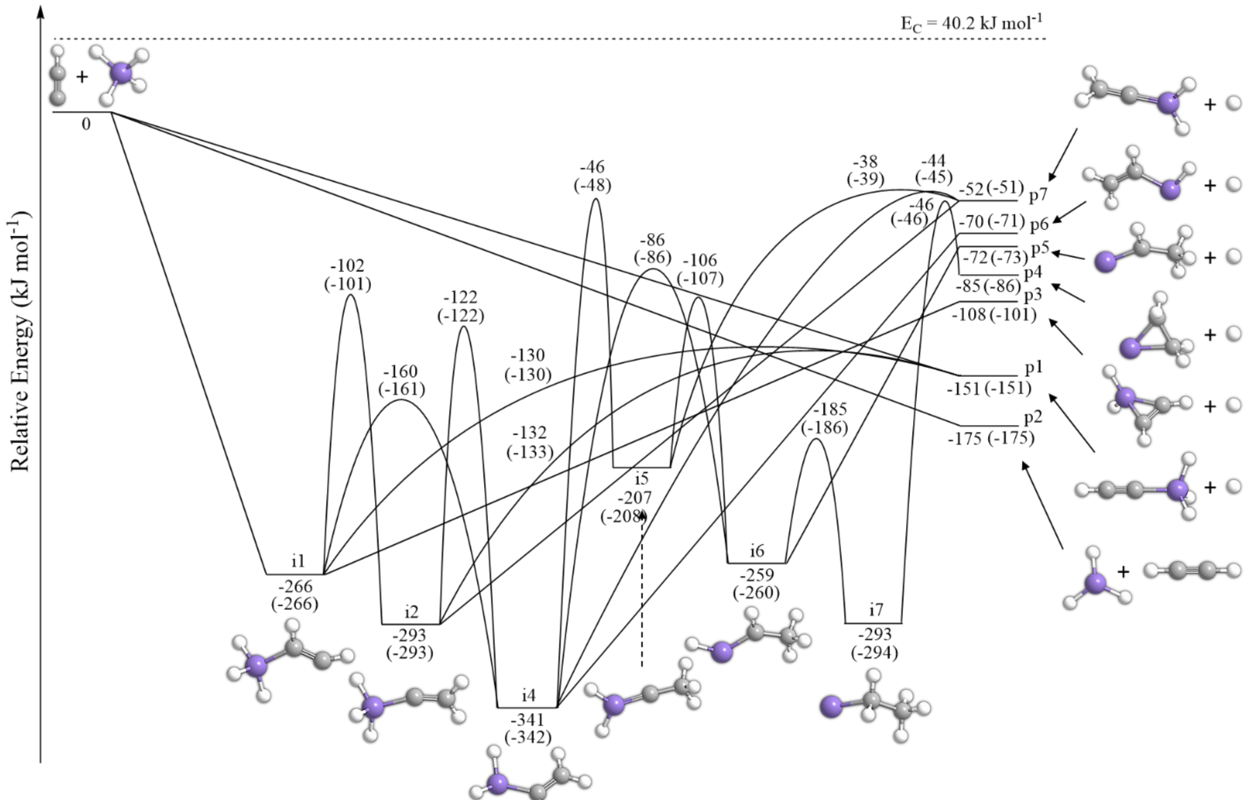

Fig. S2. Potential energy surface (PES) showing H loss products. Schematic PES for the reaction of ethynyl radicals (C_2H) with silane (SiH_4) at the CCSD(T)-F12/cc-pVTZ-F12//B2PLYP-D3/cc-pV(T+d)Z + ZPE(B2PLYP-D3/cc-pV(T+d)Z) level. Energies for the D1-ethynyl (C_2D)–silane (SiH_4) system are shown in parenthases. Carbon atoms are gray, silicon is purple, and hydrogen is white.

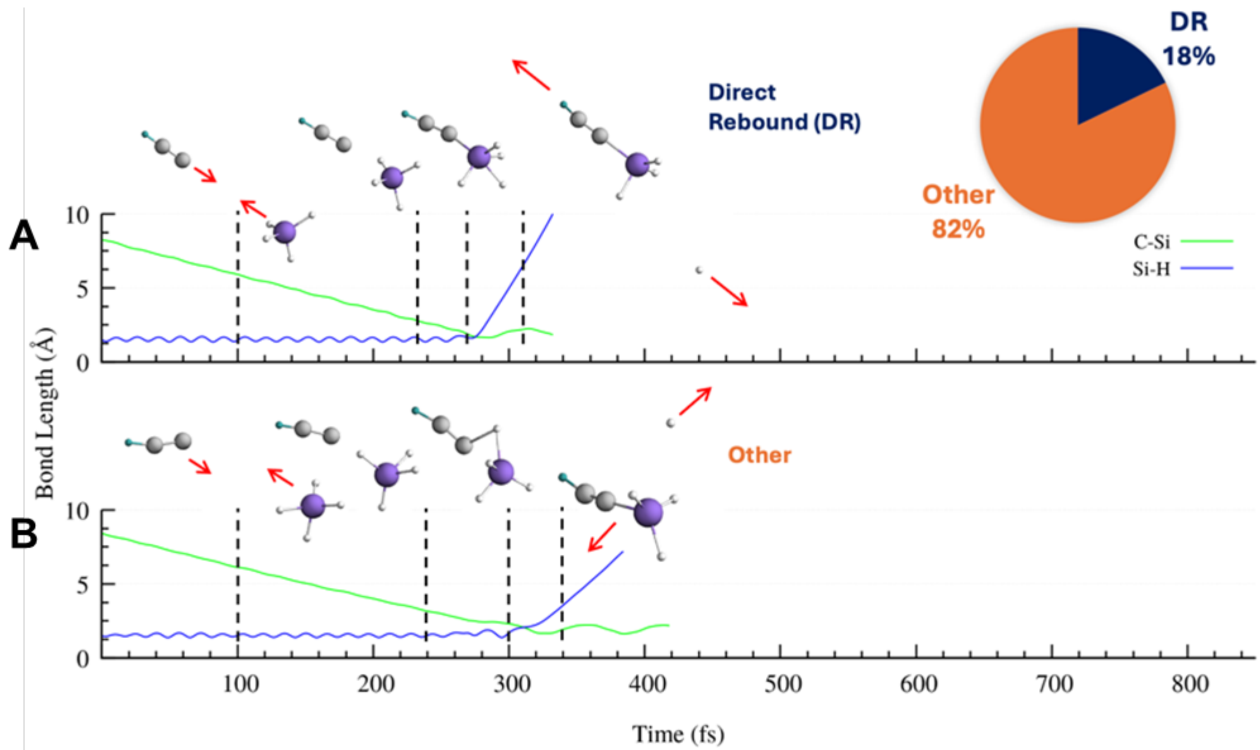

Fig. S3. Representative trajectories for the direct mechanisms. Key distances of the carbon–silicon (green line) and silicon–leaving-hydrogen-atom (blue line) versus time for the rebound (**A**) and other (**B**) direct reaction mechanisms with snapshots inserted from representative trajectories. The pie chart represents the percentage of reactive trajectories which follow rebound (dark blue area) and other (orange area) direct mechanisms.

Table S1. Deviation of the dynamics computational methods. RMSD in kJ mol^{-1} of each candidate method with respect to the benchmark method.

Theory/Basis Set	MP2	B3LYP	PBE0
6-31+G(d) (*69*)	40.26	10.08	14.38
6-31++G(d,p) (*69*)	32.52	10.21	14.86
cc-pVDZ (*57*)	31.64	**9.47**	13.39
def2-SVP (*70*)	31.73	**9.71**	15.82
def2-SVPD (*70*)	32.81	10.05	15.86
def2-TZVP (*70*)	30.40	**7.33**	12.48
def2-TZVPP (*70*)	26.89	**7.71**	12.79

Data S1. Calculated parameters of all species. Optimized Cartesian coordinates (Å), and vibrational frequencies (cm^{-1}) and T1 diagnostic of reactants, products, intermediates, and transition states involved in the ethynyl radical (C_2H) plus silane (SiH_4) reaction.

REACTANTS

C_2H

C	0.00000000146191	0.00000000220594	-0.70844729709338
C	-0.00000000292488	-0.00000000441126	0.49428100547783
H	0.00000000146297	0.00000000220532	1.55576329161555

Frequencies

590.11
590.11
2106.08
3482.03
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01672699

SiH4

Si	-0.00001332228026	-0.00000000222891	0.00000331102526
H	-0.00001030170425	-0.00000000793993	1.47600156518390
H	1.39157061199139	0.00000001364874	-0.49200940255825
H	-0.69577299988246	-1.20516836239159	-0.49199472810344
H	-0.69577298822443	1.20516835881168	-0.49199474544747

Frequencies

938.08
939.63
941.24
993.49
994.60
2263.75
2268.98
2269.06
2269.20
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01148048

PRODUCTS

p1

Si	1.06162311933641	-0.00007352059843	0.00006522838756
H	1.55027761511748	0.49525710315592	1.30012461081514
H	1.55095773841646	0.87793576554854	-1.07879500462537
H	1.55036174742045	-1.37362866672482	-0.22075924998399
C	-0.76436869375482	0.00015830840292	-0.00032077571727
C	-1.97599576749444	-0.00004185019798	0.00024293848432
H	-3.03775853904155	-0.00017973958615	0.00065437263961

Frequencies
229.91
229.97
637.29
694.25
694.25
709.69
709.70
957.07
969.22
969.41
2104.00
2267.79
2269.03
2269.27
3471.99
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01346734

p3

Si	-0.42158286715828	0.07488151716422	-0.67162197860765
H	0.44674751386367	0.15044588108155	2.02319064690855
H	-1.15329612164573	1.22876870941426	-1.22269989439297
H	-0.93283700088233	-1.19083395145836	-1.22587716713149
C	0.39277538345603	0.14633061621893	0.94517205877314
C	1.27487326317730	0.22833826515702	-0.05480609909307
H	2.34706482918934	0.32648896242239	-0.13118456645650

Frequencies

582.71
596.79
673.43
705.55
716.99
790.55
924.37
975.67
1010.87
1141.52
1518.66
2261.82
2266.05
3199.42
3222.47
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01282210

p4

Si	-0.67902137078277	-0.29542878986675	-0.62862286502748

H	0.47447104841153	0.32063707402354	1.60657011329580
C	0.50446697328489	0.59651944458595	0.55887099134482
C	1.20566892245362	-0.33982403600966	-0.39756072748567
H	1.64444905162926	-1.24369076532077	0.00889828491811
H	1.82174469923042	0.09816357925630	-1.17429597644679
H	0.65105099203597	1.66163824449683	0.42183499010223

Frequencies

421.06
599.85
609.95
653.53
724.69
918.54
956.77
1048.95
1215.27
1423.55
1436.31
3110.14
3117.70
3174.36
3194.18
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01273538

p5

Si	-1.20362659337936	-0.59351400124092	-0.12163875479135
H	0.17149104911034	0.82813847384918	0.91698664670142
C	0.36333781961967	0.00554146138493	0.20382710126987
C	1.81073124886914	-0.19848606805979	-0.13508339721924
H	2.39691234343567	-0.43532019755343	0.75440978364727
H	1.94325165690479	-1.01237817994327	-0.84513740034839
H	2.24610184908849	0.70002957463276	-0.57542789638529

Frequencies

109.70
187.04
541.47
687.32
900.95
1041.13
1158.30
1325.66
1415.38
1497.87
1511.02
2946.13
3035.52
3084.24
3118.70
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01468830

p6

Si	0.95841316139332	-0.53837122272724	-0.09673876910652
H	1.84330718246562	0.44352747608340	0.65458286456557
C	-0.66968769095948	0.31343226267557	0.28750256570898
C	-1.79201157812655	-0.23713195494337	-0.20722843365629

H -0.76859567426822 1.21777631042585 0.87843009881511
H -2.77860406643567 0.18044167333361 -0.04176750005266
H -1.74990332505422 -1.14143395178628 -0.80442506852714

Frequencies

123.87
289.93
502.20
670.31
822.51
1030.86
1035.46
1051.28
1298.88
1431.77
1613.35
2038.66
3120.77
3147.09
3205.28
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01363965

p7
Si 0.99436226358022 -0.56618251457043 0.15151783661986
H 1.87566997502431 0.58112148576267 0.38497843617565
C -0.65663615556965 -0.36133266646998 -0.12623182737186
C -1.93779338348966 -0.20057970114451 -0.34663757902363
H -2.66337876721283 -0.18802414008906 0.46112952395701
H -2.33586555268488 -0.07181640002204 -1.34865705546399
H 1.60549052422313 -1.89754124360763 0.17718231674793

Frequencies

174.84
240.87
405.26
663.63
663.96
766.75
943.89
963.08
1018.72
1445.95
1794.22
2305.92
2326.26
3099.66
3164.53
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01507913

INTERMEDIATES

i1

Si	-1.04120847742225	-0.09595383504665	-0.43639675248801
H	0.45823474474887	0.66439977321315	1.51512983021557
H	-1.72731472360011	1.19370577569384	-0.66812696861234
H	-0.72344891610360	-0.73123433059603	-1.72844100748126
H	-1.95374405592786	-0.96441994963803	0.33782751278226
C	0.53512662633929	0.19110892041377	0.53140841764773
C	1.70872858361279	-0.14720524044786	0.07363481864326
H	2.74362621835288	-0.11040211359219	0.37496514929279

Frequencies

203.48
262.83
524.59
623.82
683.91
728.79
867.39
868.99
951.30
967.02
980.56
1170.54
1655.21
2245.24
2246.25
2272.98
3025.90
3237.92
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01704178

i4

Si	1.00242759114693	-0.18744825743395	-0.21805744349478
H	1.96579044262332	0.08609699614580	0.87143926392091
C	-0.70799890190654	0.38298476546374	0.18443113892889
C	-1.81615416124095	-0.26952709181597	-0.18658361478132
H	-0.82468655387063	1.32809662014097	0.70476565835903
H	-2.80592277377591	0.11102821134536	0.02987955535026
H	-1.77053763396141	-1.21299065078440	-0.71551880053594
H	1.01424434098519	-1.61449915306155	-0.61230844774705

Frequencies

249.98
287.90
489.88
628.70
684.34
721.58
935.36
987.24
1033.94
1053.79
1304.31
1449.70
1647.40

2217.87
2244.14
3138.91
3150.99
3223.43
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01762348

i2

Si	-1.15909693235212	-0.07646277586191	-0.48544294948820
H	-1.82479918910650	1.22980079869831	-0.31748516682781
H	-1.26071095937194	-0.48304478597256	-1.90751425872853
H	-1.84097662661076	-1.08646286767533	0.34689561772738
C	0.57440652018149	0.06459758191339	0.05017884908164
C	1.87558724017018	0.03505997702157	-0.02124115678785
H	2.51262347226160	0.27589455508357	0.82672031262350
H	2.39988721482805	-0.23356666320705	-0.93863287760013

Frequencies

129.10
218.82
319.75
627.93
656.35
705.78
942.18
948.14
956.99
968.44
969.76
1424.47
1758.24
2216.72
2259.77
2262.62
3057.82
3124.38
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01597262

i6

Si	-1.72223683738152	-0.67899573062008	-0.13494303942036
H	-2.99463009834926	-0.32828124244173	0.55570756896875
C	-0.29112936137527	0.17517349035113	0.23008465042852
C	1.10557323813092	0.00387651734326	-0.28556323813828
H	-0.45467791076750	0.99491571353230	0.92872863995645
H	1.80411271544763	-0.18754308383197	0.53164864012480
H	1.45375403611332	0.90406105585783	-0.79590667967749
H	1.18367521818168	-0.82531772019075	-0.98659554224240

Frequencies

185.20
258.16
292.44
532.23
667.68
844.30
999.17
1056.15

1158.25
1342.62
1422.30
1495.12
1514.04
2165.15
3030.81
3077.75
3100.64
3120.45
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01624596

i5

Si	-1.09588099225871	-0.98453138587485	0.02530887439669
H	-2.10675327573857	-0.31022925158377	0.85323407188340
C	0.49551592099904	-0.49888675596409	-0.02086601802513
C	1.90773361321269	-0.16652035171231	-0.14338138009520
H	2.41552148606527	-0.18906286717545	0.82353637845676
H	2.42319622084148	-0.88436558259386	-0.79102806470487
H	2.05688502231650	0.82341067671335	-0.57971861722830
H	-1.61644891543771	-2.12137946180901	-0.75167701468334

Frequencies

121.23
242.24
258.13
504.96
614.48
705.77
967.58
1001.46
1041.62
1400.21
1471.89
1476.17
1483.76
2270.18
2283.41
3002.92
3058.51
3082.75
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01587254

i7

Si	-1.18558862044069	-0.07461803414022	-0.33618833394666
H	0.35536409981864	0.24372909369418	1.44667531264417
C	0.48846978889156	0.47375877646368	0.37587609145401
C	1.76615372558846	-0.18980363382935	-0.15326309007966
H	2.64988802373708	0.13307997883455	0.39804771929897
H	1.70299478057328	-1.27467872333964	-0.08059887032451
H	1.92607778417892	0.05473789728650	-1.20272465241941
H	0.56935875765274	1.56488937503030	0.34591835337309

Frequencies

205.72
260.84
449.58

613.79
904.59
962.77
1019.34
1231.32
1254.14
1409.54
1423.19
1510.41
1519.74
2953.21
3036.49
3044.22
3110.04
3122.35
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01211346

TRANSITION STATES

TS1: i1 – i4

Si	-1.06426958438164	-0.04341820443064	-0.32627455675262
H	0.63353462407756	0.72745624686887	1.71056075423981
H	-1.80142544613904	1.14333171190468	-0.82801052902466
H	-2.04397121275195	-1.03298816143266	0.18851528289338
C	0.40927999303197	0.29865254952733	0.74370966669119
C	1.28095611278432	-0.19398978879810	-0.12771458011438
H	2.35966511950820	-0.31611955321252	-0.16457460583947
H	0.22623039387059	-0.58292480042696	-1.19621043209327

Frequencies

1698.96 i
284.90
504.88
599.99
703.87
709.20
722.65
889.36
932.80
963.46
997.51
1165.81
1564.39
1755.85
2192.26
2213.28
3132.65
3199.78
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01954195

TS2: i1 – p1

Si	-1.04423214459149	-0.11550705221300	-0.47915091134656
H	-1.64193414451133	1.22858750916664	-0.53950638374157
H	-1.04891664115412	-0.72534271054816	-1.82368971993403
H	-1.79936035232725	-0.96437338334014	0.45788451123757
C	0.69351433186557	0.01130032253287	0.10514737516616
C	1.89890653792671	-0.11484000248837	0.23731406762565
H	2.94106392034477	-0.17028417373853	0.43455897963771
H	0.00095949244715	0.85045949062870	1.60744208135507

Frequencies

679.64 i
218.58
278.03
310.62
450.55
636.19
684.56
699.29
704.81
727.15
954.24
967.46
975.20

2070.43
2259.23
2278.83
2283.39
3467.26
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01873242

TS3: i1 – i2

Si	-1.12508548086112	-0.11562021272207	-0.50549106721671
H	-1.76444817733344	1.19663174275035	-0.71751085979867
H	-0.92789753784043	-0.77641241782075	-1.81754174198865
H	-1.99928219784775	-0.95786014002523	0.33238303203409
C	0.45670277219687	0.14815200033861	0.39586736011010
C	1.73626625574464	0.13466476692788	0.61141101743486
H	0.93124483382404	0.53857386039369	1.51232484932439
H	2.69249853211719	-0.16812959984250	0.18855841010059

Frequencies

1976.81 i
192.03
201.93
290.36
543.86
598.29
660.42
704.74
885.34
951.01
966.14
968.27
1779.71
2216.49
2265.00
2267.93
2409.39
3068.01
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01421002

TS4: i4 – i2

Si	-1.39651939828009	-0.00782453693219	-0.43418462186376
H	-2.18242342466352	1.16858888622297	-0.03234827582741
H	-1.79255797752488	-0.50824475938113	-1.77925678619775
H	-0.77252354059361	-0.60298804954816	0.90724512448439
C	0.29369599917324	0.12974877738601	0.08208029331818
C	1.57474204238366	-0.02474455200031	0.34903089900228
H	1.95481848696525	-0.23645443685076	1.34233987588870
H	2.32076881253995	0.08192067110357	-0.43490650880464

Frequencies

1629.55 i
171.94
315.15
504.36
611.29
642.04
679.46
897.33

904.91
975.21
999.85
1437.13
1689.78
1904.28
2152.07
2282.43
3088.35
3163.19
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01748318

TS5: i2 – p1

Si	-1.37415486079575	-0.07513835293244	-0.20250112931413
H	-1.78935695262346	1.15767069870577	0.49267843133603
H	-1.81149432414046	-0.02378732310925	-1.60930946031476
H	-1.96928876103319	-1.24789341553743	0.46327379121906
C	0.44567224528551	-0.22102647675417	-0.14434274823694
C	1.65699711110582	-0.27087923830737	-0.02073125086449
H	2.68988270174507	-0.51873742122930	-0.06077460120384
H	2.15174284045647	1.19979152916418	1.08170696737907

Frequencies

722.74 i
150.08
189.15
244.72
453.91
638.12
697.36
697.76
710.13
865.22
952.83
969.67
970.53
2085.37
2265.37
2271.66
2274.32
3449.96
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01756825

TS6: i4 – i6

Si	-1.27659623572154	-0.46847356776671	-0.29855986313387
H	-2.63383489663363	-0.94220755539350	0.14456606294371
C	-0.21322194723963	0.61610204367238	0.51598862167002
C	1.02743175456696	0.12960006267608	-0.14055988290254
H	-0.24195795312185	1.40726567852455	1.24792683533979
H	1.76323740533366	-0.39636888270463	0.46006089689484
H	1.43609623328110	0.63561820693266	-1.01015924701957
H	0.13884563953494	-0.98153698594083	-0.91926342379237

Frequencies

1545.94 i
333.28
492.73

565.37
582.33
866.43
894.73
937.63
1019.42
1068.53
1144.41
1466.98
1702.77
1826.27
2183.42
3085.86
3169.26
3229.49
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.02113635

TS7: i4 – i5

Si	-1.38162752750326	-0.67717594933109	0.39741865259959
H	-2.51346228534050	-0.07072469195009	1.13375799851159
C	-0.06380253808361	0.51737333856021	0.04954380679690
C	1.25264607559996	0.31434524909181	-0.35207816766588
H	0.99194275147699	0.60630152435885	0.84981438301152
H	1.88285383408041	1.17101724434475	-0.58563533937647
H	1.69546188958536	-0.65618249634761	-0.58908809689194
H	-1.86401219981535	-1.20495421872684	-0.90373223698531

Frequencies

1191.05 i
210.28
278.19
425.66
575.11
654.26
697.09
955.98
1023.20
1082.46
1268.72
1371.39
1523.17
2204.28
2225.48
2243.43
3018.93
3111.62
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.03544802

TS8: i4 – p7

Si	1.48267153734249	-0.30709319556549	-0.03767073492084
H	2.41840417200479	0.78274751717990	-0.32061656283038
C	-0.18639651741804	-0.07004105881811	-0.18667132216921
C	-1.44928867415075	0.02362816813891	-0.52364863223875
H	-2.18393418967410	0.47117298361265	0.13557331176207
H	-1.80690046462080	-0.34423262182231	-1.47955625987268
H	2.01147718695405	-1.45343873804235	0.70268959454905
H	-0.28603305043764	0.89725794531680	1.70990060572074

Frequencies

593.52 i
217.05
257.25
327.26
363.65
515.00
662.03
700.96
777.79
946.40
972.21
1018.21
1435.74
1789.61
2314.13
2336.94
3117.77
3192.02
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01952866

TS9: i6 – i5

Si	-1.76260195608639	-0.37367794024724	-0.58829472163641
H	-1.46304106033434	0.45922899870854	0.67829399402802
H	-2.32890367290726	-1.67692985595047	-0.10988532072111
C	-0.07217095373388	-0.42919764984055	-0.10371065316091
C	1.14870537650600	0.36340262862536	0.01741445395698
H	1.63491295904534	0.19866563732334	0.98071212287297
H	1.84881593752951	0.02054447311213	-0.75010969712808
H	0.99428336998103	1.43796370826890	-0.12441917821146

Frequencies

927.03 i
201.39
221.32
383.85
645.92
665.20
859.59
977.02
1023.29
1247.62
1390.79
1450.37
1471.88
1972.77
2112.07
3001.62
3068.75
3089.16
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.03765285

TS10: i6 – i7

Si	-2.01967782327599	-0.39453015279842	-0.66347662415851
H	-1.75274550016134	-0.43532239129903	0.90147846641746
C	-0.49600745267453	0.30298393150120	0.03045988173282
C	0.93163707673430	-0.09101705651509	-0.20904108307321

H	1.42339995739208	-0.39792291291963	0.71515799695656
H	1.02295261517703	-0.89414763151243	-0.93626829073369
H	1.48187343969385	0.78182940893809	-0.57498227700298
H	-0.59143331288539	1.12812780460531	0.73667192986155

Frequencies

1079.99 i
179.29
279.26
591.19
688.54
926.59
1011.10
1061.93
1106.96
1311.26
1393.39
1483.10
1500.74
1804.49
3020.56
3084.99
3086.10
3135.78
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.03243384

TS11: i5 – p7

Si	-1.68379844738846	-0.40741150231382	0.13428920206986
H	-2.75195319607718	0.23705375312280	0.90336286966790
C	-0.10922950124325	0.17317735882270	0.16194966558391
C	1.13922262215365	0.59091826330959	0.15094261139399
H	1.47571484782075	1.36853862072000	-0.52728745870491
H	1.85185487804780	0.28223109670580	0.90905851281679
H	-2.05422706624411	-1.58338823573300	-0.65895112596144
H	2.13241486293081	-0.66111835463406	-1.07336427686611

Frequencies

594.16 i
198.72
222.51
338.60
376.99
468.70
665.86
768.01
804.86
951.58
996.97
1030.56
1450.26
1784.90
2304.18
2324.15
3105.01
3171.74
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.01919701

TS12: i7 – p4

Si	-1.74240685772549	-0.45402425127277	-0.67881298555499
H	-0.54863450809619	0.29155907044268	1.51307252889599
C	-0.57684860334160	0.49394237808123	0.44804008869594
C	0.27549904688892	-0.36356649652645	-0.44462898555653
H	0.50115241641467	-1.39249729421439	-0.19178750452455
H	0.77070504656640	0.03069981207462	-1.31633258225697
H	-0.49164383155085	1.55708450787428	0.24691579068293
H	1.81217729084416	-0.16319872645920	0.42353464961817

Frequencies

1078.66 i
295.46
454.95
494.13
569.61
664.73
755.07
875.05
926.66
1000.44
1059.61
1202.25
1421.08
1444.96
3105.81
3139.44
3173.20
3252.52
CCSD(T)-F12/cc-pVTZ-F12 - T1 diagnostic: 0.02428007

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm^{-1}) of reactants, products, intermediates, and transition states involved in the D1-ethynyl radical (C_2D) plus silane (SiH_4) reaction.

REACTANTS

CCD

C	0.00000000146191	0.00000000220594	-0.70844729709338
C	-0.00000000292488	-0.00000000441126	0.49428100547783
D	0.00000000146297	0.00000000220532	1.55576329161555

Frequencies

452.599382
452.6048
1955.229304
2706.176905

INTERMEDIATES

i1

Si	-1.04120847742225	-0.09595383504665	-0.43639675248801
H	0.45823474474887	0.66439977321315	1.51512983021557
H	-1.72731472360011	1.19370577569384	-0.66812696861234
H	-0.72344891610360	-0.73123433059603	-1.72844100748126
H	-1.95374405592786	-0.96441994963803	0.33782751278226
C	0.53512662633929	0.19110892041377	0.53140841764773
C	1.70872858361279	-0.14720524044786	0.07363481864326
D	2.74362621835288	-0.11040211359219	0.37496514929279

Frequencies

201.627985
246.742646
457.087832
584.948019
626.747373
673.456819
795.808121
818.522218
951.161655
966.919138
980.510715
1154.005005
1612.861255
2245.232416
2246.242412
2272.97598
2414.021143
3026.859481

i4

Si	1.00242759114693	-0.18744825743395	-0.21805744349478
H	1.96579044262332	0.08609699614580	0.87143926392091
C	-0.70799890190654	0.38298476546374	0.18443113892889
C	-1.81615416124095	-0.26952709181597	-0.18658361478132
H	-0.82468655387063	1.32809662014097	0.70476565835903
D	-2.80592277377591	0.11102821134536	0.02987955535026
H	-1.77053763396141	-1.21299065078440	-0.71551880053594
H	1.01424434098519	-1.61449915306155	-0.61230844774705

Frequencies

246.408122
282.178525
419.435426
622.612444
667.329226
685.921224
884.894255
914.423082
941.62481
1042.488541
1274.813878
1340.010429
1611.983586
2217.85273
2244.132002

2345.030148
3150.151383
3183.269421

i2

Si	-1.15909693235212	-0.07646277586191	-0.48544294948820
H	-1.82479918910650	1.22980079869831	-0.31748516682781
H	-1.26071095937194	-0.48304478597256	-1.90751425872853
H	-1.84097662661076	-1.08646286767533	0.34689561772738
C	0.57440652018149	0.06459758191339	0.05017884908164
C	1.87558724017018	0.03505997702157	-0.02124115678785
H	2.51262347226160	0.27589455508357	0.82672031262350
D	2.39988721482805	-0.23356666320705	-0.93863287760013

Frequencies

122.254545
205.574231
299.774997
623.019079
649.908735
705.752779
816.627936
858.532462
956.774213
965.840795
969.518935
1284.613196
1741.408768
2216.652813
2258.566549
2262.251562
2262.625014
3110.678868

i6

Si	-1.72223683738152	-0.67899573062008	-0.13494303942036
H	-2.99463009834926	-0.32828124244173	0.55570756896875
C	-0.29112936137527	0.17517349035113	0.23008465042852
C	1.10557323813092	0.00387651734326	-0.28556323813828
H	-0.45467791076750	0.99491571353230	0.92872863995645
D	1.80411271544763	-0.18754308383197	0.53164864012480
H	1.45375403611332	0.90406105585783	-0.79590667967749
H	1.18367521818168	-0.82531772019075	-0.98659554224240

Frequencies

166.411217
254.754031
283.66967
521.51122
664.819789
780.569495
931.271387
988.734342
1148.986075
1279.266368
1316.489216
1379.770547

1483.919883
2165.135962
2242.017054
3053.117281
3100.23041
3116.675954

i5

Si	-1.09588099225871	-0.98453138587485	0.02530887439669
H	-2.10675327573857	-0.31022925158377	0.85323407188340
C	0.49551592099904	-0.49888675596409	-0.02086601802513
C	1.90773361321269	-0.16652035171231	-0.14338138009520
H	2.41552148606527	-0.18906286717545	0.82353637845676
H	2.42319622084148	-0.88436558259386	-0.79102806470487
D	2.05688502231650	0.82341067671335	-0.57971861722830
H	-1.61644891543771	-2.12137946180901	-0.75167701468334

Frequencies

119.612969
231.741632
261.306273
501.624495
614.336685
685.802023
870.802763
960.984454
980.506246
1284.701832
1308.163946
1449.138039
1479.916287
2242.580961
2270.204501
2283.425074
3015.800699
3066.994855

i7

Si	-1.18558862044069	-0.07461803414022	-0.33618833394666
H	0.35536409981864	0.24372909369418	1.44667531264417
C	0.48846978889156	0.47375877646368	0.37587609145401
C	1.76615372558846	-0.18980363382935	-0.15326309007966
D	2.64988802373708	0.13307997883455	0.39804771929897
H	1.70299478057328	-1.27467872333964	-0.08059887032451
H	1.92607778417892	0.05473789728650	-1.20272465241941
H	0.56935875765274	1.56488937503030	0.34591835337309

Frequencies

181.024242
253.688714
448.666754
595.005224
819.912283
885.974462
1014.761161
1186.094273
1217.189463

1332.215249
1354.925103
1409.598006
1488.001139
2256.804088
2953.370871
3036.58643
3076.416995
3121.799931

PRODUCTS

p1

Si	1.06162311933641	-0.00007352059843	0.00006522838756
H	1.55027761511748	0.49525710315592	1.30012461081514
H	1.55095773841646	0.87793576554854	-1.07879500462537
H	1.55036174742045	-1.37362866672482	-0.22075924998399
C	-0.76436869375482	0.00015830840292	-0.00032077571727
C	-1.97599576749444	-0.00004185019798	0.00024293848432
D	-3.03775853904155	-0.00017973958615	0.00065437263961

Frequencies

216.715670
216.773099
559.077619
559.083847
628.056195
694.328219
694.334544
957.073264
969.214880
969.410587
1970.463234
2267.786433
2269.024709
2269.228906
2685.076660

p3

Si	-0.42158286715828	0.07488151716422	-0.67162197860765
H	0.44674751386367	0.15044588108155	2.02319064690855
H	-1.15329612164573	1.22876870941426	-1.22269989439297
H	-0.93283700088233	-1.19083395145836	-1.22587716713149
C	0.39277538345603	0.14633061621893	0.94517205877314
C	1.27487326317730	0.22833826515702	-0.05480609909307
D	2.34706482918934	0.32648896242239	-0.13118456645650

Frequencies

582.711615
596.794345
673.431045
705.551542
716.991016
790.550537
924.374545
975.670513
1010.872351
1141.519209
1518.663918
2261.818849
2266.046471
3199.424402
3222.472891

p4

Si	-0.67902137078277	-0.29542878986675	-0.62862286502748

H	0.47447104841153	0.32063707402354	1.60657011329580
C	0.50446697328489	0.59651944458595	0.55887099134482
C	1.20566892245362	-0.33982403600966	-0.39756072748567
H	1.64444905162926	-1.24369076532077	0.00889828491811
H	1.82174469923042	0.09816357925630	-1.17429597644679
D	0.65105099203597	1.66163824449683	0.42183499010223

Frequencies

375.733739
573.846143
607.324915
620.026485
640.148117
849.665605
943.772856
1022.410489
1151.207182
1293.193092
1430.669004
2311.568179
3113.182989
3150.232705
3185.096195

p5

Si	-1.20362659337936	-0.59351400124092	-0.12163875479135
H	0.17149104911034	0.82813847384918	0.91698664670142
C	0.36333781961967	0.00554146138493	0.20382710126987
C	1.81073124886914	-0.19848606805979	-0.13508339721924
H	2.39691234343567	-0.43532019755343	0.75440978364727
H	1.94325165690479	-1.01237817994327	-0.84513740034839
D	2.24610184908849	0.70002957463276	-0.57542789638529

Frequencies

108.271607
167.536489
528.777904
675.590941
816.610049
944.068614
1142.544531
1276.222072
1305.746067
1368.131491
1483.982870
2247.003106
2946.175361
3057.495977
3114.566224

p6

Si	0.95841316139332	-0.53837122272724	-0.09673876910652
H	1.84330718246562	0.44352747608340	0.65458286456557
C	-0.66968769095948	0.31343226267557	0.28750256570898
C	-1.79201157812655	-0.23713195494337	-0.20722843365629
H	-0.76859567426822	1.21777631042585	0.87843009881511
D	-2.77860406643567	0.18044167333361	-0.04176750005266

H	-1.74990332505422	-1.14143395178628	-0.80442506852714

Frequencies

119.310354
280.407541
438.160942
643.345647
794.058741
913.940689
934.515225
1048.968502
1259.087374
1339.063809
1568.503902
2038.657219
2332.070690
3147.075451
3163.431237

p7

Si	0.99436226358022	-0.56618251457043	0.15151783661986
H	1.87566997502431	0.58112148576267	0.38497843617565
C	-0.65663615556965	-0.36133266646998	-0.12623182737186
C	-1.93779338348966	-0.20057970114451	-0.34663757902363
H	-2.66337876721283	-0.18802414008906	0.46112952395701
H	-2.33586555268488	-0.07181640002204	-1.34865705546399
D	1.60549052422313	-1.89754124360763	0.17718231674793

Frequencies

170.668988
229.516491
359.069539
560.787234
637.457279
760.252604
857.130563
963.070884
1017.517490
1445.810007
1666.875007
1794.353771
2315.499185
3099.660308
3164.528856

TRANSITION STATES

TS1: i1 – i4

Si	-1.06426958438164	-0.04341820443064	-0.32627455675262
H	0.63353462407756	0.72745624686887	1.71056075423981
H	-1.80142544613904	1.14333171190468	-0.82801052902466
H	-2.04397121275195	-1.03298816143266	0.18851528289338
C	0.40927999303197	0.29865254952733	0.74370966669119
C	1.28095611278432	-0.19398978879810	-0.12771458011438
D	2.35966511950820	-0.31611955321252	-0.16457460583947
H	0.22623039387059	-0.58292480042696	-1.19621043209327

Frequencies

1698.274434 i
273.468562
479.553498
530.605376
637.822261
667.924371
706.641728
827.690127
850.449389
962.551072
982.859402
1138.373828
1528.695458
1754.788223
2192.224116
2213.260802
2332.365398
3196.708896

TS2: i1 – p1

Si	-1.04423214459149	-0.11550705221300	-0.47915091134656
H	-1.64193414451133	1.22858750916664	-0.53950638374157
H	-1.04891664115412	-0.72534271054816	-1.82368971993403
H	-1.79936035232725	-0.96437338334014	0.45788451123757
C	0.69351433186557	0.01130032253287	0.10514737516616
C	1.89890653792671	-0.11484000248837	0.23731406762565
D	2.94106392034477	-0.17028417373853	0.43455897963771
H	0.00095949244715	0.85045949062870	1.60744208135507

Frequencies

679.642474 i
212.426420
262.548007
302.209362
427.670966
551.141774
574.236651
649.765878
694.568847
704.497912
954.232281
967.454007
975.197955
1944.949839

2259.234093
2278.822429
2283.385648
2672.588913

TS3: i1 – i2

Si	-1.12508548086112	-0.11562021272207	-0.50549106721671
H	-1.76444817733344	1.19663174275035	-0.71751085979867
H	-0.92789753784043	-0.77641241782075	-1.81754174198865
H	-1.99928219784775	-0.95786014002523	0.33238303203409
C	0.45670277219687	0.14815200033861	0.39586736011010
C	1.73626625574464	0.13466476692788	0.61141101743486
H	0.93124483382404	0.53857386039369	1.51232484932439
D	2.69249853211719	-0.16812959984250	0.18855841010059

Frequencies

1969.593239 i
180.694776
191.198233
290.527163
448.521973
587.058313
660.124816
694.831116
703.238441
950.494227
966.025595
968.071603
1726.901088
2216.356260
2264.766644
2267.866194
2273.593011
2434.035124

TS4: i4 – i2

Si	-1.39651939828009	-0.00782453693219	-0.43418462186376
H	-2.18242342466352	1.16858888622297	-0.03234827582741
H	-1.79255797752488	-0.50824475938113	-1.77925678619775
H	-0.77252354059361	-0.60298804954816	0.90724512448439
C	0.29369599917324	0.12974877738601	0.08208029331818
C	1.57474204238366	-0.02474455200031	0.34903089900228
D	1.95481848696525	-0.23645443685076	1.34233987588870
H	2.32076881253995	0.08192067110357	-0.43490650880464

Frequencies

1627.918362 i
167.015175
298.058695
458.999553
604.961690
636.346451
660.147978
811.274321
862.462269
899.097323
973.819884

1293.899405
1671.501700
1904.130702
2151.991424
2282.418700
2314.976060
3109.554247

TS5: i2 – p1

Si	-1.37415486079575	-0.07513835293244	-0.20250112931413
H	-1.78935695262346	1.15767069870577	0.49267843133603
H	-1.81149432414046	-0.02378732310925	-1.60930946031476
H	-1.96928876103319	-1.24789341553743	0.46327379121906
C	0.44567224528551	-0.22102647675417	-0.14434274823694
C	1.65699711110582	-0.27087923830737	-0.02073125086449
D	2.68988270174507	-0.51873742122930	-0.06077460120384
H	2.15174284045647	1.19979152916418	1.08170696737907

Frequencies

708.430245 i
150.291982
183.100867
228.986992
451.274305
566.396666
624.255579
680.437254
698.963068
702.953532
952.810600
969.661724
970.521961
1959.533292
2265.325800
2271.658887
2274.319652
2660.833460

TS6: i4 – i6

Si	-1.27659623572154	-0.46847356776671	-0.29855986313387
H	-2.63383489663363	-0.94220755539350	0.14456606294371
C	-0.21322194723963	0.61610204367238	0.51598862167002
C	1.02743175456696	0.12960006267608	-0.14055988290254
H	-0.24195795312185	1.40726567852455	1.24792683533979
D	1.76323740533366	-0.39636888270463	0.46006089689484
H	1.43609623328110	0.63561820693266	-1.01015924701957
H	0.13884563953494	-0.98153698594083	-0.91926342379237

Frequencies

1545.548247 i
287.044415
490.727301
549.782280
572.217314
775.951695
861.929202
910.635507

947.074502
1061.615833
1138.634030
1321.351772
1683.929044
1800.075346
2156.092231
2311.937939
3124.743015
3229.445674

TS7: i4 – i5

Si	-1.38162752750326	-0.67717594933109	0.39741865259959
H	-2.51346228534050	-0.07072469195009	1.13375799851159
C	-0.06380253808361	0.51737333856021	0.04954380679690
C	1.25264607559996	0.31434524909181	-0.35207816766588
H	0.99194275147699	0.60630152435885	0.84981438301152
D	1.88285383408041	1.17101724434475	-0.58563533937647
H	1.69546188958536	-0.65618249634761	-0.58908809689194
H	-1.86401219981535	-1.20495421872684	-0.90373223698531

Frequencies

1170.531513 i
204.074245
276.018696
396.912039
543.867835
634.724922
684.282079
905.347383
964.659446
1003.063062
1165.431409
1311.478954
1409.056159
2204.271952
2225.429192
2240.935675
2272.073154
3037.229209

TS8: i4 – p7

Si	1.48267153734249	-0.30709319556549	-0.03767073492084
H	2.41840417200479	0.78274751717990	-0.32061656283038
C	-0.18639651741804	-0.07004105881811	-0.18667132216921
C	-1.44928867415075	0.02362816813891	-0.52364863223875
D	-2.18393418967410	0.47117298361265	0.13557331176207
H	-1.80690046462080	-0.34423262182231	-1.47955625987268
H	2.01147718695405	-1.45343873804235	0.70268959454905
H	-0.28603305043764	0.89725794531680	1.70990060572074

Frequencies

590.649186 i
202.955203
255.512708
321.653628
355.934509

511.367283
600.545061
664.569883
745.273696
885.112595
897.829542
954.361408
1299.151495
1771.082810
2314.118649
2329.748825
2336.934357
3151.863025

TS9: i6 – i5

Si	-1.76260195608639	-0.37367794024724	-0.58829472163641
H	-1.46304106033434	0.45922899870854	0.67829399402802
H	-2.32890367290726	-1.67692985595047	-0.10988532072111
C	-0.07217095373388	-0.42919764984055	-0.10371065316091
C	1.14870537650600	0.36340262862536	0.01741445395698
D	1.63491295904534	0.19866563732334	0.98071212287297
H	1.84881593752951	0.02054447311213	-0.75010969712808
H	0.99428336998103	1.43796370826890	-0.12441917821146

Frequencies

926.591999 i
197.180888
200.063132
378.130099
624.630406
662.214594
844.885062
881.757151
957.238838
1215.115086
1274.102792
1321.436858
1431.490725
1972.717210
2112.065357
2250.324135
3016.209141
3071.054843

TS10: i6 – i7

Si	-2.01967782327599	-0.39453015279842	-0.66347662415851
H	-1.75274550016134	-0.43532239129903	0.90147846641746
C	-0.49600745267453	0.30298393150120	0.03045988173282
C	0.93163707673430	-0.09101705651509	-0.20904108307321
D	1.42339995739208	-0.39792291291963	0.71515799695656
H	1.02295261517703	-0.89414763151243	-0.93626829073369
H	1.48187343969385	0.78182940893809	-0.57498227700298
H	-0.59143331288539	1.12812780460531	0.73667192986155

Frequencies

1079.736356 i
158.063932

276.405548
568.387213
663.348362
883.727711
923.738129
1045.363650
1097.088508
1259.897107
1276.642228
1366.620198
1467.953177
1804.428619
2256.971164
3032.620235
3086.040195
3128.446923

TS11: i5 – p7

Si	-1.68379844738846	-0.40741150231382	0.13428920206986
H	-2.75195319607718	0.23705375312280	0.90336286966790
C	-0.10922950124325	0.17317735882270	0.16194966558391
C	1.13922262215365	0.59091826330959	0.15094261139399
D	1.47571484782075	1.36853862072000	-0.52728745870491
H	1.85185487804780	0.28223109670580	0.90905851281679
H	-2.05422706624411	-1.58338823573300	-0.65895112596144
H	2.13241486293081	-0.66111835463406	-1.07336427686611

Frequencies

592.750126 i
197.080025
213.057307
333.105879
372.813286
461.788456
647.586691
668.488393
774.704254
893.431793
933.441644
952.942423
1315.168498
1769.580478
2304.088924
2311.109925
2324.150274
3140.505622

TS12: i7 – p4

Si	-1.74240685772549	-0.45402425127277	-0.67881298555499
H	-0.54863450809619	0.29155907044268	1.51307252889599
C	-0.57684860334160	0.49394237808123	0.44804008869594
C	0.27549904688892	-0.36356649652645	-0.44462898555653
D	0.50115241641467	-1.39249729421439	-0.19178750452455
H	0.77070504656640	0.03069981207462	-1.31633258225697
H	-0.49164383155085	1.55708450787428	0.24691579068293
H	1.81217729084416	-0.16319872645920	0.42353464961817

Frequencies

1059.487535 i
284.492995
435.782918
490.616958
565.070044
644.685149
682.448387
735.691294
879.812668
998.428411
1038.115135
1148.396416
1309.092818
1427.592547
2319.516028
3105.876331
3173.166332
3232.631157

Data S2. IRC trajectories for all transition states.

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