

Supplementary material

Can Third-Body Stabilization of Bimolecular Collision Complexes in Cold Molecular Clouds Happen?

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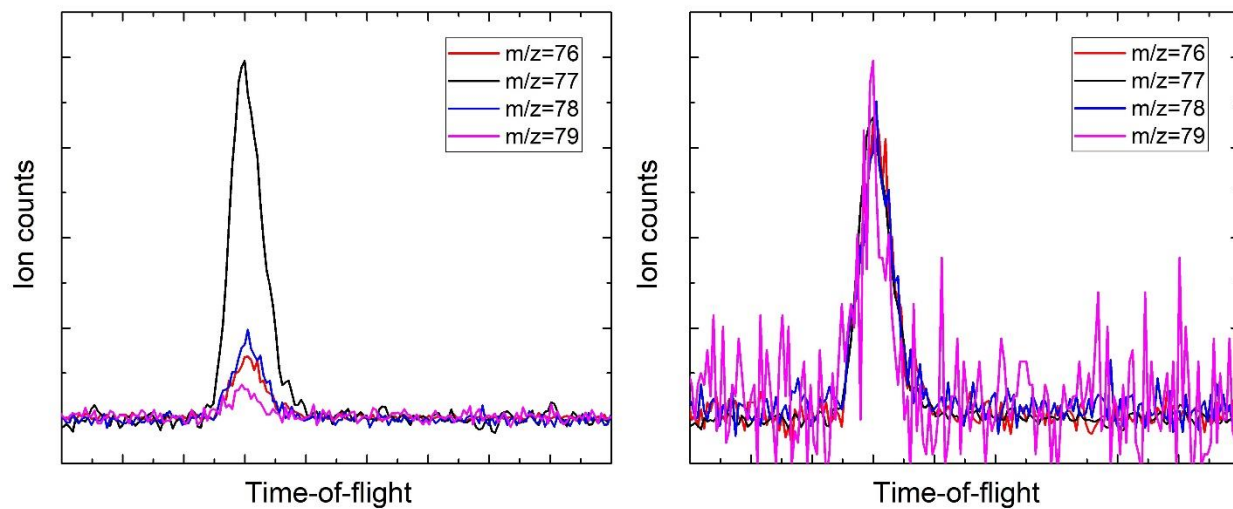


Figure S1. Time-of-flight spectra recorded at the CM angles for $m/z = 76, 77, 78,$ and 79 for the reaction of the ground state atomic silicon ($\text{Si}(^3\text{P})$) with diacetylene ($\text{C}_4\text{H}_2; \text{X}^1\Sigma_g^+$). The left and right panels depict raw and scaled TOF spectra, respectively.

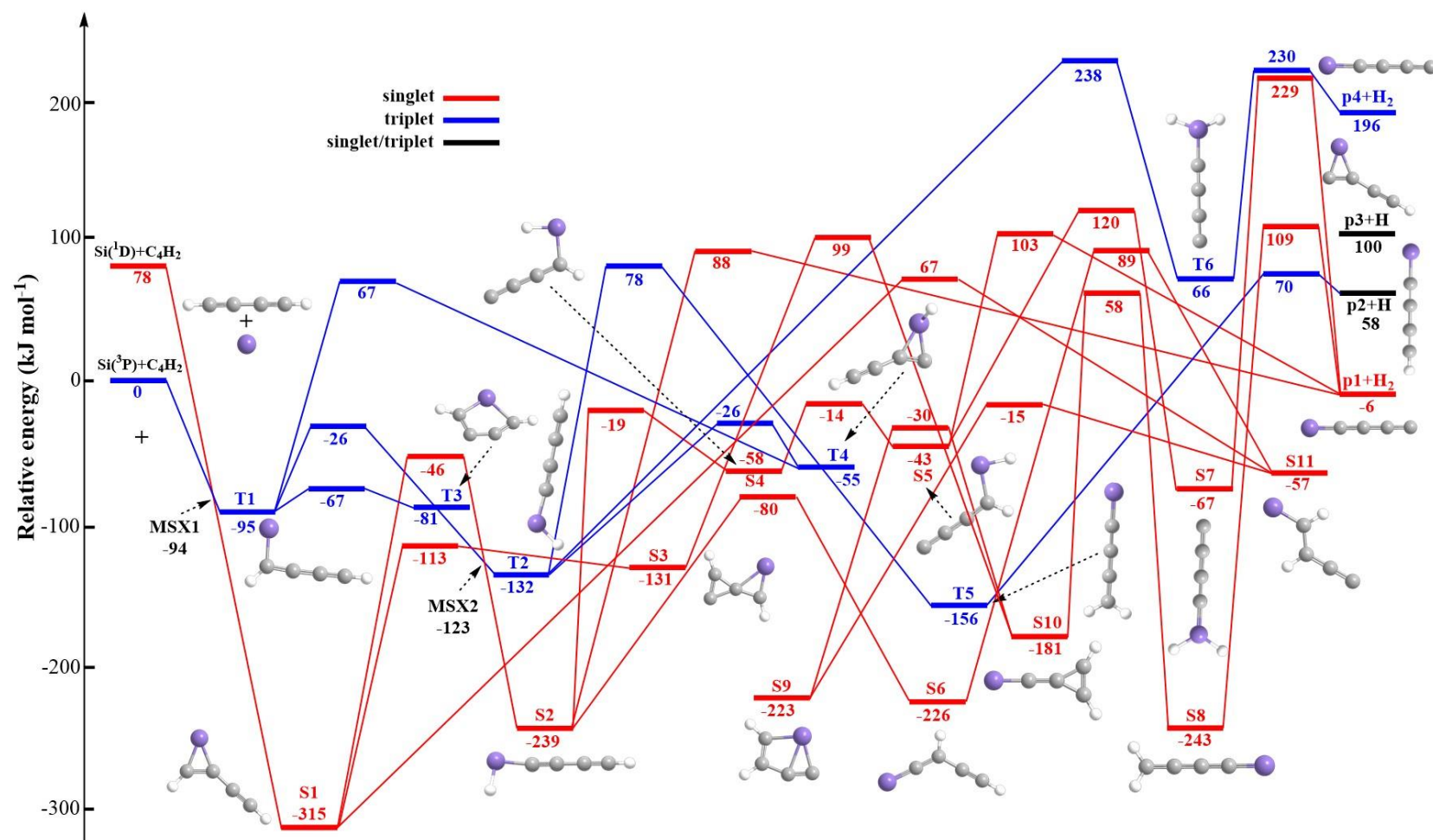


Figure S2. Potential energy surface for the reaction of atomic silicon with diacetylene. The cartesian coordinates and vibrational frequencies are compiled in the Table S2.

Table S1. Peak Velocity (v_p) and Speed Ratio (S) of the Silicon (Si) and Diacetylene (HCCCCH) Beams along with the Corresponding Collision Energy (E_c) and Center-of-Mass Angle (θ_{CM}) for the reactive scattering experiment.

beam	v_p (m s ⁻¹)	S	E_c (kJ mol ⁻¹)	θ_{CM} (deg)
Si	998 ± 18	4.6 ± 0.6		
C ₄ H ₂	630 ± 20	9.2 ± 0.3	12.5 ± 0.4	48.4 ± 0.5

Table S2. Optimized Cartesian coordinates (Å) and vibrational frequencies (cm⁻¹) for the reactants, products, intermediates, saddle points, and crossing seam minima (MSX) for the singlet and triplet surfaces of the silicon (Si) plus diacetylene (HCCCCH; X¹Σ_g⁺) reaction.

C₄H₂

C	-0.4202024975	1.5302594222	-0.0001327735	
C	-0.4127621102	0.3313748643	-0.0000037993	
C	-0.4042471034	-1.0407551309	0.0000987768	
C	-0.3968065745	-2.2396398948	0.0002181178	
H	-0.4267819164	2.5928731354	0.0000242138	
H	-0.3902314280	-3.3022539864	-0.0002333871	

Frequencies

235.155	235.259	536.857	
536.883	697.521	697.591	
701.838	702.001	911.079	
2148.800	2333.367	3481.505	3482.191

P1 - singlet

SiC₄

Si	-1.1680679436	0.1612521391	-0.0000217607	
C	0.5119765240	0.1362298522	0.0000984953	
C	1.7765642205	0.1176003038	0.0000625176	
C	3.0732618790	0.0985318033	0.0000600076	
C	4.3388012302	0.0800483218	0.0001292310	

Frequencies

87.632	87.707	211.007	
211.044	588.351	588.366	
595.516	1212.592	1942.391	2205.345

H₂

H	-0.6928913511	0.0670987046	0.0000000000	
H	0.0505413911	0.0781947254	0.0000000000	

Frequencies

4432.825

P2 - singlet/triplet

SiC₄H

C	-0.6885560034	-0.1457503542	0.0214775177	
C	0.6678386708	-0.1331852355	0.1022681208	
C	1.8687435183	-0.1220579483	0.1735138012	
H	2.9296161492	-0.1122297795	0.2364953951	
C	-1.9128225936	-0.1571334499	-0.0517699785	
Si	-3.6911642941	-0.1736648211	-0.1588397032	

Frequencies

91.777	119.214	277.497	
323.926	492.340	507.992	
573.650	634.002	739.477	
1046.337	2061.270	2226.629	3478.237

P3 - singlet/triplet

SiC₄H

C	-1.7776990658	-1.1001662557	0.0000000000	
C	-0.7123748882	-0.3369223959	-0.0000000000	
C	0.6698801540	-0.1889313750	0.0000000000	
C	1.8577060572	-0.0180151505	-0.0000000000	
H	2.9117511823	0.1172757168	0.0000000000	
Si	-2.3409352194	0.6332772103	0.0000000000	

Frequencies

122.204	212.403	420.385	
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531.035 601.117 655.184
735.282 762.568 913.533
1707.853 2227.204 3479.774

P4 - triplet

SiC₄ - triplet

Si -1.2569733340 0.1631611839 -0.0000000000
C 0.5309077273 0.1354543616 0.0000000000
C 1.7793830944 0.1171227181 -0.0000000000
C 3.0958494307 0.0980121615 0.0000000000
C 4.3833689915 0.0799119951 0.0000000000

Frequencies

98.778 99.784 238.609
299.208 400.052 492.144
559.823 1032.287 1799.069 1940.610

INTERMEDIATES - singlets

S1

Si -4.1777613212 -0.5273755444 0.0000000000
C -3.2411037021 -2.0957756780 -0.0000000000
C -2.0851389427 -2.8836927917 -0.0000000000
C -4.5720904230 -2.2895241626 -0.0000000000
C -1.0718303746 -3.5276831780 0.0000000000
H -5.1904804280 -3.1761223935 -0.0000000000
H -0.1789231483 -4.1036180219 0.0000000000

Frequencies

166.232 206.449 470.059
519.908 600.755 636.452
757.776 792.272 904.428
995.043 1102.989 1590.627
2218.641 3217.814 3479.892

S2

Si -3.7776331502 -0.7009354069 -0.3656558602
C -2.2320087120 -1.6484892675 -0.1497743929
C -1.1538402544 -2.2121737526 -0.1263945943
C 0.0505133063 -2.8536362082 -0.0845733920
C 1.1099019090 -3.4180013505 -0.0474701866
H -4.4277331705 -1.3053042129 0.8640425258
H 2.0475963620 -3.9172388413 -0.0150264497

Frequencies

97.258 109.401 278.016
298.435 479.429 527.639
568.338 660.453 728.401
823.604 1036.230 2074.947
2141.567 2290.649 3479.199

S3

Si -0.3262368437 -0.3902286917 0.9822024869
C -1.6560126114 -0.1230013609 -0.0689669378
C -0.6335057144 0.0965150893 -0.9964172920
C 0.6234318983 0.2417264002 -1.6107012650
C -0.4044531047 0.4437204799 -2.4303168511
H -2.6988582365 -0.0546346764 -0.3300370022
H 1.6778230605 0.1892937234 -1.4049817126

Frequencies

180.379 185.104 325.024
467.868 712.676 744.379
826.633 889.067 968.522
1038.110 1108.765 1350.638

1651.410 3259.081 3282.321
S4
Si -0.0907206772 -0.3352708695 2.0579959914
H 2.1145506860 -0.9010023887 0.7306712697
H -1.2273509074 0.1737867041 1.1984792058
C 1.1017388522 -0.5414697867 0.6290385352
C 0.5329944818 -0.1943077307 -0.4780610384
C -0.0694287225 0.1610795642 -1.5655062161
C -0.6137603734 0.4974595258 -2.6588636022

Frequencies
110.620 165.352 202.297
284.759 488.118 570.623
678.263 705.356 857.199
928.498 1107.250 1781.008
2102.867 2173.280 3237.669

S5
Si -0.4212596842 -0.0045251922 1.9559816708
H 1.9527406397 0.0099473456 0.7902278220
H 0.6390618511 -0.0033084733 3.0437255353
C 0.8890150403 0.0045004488 0.5837878197
C 0.4562777297 0.0022564415 -0.6346092268
C -0.0545026577 -0.0008655457 -1.8171585618
C -0.5477609221 -0.0046118389 -2.9881134714

Frequencies
86.518 157.086 187.580
228.486 519.376 563.450
618.702 679.024 824.418
944.882 1082.291 1774.448
2070.102 2173.549 3195.429

S10
Si 0.0460279858 -0.1581811327 2.0318429570
C -0.1193328913 -0.0047363554 0.3904974371
C -0.2514493751 0.1179097604 -0.9233238994
C 0.2506546158 0.4311151188 -2.2159327903
C -1.0042735184 0.0375632613 -2.1265895820
H -1.9318356230 -0.1830885837 -2.6265462432
H 1.0657723389 0.7560123750 -2.8394948767

Frequencies
131.282 154.018 469.155
505.494 568.336 755.625
917.158 930.211 958.761
1118.818 1269.756 1590.641
1818.888 3258.346 3296.417

S7
Si 0.3261168658 -0.5000792490 -0.0150536334
H 1.0664690377 -1.7663650444 -0.0998839764
H 1.1515197281 0.7066838958 -0.1606012517
C -1.3316230846 -0.4368309988 0.2299705507
C -2.5706892217 -0.3876480559 0.4132734387
C -3.8592787156 -0.3363699468 0.6040416648
C -5.1083106346 -0.2860471849 0.7889971481

Frequencies
84.560 94.199 217.505
217.714 555.617 584.579
592.646 631.850 674.228
973.997 1210.281 1968.357

2209.428 2315.856 2334.039
S8
Si -4.0671203503 0.6947842883 -0.0253318670
C -3.0049236749 -0.6110556977 -0.0058969761
C -2.1928733149 -1.6086054343 0.0089608240
C -1.3900666124 -2.5945507509 0.0236146878
C -0.5642137304 -3.6074844647 0.0387357762
H 0.5102732054 -3.4621899030 0.0056603226
H -0.9231512242 -4.6300853836 0.0848283286

Frequencies
99.002 117.089 252.731
271.954 500.009 575.738
608.517 961.997 1034.425
1150.080 1468.048 1792.505
2177.315 3125.663 3205.129

S9
H -0.8699760271 -0.0650827207 -2.7466779329
H 1.6565004678 0.6128438657 -2.1855023906
Si 0.7219179534 0.2611812543 0.4429877472
C -0.8983798113 -0.8170150847 0.6733304766
C -0.9148419888 -0.5634186025 -0.5505769336
C 0.9302608481 0.1992111506 -1.4989657216
C -0.3266652020 -0.1228819919 -1.8125157206

Frequencies
120.142 338.099 444.743
517.438 570.487 712.883
766.204 939.887 1007.528
1086.248 1299.282 1579.802
1975.703 3194.027 3221.110

S6
Si -5.0889945006 -0.4415351377 0.6166850668
C -3.6937563672 -0.9468271516 -0.1744993771
C -2.5976513172 -1.3397302113 -0.8101096602
C -1.5682365911 -2.1250393033 -0.2225700673
C -0.6855799569 -2.7868190642 0.2469572830
H -2.4350766004 -1.0651892350 -1.8518311606
H 0.0900118959 -3.3737692400 0.6753851068

Frequencies
112.444 204.646 312.600
337.114 535.508 690.860
718.951 812.460 881.799
1022.872 1307.317 1753.532
2228.962 3108.439 3478.919

S11
Si -4.2887012806 -0.8006874867 1.3897382152
C -2.8985223479 -1.6901817301 0.8881772074
C -2.2996286337 -1.6370166635 -0.4019061122
C -1.2176428905 -2.3396785731 -0.7802898477
C -0.2021874657 -2.9915500999 -1.1558537325
H -2.7478155351 -0.9775949661 -1.1448835868
H -2.4175303578 -2.3611559939 1.6010964748

Frequencies
85.627 93.425 194.255
262.440 500.143 769.532
822.311 932.437 1108.416
1196.209 1252.975 1493.465

2050.162 3103.213 3115.101
INTERMEDIATES - triplets
T1
Si -2.3056643688 -0.1631132326 0.0000000000
C -2.8555634572 -1.9253936744 -0.0000000000
C -1.6585660256 -2.4333733664 -0.0000000000
C -0.4029491404 -2.8727130367 -0.0000000000
C 0.7488803094 -3.2639021146 0.0000000000
H -3.8071874061 -2.4463086244 -0.0000000000
H 1.7541381488 -3.6075561510 0.0000000000
Frequencies
90.500 206.480 285.473
415.444 480.471 501.999
559.934 604.311 608.624
884.499 948.905 1701.557
2039.144 3156.883 3473.353
T2
Si -4.0416020768 0.7999269161 0.0000000014
C -3.0115057929 -0.6421098935 0.0000000006
C -2.2158012344 -1.5641003454 0.0000000004
C -1.3431747792 -2.6110925277 0.0000000000
C -0.5724561291 -3.5330801947 -0.0000000003
H -5.5119646131 0.6175191306 -0.0000000016
H 0.1076158134 -4.3497035943 -0.0000000005
Frequencies
110.245 119.537 289.861
324.946 511.502 524.151
553.556 666.335 694.456
713.919 1061.134 2126.306
2224.758 2267.396 3479.424
T5
Si -4.0977764250 0.7258704684 -0.0076107323
C -2.9962476736 -0.6240093587 0.0042698272
C -2.1935949861 -1.6080817666 0.0129185578
C -1.3814900280 -2.6039117074 0.0216873969
C -0.5558587931 -3.6150959913 0.0306154686
H 0.5157960095 -3.4590053441 0.0248670216
H -0.9223807353 -4.6340456995 0.0439574708
Frequencies
103.033 111.537 284.182
333.133 470.737 513.944
520.058 813.813 962.059
1044.342 1411.614 1724.833
1918.817 3146.951 3231.330
T6
Si 0.5101522838 -0.4854238768 0.3133688333
H 0.9635641636 -1.7438480052 -0.3123472511
H 1.0575138956 0.7190577710 -0.3425184591
C -1.3154094328 -0.4191853247 0.3691364748
C -2.5340399439 -0.3883273619 0.4642088087
C -3.8660553077 -0.3570668844 0.5824304980
C -5.1415851584 -0.3318599581 0.6865107655
Frequencies
101.492 106.839 249.653
263.662 446.708 487.525
526.389 648.668 687.782

925.882	1015.670	1929.661
2178.250	2262.722	2289.070

T3

Si	-2.9108075954	-1.4247236488	-0.7047871738
C	-3.8094611210	-3.4196018727	0.5568319103
C	-2.4660550542	-3.3762177792	0.3408054595
C	-4.3912970912	-2.3352750637	0.0231533890
C	-1.4833388234	-2.7659331021	-0.1457414855
H	-5.4278888489	-2.0363566421	0.0010366370
H	-0.4443329925	-2.6455595693	-0.3607885308

Frequencies

264.915	349.337	392.983
408.753	545.612	603.253
708.737	733.320	795.055
1041.876	1163.102	1463.360
1818.915	3237.576	3393.716

T4

Si	-3.9379140815	-0.0680703577	-0.2416956866
C	-2.2739761315	0.1274767768	-0.9763834547
C	-2.3334088625	-1.0662616899	-0.4509733920
C	-1.7422792357	-2.2863280390	-0.1417623447
C	-1.2742396860	-3.3526800637	0.1463811889
H	-4.2278525053	0.5080168793	1.1091164691
H	-0.8469938667	-4.2935806693	0.3944589970

Frequencies

158.608	211.118	417.678
493.349	541.772	581.394
675.272	695.698	708.886
751.141	914.337	1716.309
2133.049	2232.107	3479.700

TRANSITION STATES - singlets

TS_S1_S2

Si	-0.0880527217	-0.3016927957	-1.9894539478
H	0.1115933265	-1.5083140304	3.2346851995
H	0.2951724849	1.7445083460	-1.3421856415
C	-0.1807354620	0.9862378993	0.5994817639
C	-0.0387775934	-0.0083694101	1.5292717029
C	0.2029150115	0.8232362895	-0.7106526297
C	0.0607762141	-0.8376740186	2.4121255027

Frequencies

-237.693	126.056	248.777
367.535	377.853	479.164
590.550	783.924	816.596
957.879	1140.532	1385.460
2070.217	2798.231	3472.701

TS_S1_S3

C	0.1434371090	-0.3424728242	-2.6305028611
C	-0.0400249253	0.3356309087	-1.5437791050
H	-0.2167568516	1.3720852280	-1.8723995238
C	0.0048257807	-1.1104158934	0.6127547718
C	0.0247424955	0.0031214216	-0.1332346563
Si	0.1690976912	0.3723714264	1.6421896027
H	-0.0857140396	-2.1674638470	0.4064363617

Frequencies

-108.975	43.775	293.105
357.860	574.551	661.831

785.987	902.140	979.091
1003.151	1122.323	1594.888
1779.960	3025.540	3219.720

TS_S1_S11

C	-0.0001118953	0.4107366897	-2.6669547176
C	0.0000956143	-0.1761607843	-1.5531812487
H	-0.0004259743	0.8495653988	-0.7005040944
C	0.0003476490	-1.1267717005	0.9159958279
C	0.0000975125	-0.3220913200	-0.1645227810
Si	-0.0003165024	0.5266296225	1.5749964270
H	0.0007740362	-2.2038359164	0.9871890670

Frequencies

-1559.624	156.154	167.458
327.786	386.518	433.976
552.850	812.746	838.944
933.957	1096.134	1543.502
1976.595	2180.686	3239.968

TS_S2_S4

Si	-0.7929353482	-0.4670054267	-1.0845612995
C	-0.3209535975	-0.8456782837	2.4641392407
C	0.0649842342	-0.0254644347	1.5776644251
H	0.3445908940	-1.4280895396	-0.8607529347
C	0.1980710669	1.1823207568	-0.6420165746
C	0.2780152105	0.7605359958	0.5494853940
H	0.2356676502	2.1134292422	-1.1749220411

Frequencies

-193.080	163.120	189.915
376.298	505.916	566.739
584.861	645.372	802.357
867.703	1010.173	1829.933
2112.489	2134.992	3320.194

TS_S2_P1

Si	0.2274936749	0.5068302057	-1.9366201641
H	0.6260974616	-0.9792300126	-0.9168869037
H	0.6418615627	-1.3648343299	-0.0235768229
C	0.4519293041	-1.3721242816	1.3924744111
C	0.0291210324	-0.1934706274	1.4706630097
C	-0.2572731423	1.3553955879	-0.4762570300
C	-0.2193554834	0.8196400179	0.6485636199

Frequencies

-1051.836	85.812	217.177
258.133	344.377	521.466
545.177	762.223	826.773
1059.509	1157.524	1203.545
1466.954	1916.941	2056.668

TS_S2_S6

Si	-4.7082539611	-0.3537156056	0.4921349322
C	-4.1516215476	-1.7147751722	-0.4662647496
C	-2.9091861391	-1.2290026688	-0.1072367698
C	-1.7035146266	-1.9931560642	-0.0743905004
C	-0.6826563190	-2.6206479682	-0.0445581637
H	-2.6457068319	-0.1773071778	0.2272035622
H	0.2120025554	-3.1940939132	-0.0268883173

Frequencies

-347.086	140.192	214.705
360.596	566.453	688.448

740.052	814.754	913.344
976.968	1269.042	1496.360
2224.390	2584.961	3479.183

TS_S3_S10

H	-1.6145408405	0.2851473004	-3.1492796936
H	1.0995732010	-0.4017531815	-0.9346959295
Si	1.2523055621	-0.0292798996	1.3074707275
C	0.1308571316	0.2013999713	0.1013682579
C	-0.4460931456	0.1987591499	-1.1299585734
C	0.4085261970	-0.3620906287	-2.1931961726
C	-0.8306708059	0.1032233981	-2.4288912863

Frequencies

-1864.486	138.447	149.880
426.287	436.513	641.508
749.395	792.730	927.078
1037.632	1253.030	1304.015
1477.115	1759.530	3225.592

TS_S4_S5

H	-1.3646255701	1.4864533256	-0.7422842849
C	-0.5920050461	0.7317318275	-0.6054162240
Si	-0.0268045646	-0.2106768891	-2.1729954233
C	-0.1801732812	0.4623905825	0.5808008607
C	0.2823538411	0.1273875546	1.7418454626
C	0.7435687261	-0.2067659525	2.8766718884
H	1.1377042649	0.7210859213	-2.4577012995

Frequencies

-403.977	78.727	192.120
196.022	431.833	505.636
563.153	627.689	816.540
940.450	1072.062	1805.900
2071.697	2158.127	3143.358

TS_S10_S8

Si	0.0840276922	-0.0511582876	-2.3665586116
C	-0.0329857035	-0.0009247122	-0.6709229159
C	-0.0967138588	0.0477694188	0.6002013996
C	0.1115466576	0.1225496836	3.2150535930
C	-0.1932777850	-0.0169583855	1.8988739945
H	-1.1850259454	0.3288481268	2.4298564493
H	-0.2117695471	-0.7502383040	3.8013814010

Frequencies

-619.687	103.614	130.299
293.269	350.353	429.745
558.579	660.960	902.793
1024.260	1112.281	1661.464
2072.257	2515.576	3019.136

TS_S5_P1

Si	0.3041863400	0.0351967600	0.4558157000
H	0.6981295900	-1.2810771500	-0.4443513500
H	1.5913312400	-0.2937907600	-0.2019470600
C	-1.3598167900	-0.1283594100	0.1943734600
C	-2.5853056900	-0.2923143200	0.4087316100
C	-3.8650598500	-0.4568216800	0.5924721400
C	-5.1061191600	-0.6159035600	0.7882387600

Frequencies

-1568.271	78.499	158.640
196.591	252.591	348.655

529.148	562.459	602.072
684.597	1178.727	1668.950
1933.369	2187.967	2296.561

TS_S5_S7

H	-1.2524872139	-0.5119759048	-1.2326586189
C	-0.0164838562	0.2363341475	-0.4581619979
Si	-0.0925697579	-0.0588541711	-2.1870207963
C	0.0029565002	0.1075224192	0.8095173831
C	0.0187916271	-0.0073931825	2.0976836002
C	0.0312768272	-0.1264152936	3.3689733353
H	-0.2382815465	1.3199001853	-2.7482618155

Frequencies

-1350.361	81.263	104.481
236.830	267.832	505.085
547.979	592.074	632.082
799.817	1135.217	1837.878
1901.579	2154.154	2173.039

TS_S7_P1

Si	-0.1482606894	-0.0053746961	2.2655164670
H	1.2900447454	0.0041182627	1.3636647097
H	1.5301308117	0.0046195628	2.3438457737
C	0.0997743398	-0.0020663115	0.5264755330
C	0.0365429079	-0.0012574115	-0.7320161025
C	-0.0055920546	-0.0003142898	-2.0333647794
C	-0.0445885278	0.0004952478	-3.2969551192

Frequencies

-1355.282	100.179	139.422
221.146	258.098	542.572
580.366	598.040	848.325
1023.323	1163.110	1804.208
1880.352	1943.793	2189.076

TS_S8_P1

Si	-3.9242419333	0.8336237840	-0.1898360328
C	-2.9881730452	-0.5547068234	-0.0150161648
C	-2.2793266245	-1.6088199862	0.1212863351
C	-1.5565227637	-2.6612403336	0.2415846397
C	-0.9914010294	-3.7706732334	0.5742270122
H	0.1179772399	-3.7258991630	-0.6174365867
H	-0.0102964239	-4.3313593444	0.0158653573

Frequencies

-1077.795	91.931	110.567
249.886	256.390	516.523
548.432	597.836	615.251
684.245	1166.915	1645.703
1862.541	2137.369	2729.602

TS_S9_S10

H	-1.2785509032	0.0687897325	-2.5319178886
H	0.8996527867	-0.5670141399	-3.4608129563
Si	0.6794865989	0.0911598896	1.9240975192
C	-0.4160772084	0.2138618630	0.6504006648
C	-0.4276429109	0.0755110832	-0.6028879786
C	0.9124901317	-0.4493419109	-2.3647777467
C	-0.3710718048	-0.0889789074	-1.9481707239

Frequencies

-71.940	138.767	206.386
359.599	518.540	655.294

783.067 890.963 1076.735
1197.636 1254.409 1416.641
2033.809 2987.569 3087.363

TS_S9_S11

H 0.2211532341 -1.0473468102 -2.3723746579
H 0.2398164279 1.6379250224 -1.5566240622
Si 2.1475244750 1.1456709214 -0.3767628591
C -1.9519007292 -1.4739197337 0.0009018566
C -1.0241962221 -0.9787866377 -0.7129394978
C 0.7122628012 0.7162534321 -1.1888858362
C -0.0458437370 -0.4949583044 -1.4712352634

Frequencies

-430.802 116.718 188.864
209.122 364.641 565.580
750.489 836.514 1045.872
1165.694 1284.542 1426.126
2053.355 3041.271 3105.092

TS_S6_S11

Si -3.9348365617 -1.1621679254 1.5880274419
C -3.1303641546 -1.1899081743 0.1158854143
C -2.3634684707 -1.3374610013 -0.9973952642
C -1.3545365064 -2.2566561467 -0.7126886445
C -0.6018751790 -3.0924654042 -0.1433230318
H -2.5068695085 -0.8320427041 -1.9449093201
H -2.0873741415 -2.2082274215 0.5744649038

Frequencies

-1742.527 135.823 190.218
240.277 265.524 646.213
810.020 906.612 986.130
1021.200 1278.444 1494.457
1627.513 1993.773 3199.759

TRANSITION STATES - triplets

TS_T1_T2

H 0.3176373943 -1.3492994749 -1.5541038367
C 0.0234071682 0.1042488754 -0.5431194685
Si 0.1128833158 0.0254744386 -2.2983138366
C -0.0193289491 0.0721788468 0.7201876119
C -0.0512105825 0.0079068263 2.0531342509
C -0.0784914824 -0.0509529487 3.2636320584
H -0.1014239642 -0.1026251233 4.3250666306

Frequencies

-987.553 96.738 116.592
327.758 348.493 472.587
508.609 540.747 561.567
729.731 1064.592 1727.534
1830.730 2074.752 3470.930

TS_T1_T3

Si -3.1168871527 -1.3013748569 -0.7622403934
C -3.7154746650 -3.3645727578 0.5227874691
C -2.3497996187 -3.3711411184 0.3312715275
C -4.4311970894 -2.3510072446 0.0363929595
C -1.2134155255 -3.0863013078 0.0032032529
H -5.5005090774 -2.2059181897 0.1055420593
H -0.1900452116 -2.9234762950 -0.2369568751

Frequencies

-150.244 261.782 280.712

517.077	538.261	582.071
688.701	709.413	737.343
975.215	1130.520	1496.004
2068.469	3213.941	3462.678

TS_T1_T4

Si	-2.5125532956	-0.9855365145	0.5214498135
C	-1.9047569137	0.7558547137	0.3064681205
C	-0.7910457353	0.0519064174	0.2091240983
C	0.5501068046	-0.1248015729	0.0419064049
C	1.7333200582	-0.3244104950	-0.0825811696
H	-2.8227766898	-0.1263577755	-0.8005539437
H	2.7778057715	-0.4843547731	-0.1958133239

Frequencies

-843.835	163.471	210.574
375.498	466.340	530.759
636.040	651.582	699.886
718.721	913.121	1590.203
1726.523	2147.656	3476.012

TS_T2_T5

Si	-3.8225348991	-0.2276819017	0.0992096390
C	-2.5563855344	0.1700649895	-1.1445317660
C	-1.7541378662	-0.7747721797	-1.0269103872
C	-1.3800095388	-1.9261974544	-0.4372494968
C	-1.9314438965	-2.5839633342	0.4710422878
H	-3.1875359010	-1.6786295165	0.7311630964
H	-2.0046167335	-3.4102477665	1.1464184038

Frequencies

-1475.493	281.026	301.552
436.843	455.141	503.703
536.212	663.624	701.156
940.457	1136.509	1359.495
1880.076	1972.743	3380.152

TS_T2_T6

H	1.4029717232	-0.1142233550	-0.0346326644
C	1.1109833295	-0.0574221075	1.5502047212
Si	0.4134163620	-0.0470311215	-1.3749166977
H	0.6291197255	1.2904778539	-1.9893416925
C	-1.2103130258	-0.1227774630	-0.5554440631
C	-0.8857518634	0.0268646123	0.6463947289
C	-0.1281202011	0.1785449708	1.7516210476

Frequencies

-1151.253	177.287	306.014
379.616	446.341	484.399
514.224	635.715	755.652
853.335	1143.857	1242.851
1556.009	1890.471	2207.638

TS_T2_T4

Si	-4.0166331230	0.1935404318	-0.2617904527
C	-2.3744229197	0.1104389589	-1.0964066472
C	-2.1183515687	-1.0050337628	-0.5957057386
C	-1.6896492491	-2.2356548327	-0.1729095552
C	-1.3212639026	-3.3130040053	0.2072210527
H	-4.1247692018	0.0854995889	1.2181522400
H	-0.9915744045	-4.2672135424	0.5405808780

Frequencies

-456.831	137.092	217.900
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290.694	498.911	517.461
670.399	672.245	745.362
748.017	886.292	1946.879
2181.852	2244.674	3476.160

TS_T5_P2

Si	0.0057754717	0.0122312702	-2.4211254645
C	0.0018138391	-0.0078202105	-0.6228460872
C	-0.0007565408	-0.0211474761	0.6010557346
C	-0.0035945393	-0.0450402271	1.9603590164
C	-0.0055523991	0.0630562111	3.1685643997
H	0.0006945502	1.8851368026	3.5700486434
H	-0.0084807319	-0.1815387203	4.2053311477

Frequencies

-1001.677	97.200	106.545
270.426	281.623	405.618
490.619	548.629	572.993
728.749	829.956	1032.688
2059.455	2218.676	3436.990

TS_T6_P4

H	-1.3081219002	-0.6271777517	-2.2120364057
H	-1.2525486140	0.5827927801	-2.6972155011
Si	0.1559798797	0.0384989091	-2.3041092432
C	-0.0893799288	0.0837976323	-0.5211584721
C	-0.0332547691	0.0212595906	0.7219384031
C	-0.0174320644	-0.0287077660	2.0331758283
C	-0.0016966132	-0.0768946444	3.3098815106

Frequencies

-1236.278	106.609	110.791
247.589	261.830	447.690
480.352	534.373	581.545
632.730	1077.419	1693.007
1822.546	1834.566	2088.754

MSXs

MSX1

Si	-0.3226921530	-0.0020721604	-1.9492013995
C	1.1516203969	0.0010874377	-0.8613883120
C	0.7617938773	-0.0007884571	0.4155835957
C	0.0339010109	-0.0012663142	1.4963170644
C	-0.6708761692	-0.0021524618	2.5440711740
H	2.1994807522	0.0035201329	-1.1503253708
H	-0.9794901793	0.0016753828	3.5624554513

Frequencies (Effective Hessian)

MSX2

H	0.3504542651	-1.1998603534	-3.1808034699
C	0.0475345478	-0.0265799275	-0.4547660505
Si	0.1254687103	-0.1268298794	-2.2219946507
C	0.0025370412	-0.0124869294	0.7791021814
C	-0.0485810484	0.0041838445	2.1404508864
C	-0.0961110558	0.0239392462	3.3609124877
H	-0.1378705802	0.0411371489	4.4219353247

Frequencies (Effective Hessian)

3484.629	2181.180	2139.803
2006.351	1045.458	621.387
618.925	537.407	511.486
481.510	331.506	284.248
131.936	109.920	