

Supporting Information

Directed Gas Phase Preparation of Ethynylallene (CH₂CCHCCH; X¹A') via the Crossed Molecular Beam Reaction of the Methylidyne Radical (CH; X²Π) with Vinylacetylene (H₂CCHCCH; X¹A')

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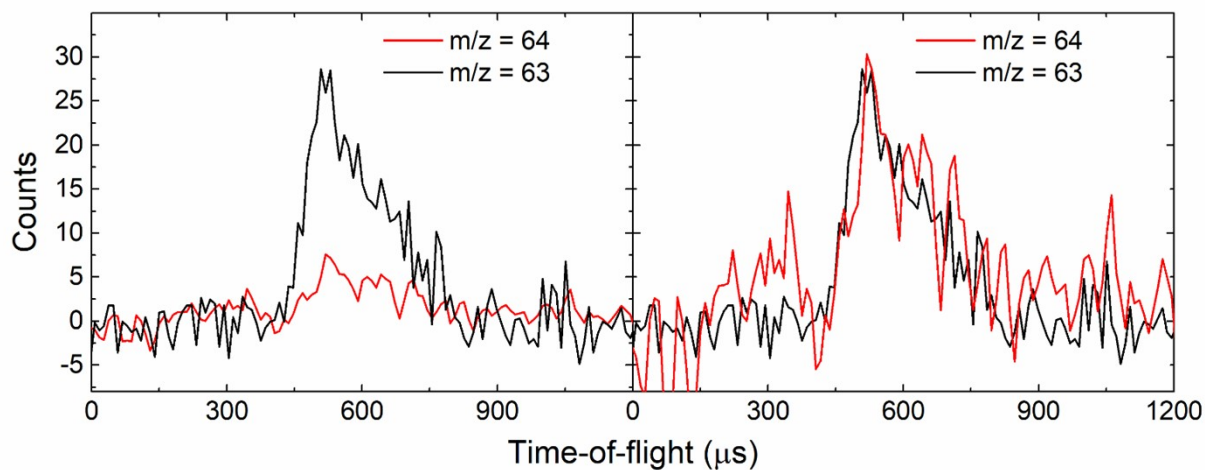


Figure S1. Time-of-flight spectra recorded at the CM angles for $m/z = 63$ ($C_5H_3^+$) and $m/z = 64$ ($C_5H_4^+$) for the reaction of the methylidyne radical (CH) with vinylacetylene (C_4H_4). The left and right panels depict raw and scaled TOF spectra, respectively. Since both traces overlap, signal at $m/z = 63$ represents a fragment of $m/z = 64$.

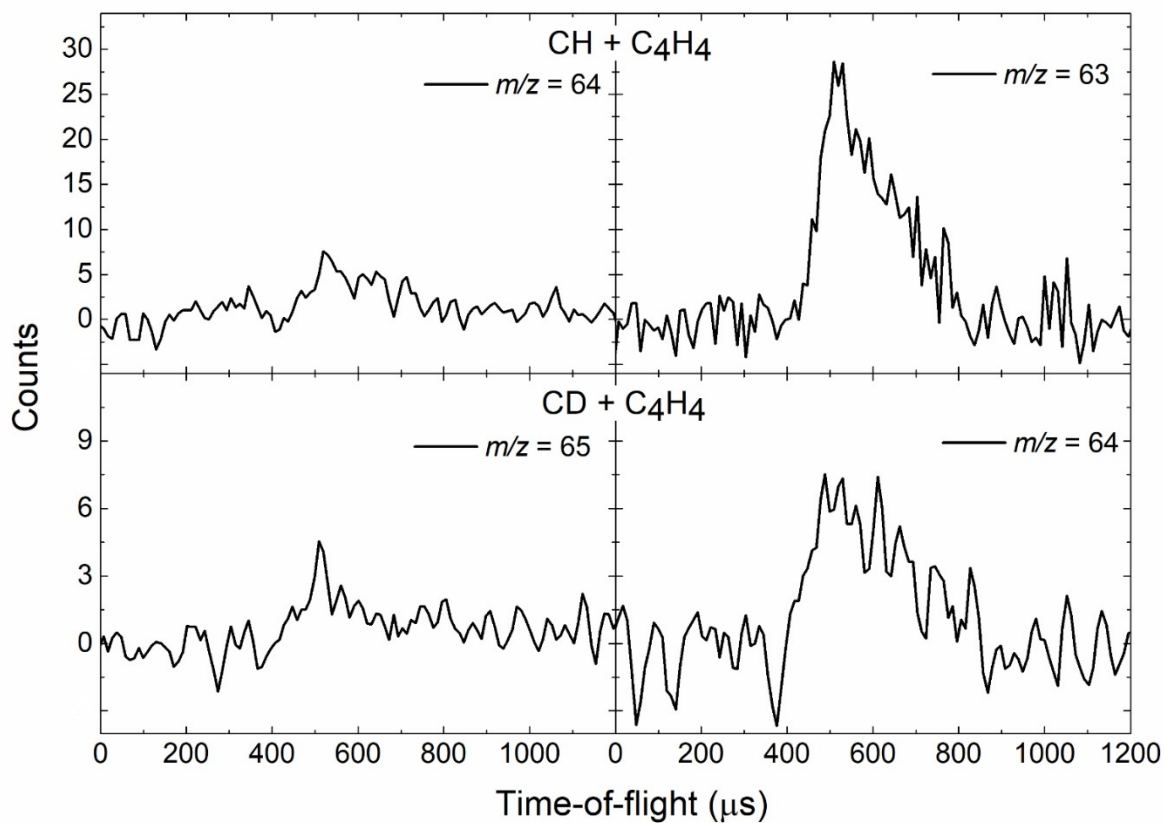


Figure S2. Time-of-flight spectra for the reaction of methylidyne radical (CH) with vinylacetylene (C₄H₄) (top), and D1-methylidyne radical (CD) with vinylacetylene (C₄H₄) (bottom).

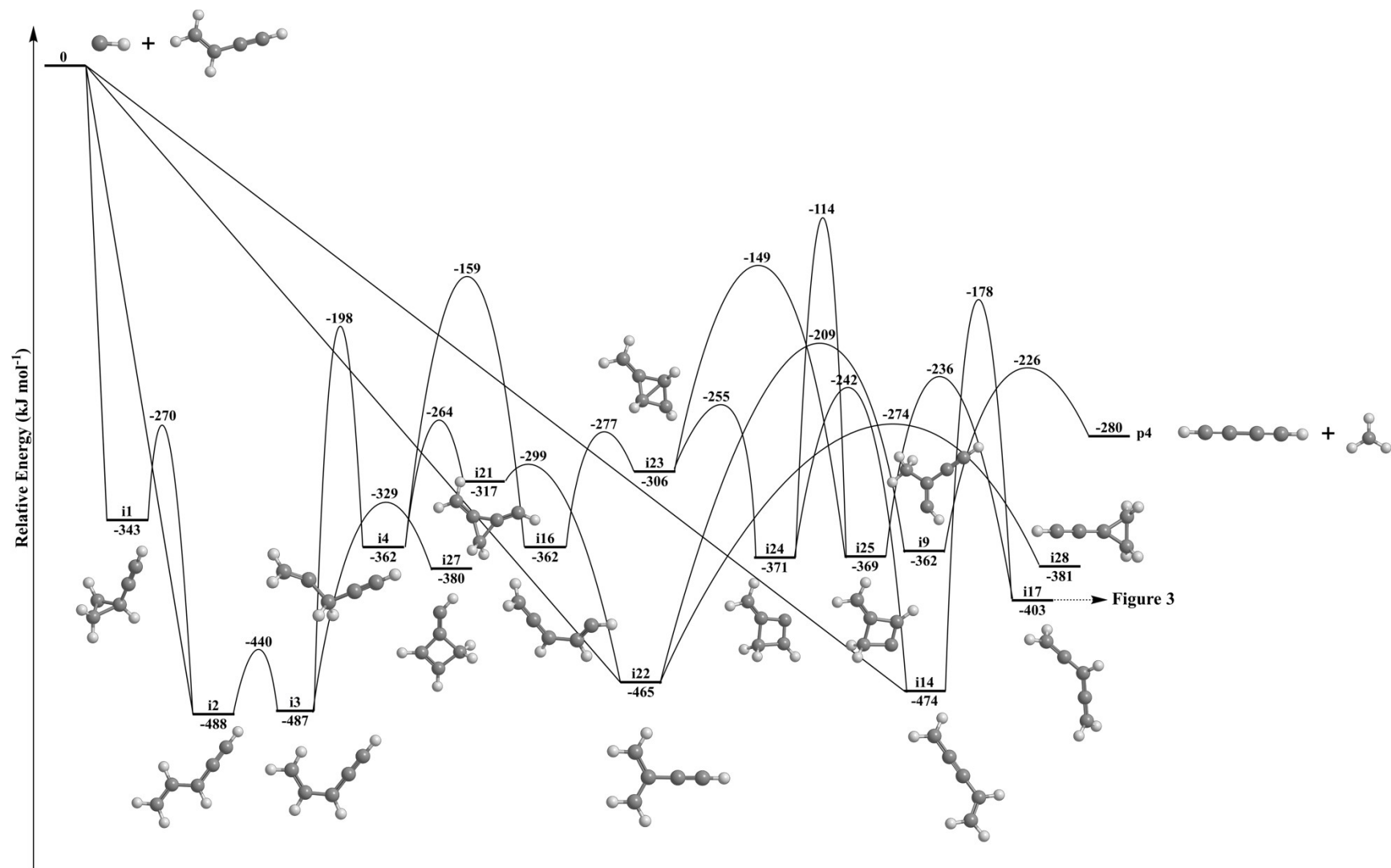


Figure S3. Portion of C_5H_5 potential energy surface (PES) leading to p4.

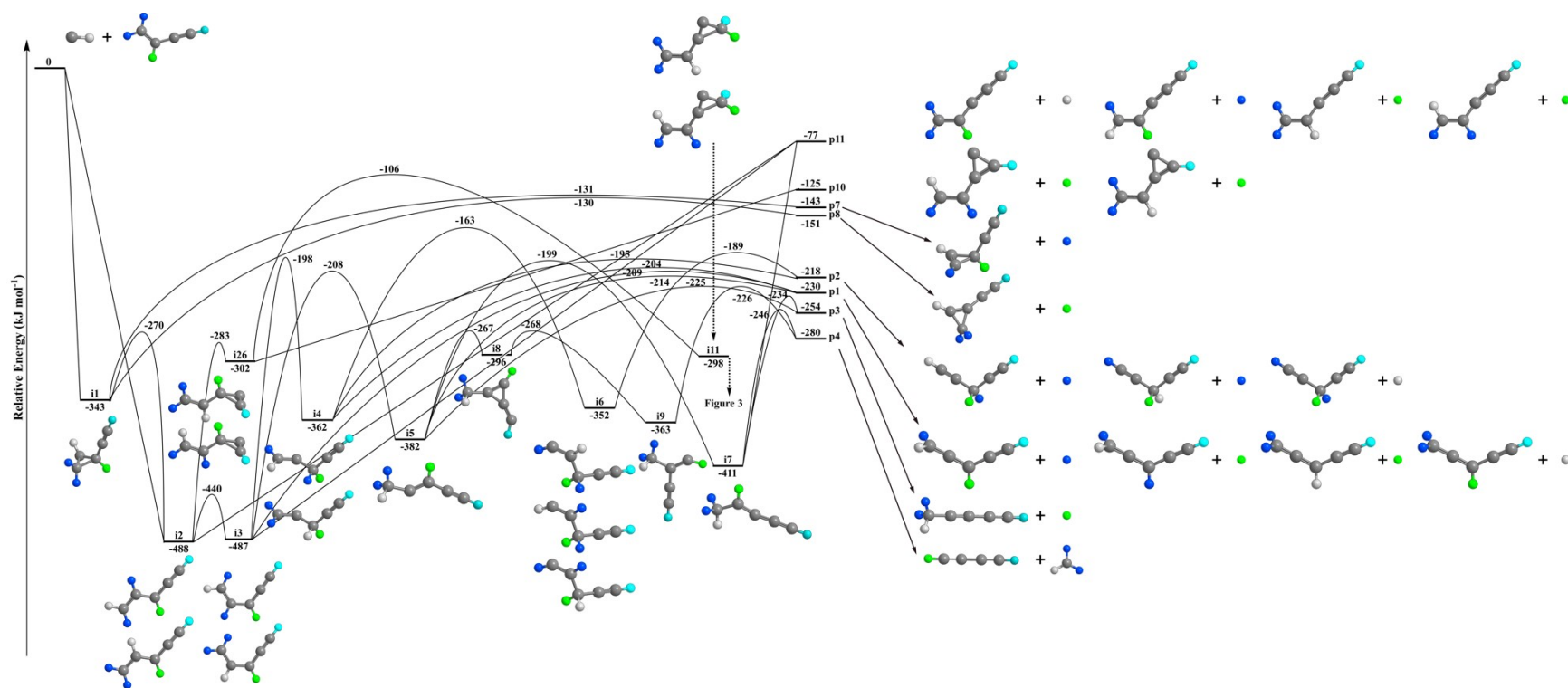


Figure S4. Portion of C_5H_5 potential energy surface (PES) leading to **p1-p4**, **p7**, **p8**, **p10**, and **p11**. H atoms from methylidyne radical, CH moiety, CH_2 moiety, and terminal CH moiety of vinylacetylene reactant are highlighted in grey, green, blue, and cyan, respectively.

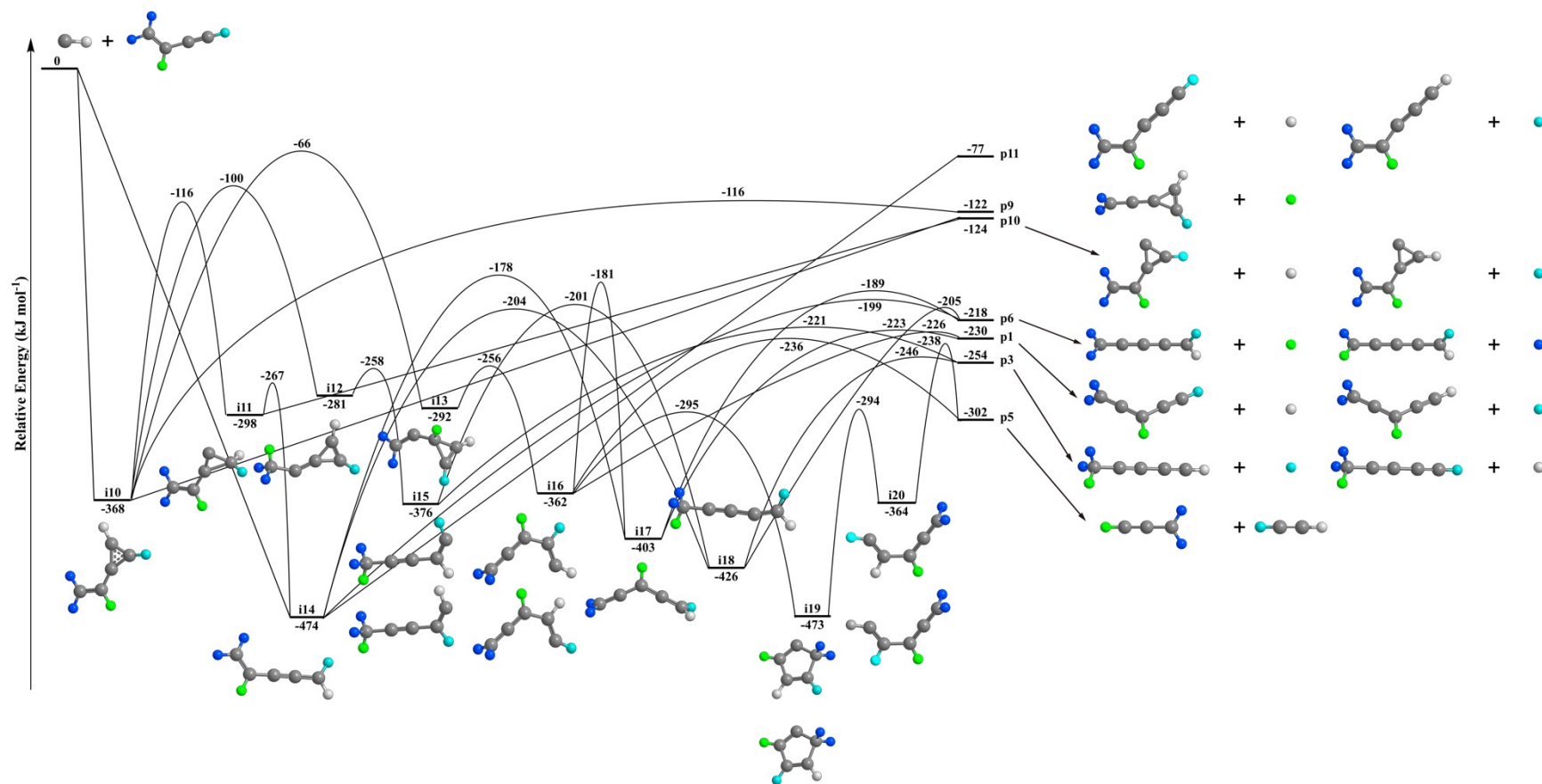


Figure S5. Portion of C₅H₅ potential energy surface (PES) leading to **p1**, **p3**, **p5**, **p6**, and **p9-p11**. H atoms from methylidyne radical, CH moiety, CH₂ moiety, and terminal CH moiety of vinylacetylene reactant are highlighted in grey, green, blue, and cyan, respectively.

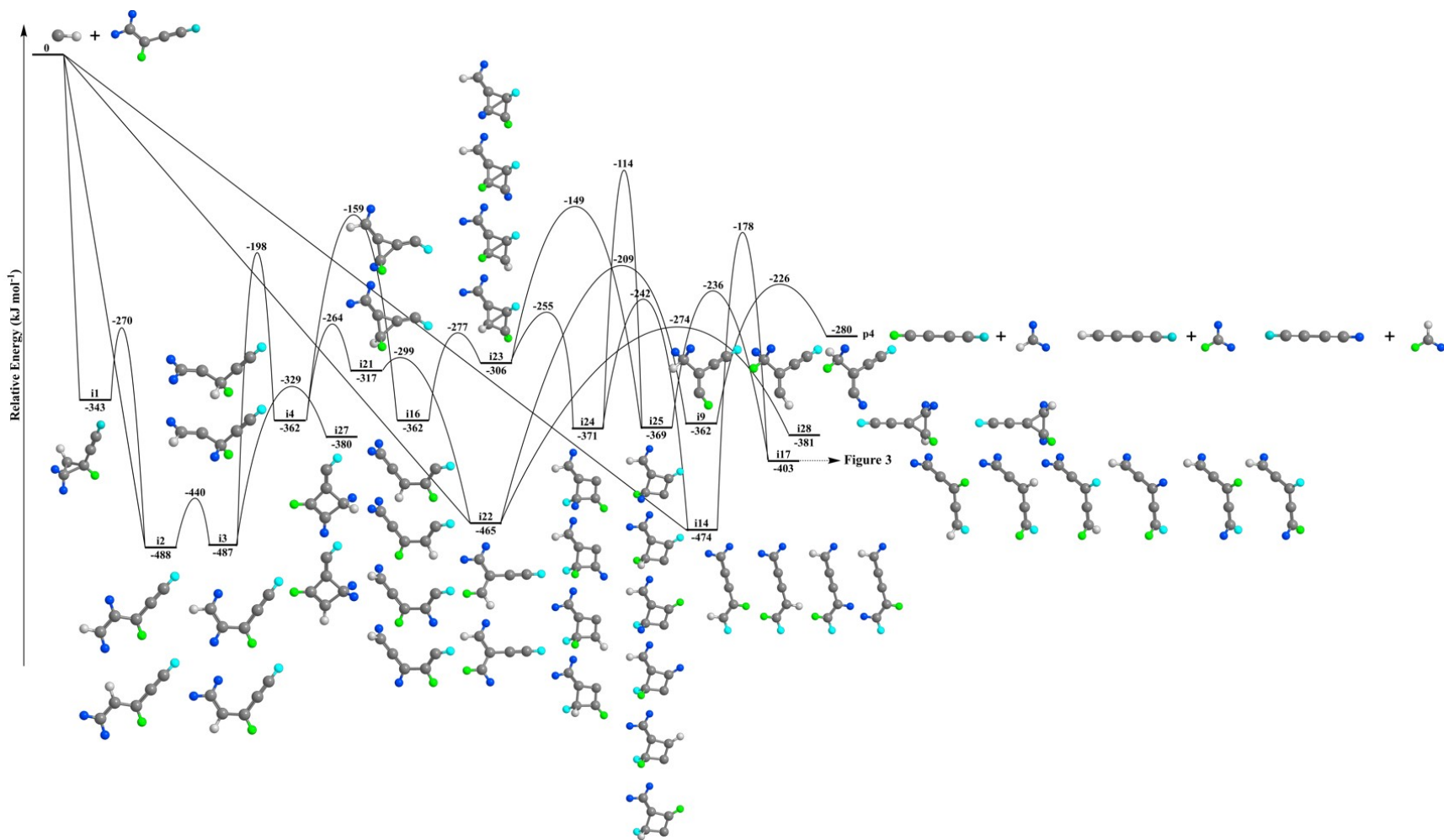


Figure S6. Portion of C_5H_5 potential energy surface (PES) leading to **p4**. H atoms from methylidyne radical, CH moiety, CH_2 moiety, and terminal CH moiety of vinylacetylene reactant are highlighted in grey, green, blue, and cyan, respectively.

Table S1. For each candidate basis set (BSX), after optimizing each reactant, product, intermediate, and transition state with B3LYP/BSX, the average time per energy gradient, *t*, and minimal root mean square difference between the calculated and benchmark energy, RMSD, is summarized below. Altogether, this comes down to 79 optimized geometries per BSX.

Basis Set	t (s)	RMSD (kJ mol⁻¹)
6-311G**¹	36.1	22.3
6-311G*¹	26.6	23.3
6-31G*²	11.6	34.0
aug-cc-pVDZ³	85.5	22.0
cc-pVDZ⁴	36.8	25.7
def2-SVP⁵	20.0	38.8
def2-SVPD⁶	49.5	36.3
aug-pc-1⁷	72.6	21.2
pc-1⁸	15.6	24.6
Sapporo-DZP-2012⁹	37.0	27.6

Table S2. Optimized Cartesian coordinates (in Å) and vibrational frequencies (in cm^{-1}) for all intermediates, transition states, reactants and products involved in the reaction of the methylidyne radical (CH) with vinylacetylene (C_4H_4).

Reactants

C_4H_4

T1 diagnostic: 0.01287890

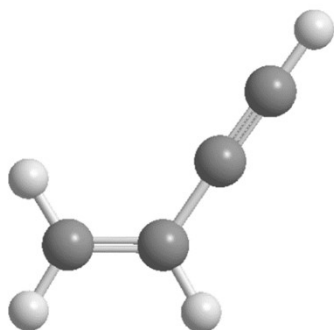
Geometry

C	-1.653366	0.376552	0.000029
C	-0.639154	-0.492868	0.000038
C	1.904944	0.173030	-0.000046
C	0.732151	-0.115565	0.000130
H	-2.675676	0.030528	-0.000564
H	-1.480234	1.442355	0.000126
H	-0.843266	-1.556279	-0.000113
H	2.931724	0.436500	-0.000353

Frequencies

221.0783	315.4624	552.7044
633.1469	663.3548	704.1720
894.6699	962.6337	1017.0962
1116.9038	1329.0382	1455.2260
1667.0524	2172.0727	3170.0959
3178.0262	3267.0649	3486.6060

Picture



CH

T1 diagnostic: 0.00907168

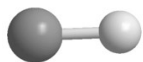
Geometry

C	0.000000	0.000000	0.159796
H	0.000000	0.000000	-0.958776

Frequencies

2874.2922

Picture



Intermediates

i10

T1 diagnostic: 0.01880906

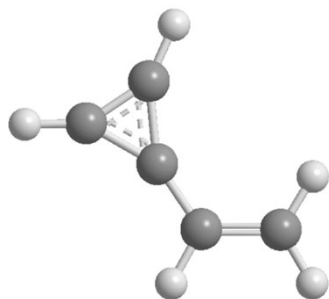
Geometries

C	2.062004	0.336706	0.000604
C	0.996262	-0.558050	-0.000230
C	-1.353892	0.807367	0.000154
C	-0.317932	-0.196148	-0.001921
C	-1.720806	-0.461897	0.000989
H	3.079911	-0.016279	0.000975
H	1.895038	1.403231	0.000818
H	1.206451	-1.620178	-0.000271
H	-1.649533	1.839321	-0.000723
H	-2.525679	-1.173958	0.001626

Frequencies

201.0853	219.0368	329.5754
513.2457	513.7433	630.9506
666.4958	770.5616	858.9631
889.7300	913.6495	978.6218
1067.5311	1107.2495	1202.5576
1392.0585	1513.3431	1546.8669
1746.2568	3170.7956	3175.0781
3265.6183	3274.2721	3310.8059

Picture



il

T1 diagnostic: 0.01398030

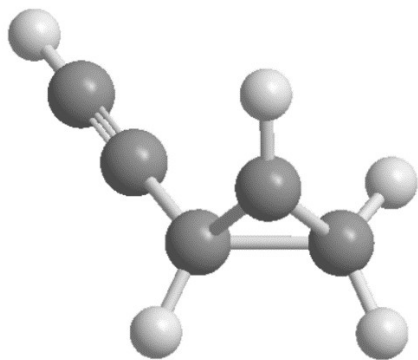
Geometries

C	1.410336	-0.608310	-0.315073
C	0.304112	-0.023847	0.592990
C	-2.212064	-0.033271	-0.212518
C	-1.065706	-0.031641	0.164548
C	1.288391	0.829550	-0.104048
H	2.181712	-1.156810	0.209522
H	1.124513	-1.027814	-1.270904
H	0.458435	-0.199432	1.650599
H	-3.221021	-0.034187	-0.536731
H	1.105950	1.623358	-0.807877

Frequencies

193.9006	208.1536	482.2092
497.4170	617.6730	664.1191
668.5362	790.3703	852.5941
872.5007	957.4549	1046.5876
1084.2441	1088.3635	1130.7767
1247.5616	1367.0306	1475.7203
2179.6452	3125.0301	3147.3425
3207.4990	3247.1506	3489.3898

Picture



i2

T1 diagnostic: 0.01812062

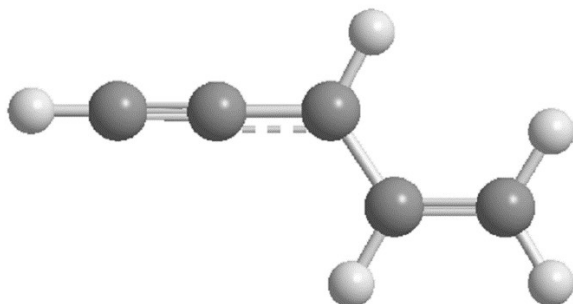
Geometries

C	1.041444	-0.398010	-0.001237
C	-0.025894	0.515580	-0.001331
C	-2.535065	-0.195454	0.001292
C	-1.366624	0.129872	-0.000974
C	2.351548	-0.032592	0.001302
H	2.640294	1.008941	0.003865
H	0.789779	-1.451028	-0.003063
H	0.194371	1.575611	-0.000836
H	-3.555887	-0.480699	0.003702
H	3.138983	-0.769198	0.002023

Frequencies

154.3067	169.1536	395.7109
428.7151	554.4461	569.2422
596.4388	661.2892	773.3620
878.8890	930.7404	1025.1386
1095.2351	1189.4992	1304.5843
1341.1267	1470.6929	1552.5700
2127.0192	3167.1838	3174.8645
3184.9369	3267.8088	3486.4777

Picture



i4

T1 diagnostic: 0.01486247

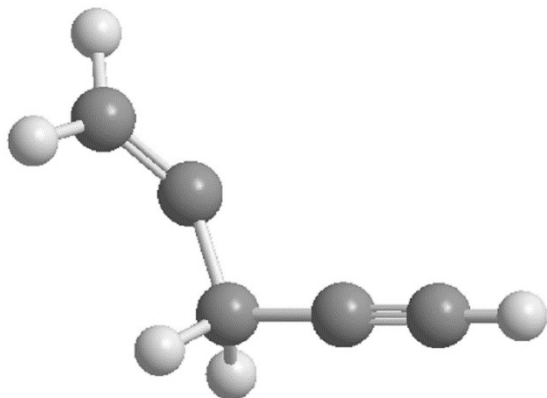
Geometries

C	-2.355916	-0.511878	0.040213
C	-1.309334	0.082814	0.027205
C	-0.039591	0.808362	0.012231
H	-0.124953	1.665671	-0.659303
C	1.108422	-0.030333	-0.394444
C	2.230999	-0.447341	0.126473
H	2.508527	-0.184667	1.147023
H	2.926783	-1.068090	-0.421869
H	-3.275324	-1.038889	0.051628
H	0.157485	1.216222	1.012459

Frequencies

90.3222	198.7730	319.2872
327.3683	438.5808	584.0483
656.2593	667.7956	867.2081
906.5111	920.0349	983.1089
1063.0492	1232.0665	1321.7958
1426.7087	1453.4784	1758.3455
2195.1683	2987.0606	3062.6438
3072.4768	3195.7392	3491.5062

Picture



i21

T1 diagnostic: 0.01797891

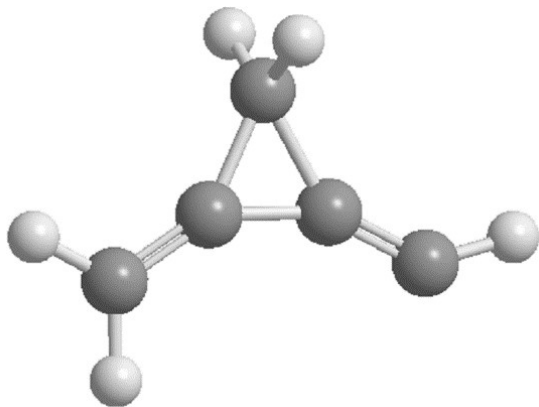
Geometries

C	1.860919	-0.788526	0.000102
H	2.921414	-0.615640	0.000759
C	0.763146	-0.118639	-0.000464
C	-0.654355	0.001361	-0.000658
C	-1.832491	-0.596388	0.000151
H	-2.746907	-0.020904	0.000902
H	-1.908132	-1.673755	-0.000199
C	0.097942	1.272110	0.000365
H	0.160996	1.844759	0.917425
H	0.161666	1.846031	-0.915853

Frequencies

233.0233	246.5765	343.9044
417.6255	630.2799	646.6875
737.1481	774.8153	883.9334
930.6503	945.1051	947.1408
1030.7666	1035.5844	1141.1538
1442.2575	1470.7533	1709.5588
1934.5083	3116.4464	3162.9044
3204.2654	3252.4972	3286.3522

Picture



i22

T1 diagnostic: 0.01209839

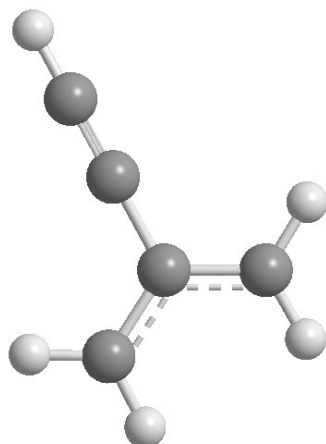
Geometries

C	-2.173060	-0.000065	-0.000552
C	-0.967888	-0.000668	0.000535
C	0.470554	-0.000012	0.000162
C	1.135551	1.216482	0.000004
H	0.595325	2.148380	0.000151
C	1.136614	-1.215932	-0.000007
H	0.597195	-2.148297	0.000125
H	2.215545	-1.242070	-0.000222
H	-3.233150	-0.000407	-0.000689
H	2.214458	1.243568	-0.000214

Frequencies

189.3743	265.6040	404.8724
536.5225	557.7664	564.6442
633.4224	658.8235	672.5129
790.3074	802.8796	818.9037
988.2965	1054.4041	1276.1834
1385.9203	1489.1667	1539.5144
2210.0346	3175.9128	3182.6758
3286.4509	3287.8588	3488.4291

Picture



i6

T1 diagnostic: 0.01472486

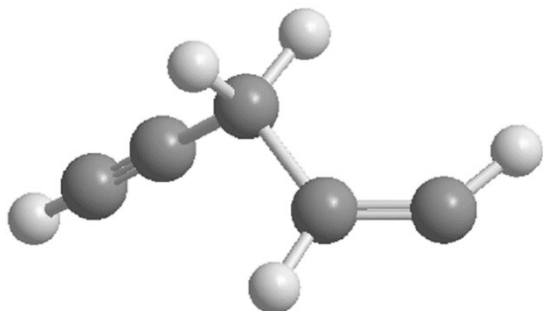
Geometries

C	-2.316815	-0.415331	-0.126125
C	-1.246005	0.132285	-0.054571
C	0.062794	0.770375	0.046043
H	0.316231	1.250734	-0.898377
C	1.151030	-0.223870	0.429430
C	2.228501	-0.438903	-0.273184
H	2.668135	-0.092664	-1.192994
H	-3.260209	-0.893405	-0.194897
H	0.019670	1.555673	0.804102
H	0.979142	-0.767669	1.352608

Frequencies

90.7223	189.0884	332.3631
372.5397	488.5946	651.9195
663.4632	686.2867	825.9810
856.0706	948.4613	974.1242
1037.5665	1215.4601	1281.7145
1324.9854	1476.9266	1691.2622
2187.7369	3049.0484	3098.9113
3146.1141	3263.7152	3490.2772

Picture



i3

T1 diagnostic: 0.01782912

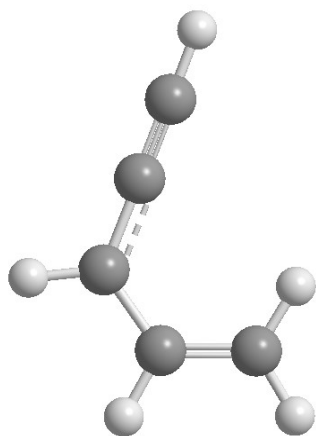
Geometries

C	1.309004	-0.404836	-0.000060
C	0.014583	-0.953355	0.000125
C	-1.155316	-0.185304	0.000009
C	1.600578	0.925386	0.000030
C	-2.169963	0.476922	-0.000038
H	2.127466	-1.113112	-0.000197
H	-0.097829	-2.028106	-0.000148
H	2.622361	1.269916	-0.000094
H	0.815347	1.666846	0.000132
H	-3.060656	1.051584	-0.000092

Frequencies

157.4819	228.7453	382.3362
443.0170	567.2678	589.2083
650.6183	662.7101	736.4461
881.9146	948.6996	1012.4735
1043.9286	1152.7749	1256.3111
1418.7016	1443.8219	1557.6593
2144.2080	3173.1862	3180.2809
3202.5596	3273.0008	3486.8484

Picture



i7

T1 diagnostic: 0.01937847

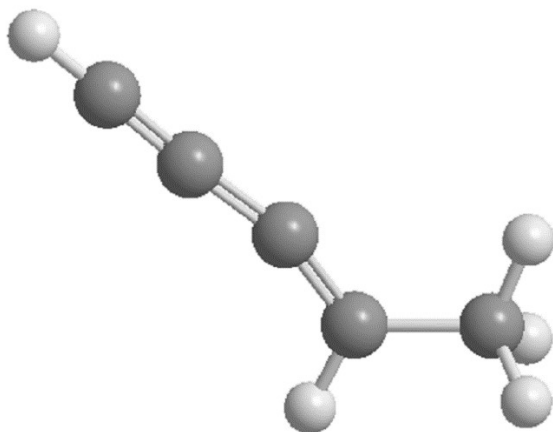
Geometries

C	2.686937	-0.153442	0.000001
C	1.473038	-0.004317	0.000002
C	0.144357	0.072001	-0.000003
C	-1.084627	0.505840	0.000001
C	-2.315455	-0.356775	0.000000
H	-2.057095	-1.411884	0.000019
H	-2.927248	-0.144638	0.877792
H	-2.927231	-0.144664	-0.877810
H	3.741098	-0.261820	-0.000006
H	-1.255025	1.583166	0.000001

Frequencies

60.5662	149.5644	218.7460
387.4329	431.8920	448.7173
509.9224	649.3925	748.3296
792.9628	1037.6026	1066.7135
1104.2129	1324.1908	1412.8147
1495.4511	1500.1806	1858.4444
2130.7973	3046.4590	3069.4163
3101.1747	3150.9075	3487.0435

Picture



i15

T1 diagnostic: 0.01393031

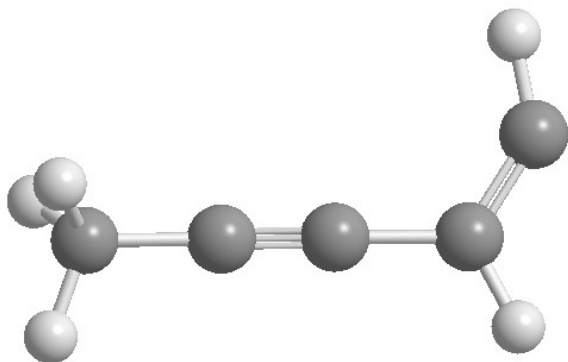
Geometries

C	0.000000	-2.470525	0.159789	-0.000050
H	0.000000	-2.766312	0.790840	-0.837576
H	0.000000	-3.009495	-0.783218	-0.081483
C	0.000000	-1.031695	-0.062381	-0.000054
C	0.000000	0.163467	-0.241726	0.000139
C	0.000000	1.573721	-0.471170	-0.000037
H	0.000000	1.904560	-1.505327	-0.000036
C	0.000000	2.464882	0.494664	-0.000033
H	0.000000	2.460060	1.571436	0.000081
H	0.000000	-2.787912	0.651208	0.919227

Frequencies

22.7792	137.3359	194.0087
311.8484	390.0079	496.2517
709.1058	720.2759	893.1096
929.4517	1060.3831	1063.0308
1184.0689	1279.9880	1425.6824
1492.9211	1493.2019	1686.0654
2325.9972	3051.6946	3115.1858
3119.2306	3133.2837	3264.3446

Picture



i18

T1 diagnostic: 0.01815963

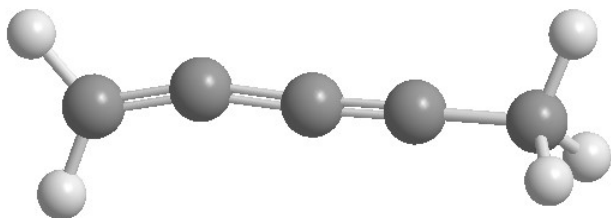
Geometries

C	2.597689	-0.037579	-0.000050
H	2.967680	-0.538924	0.894476
H	3.027604	0.964877	-0.026021
C	1.148068	0.010254	0.000186
C	-0.076534	0.040959	-0.000192
C	-1.401586	0.162762	-0.000073
C	-2.680561	-0.084728	0.000044
H	-3.418167	0.709973	0.000180
H	2.966520	-0.584223	-0.868175
H	-3.066085	-1.101705	0.000050

Frequencies

16.8846	78.3748	151.9823
178.9219	346.2929	396.1145
564.3272	679.4292	902.1574
985.6691	1044.3594	1052.8283
1144.1149	1421.3077	1454.9988
1481.6379	1487.2493	1891.5507
2216.4571	3039.3123	3085.5509
3098.9292	3110.6229	3162.3063

Picture



i8

T1 diagnostic: 0.01726084

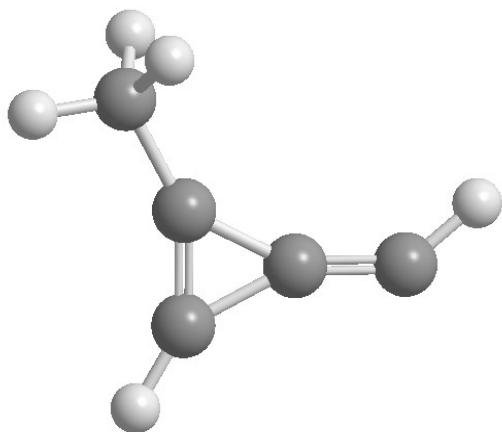
Geometries

C	2.015311	-0.633227	0.000790
C	0.905680	0.031571	-0.000532
C	-0.558365	0.157643	-0.000414
C	0.143638	1.265853	0.000028
C	-1.844125	-0.558815	0.000162
H	2.363208	-1.647022	-0.001910
H	0.168300	2.341112	0.000503
H	-1.910020	-1.203270	-0.876308
H	-1.910056	-1.201292	0.878102
H	-2.684260	0.132323	-0.000595

Frequencies

139.6456	205.7844	258.8926
434.9807	445.1756	513.2787
656.0053	757.7890	783.7415
884.1153	980.9936	1053.9972
1055.9956	1137.9951	1413.0689
1488.0153	1490.4315	1660.4093
1860.1198	3053.4198	3116.2460
3138.9860	3265.9098	3307.8085

Picture



i9

T1 diagnostic: 0.01412078

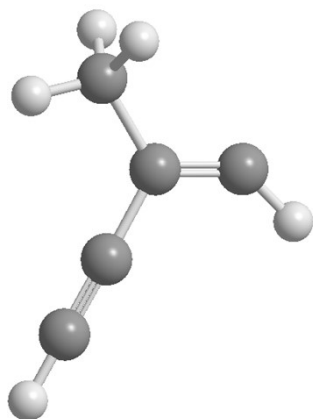
Geometries

C	2.143105	-0.219212	-0.000001
C	0.954686	-0.020812	0.000001
C	-0.463533	0.190183	-0.000004
C	-0.938721	1.423197	-0.000001
H	-0.539844	2.426712	0.000007
C	-1.352965	-1.037835	0.000001
H	-2.404243	-0.749174	-0.000048
H	-1.151629	-1.651559	-0.882383
H	-1.151694	-1.651495	0.882440
H	3.191978	-0.387612	0.000002

Frequencies

171.6784	178.1686	270.2974
368.4727	531.5220	538.6140
643.3850	678.0818	691.6875
770.8310	852.2368	1028.3141
1052.8231	1194.0462	1402.4788
1480.5736	1482.2633	1641.3951
2190.8530	3030.7571	3087.9679
3123.9399	3240.7376	3476.1282

Picture



i24

T1 diagnostic: 0.01556265

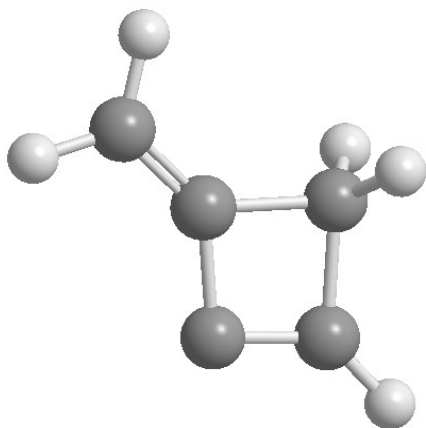
Geometries

C	-1.884228	-0.045426	-0.000051
H	-2.414243	0.895562	0.000074
C	-0.561107	-0.083409	-0.000101
C	0.570546	0.967510	0.000195
H	0.599503	1.581689	0.899593
C	1.539295	-0.226098	-0.000096
C	0.513648	-1.080263	-0.000076
H	-2.466277	-0.955118	-0.000145
H	0.599586	1.582328	-0.898748
H	2.612511	-0.298345	-0.000002

Frequencies

217.4237	347.5997	526.1883
718.2350	723.6699	789.0217
846.2966	897.1456	911.6564
961.6099	986.0730	1096.3229
1109.2509	1189.8055	1233.3566
1448.5542	1471.7341	1615.2772
1764.7891	3057.4322	3123.4062
3168.3076	3255.8330	3270.0499

Picture



i14

T1 diagnostic: 0.02096690

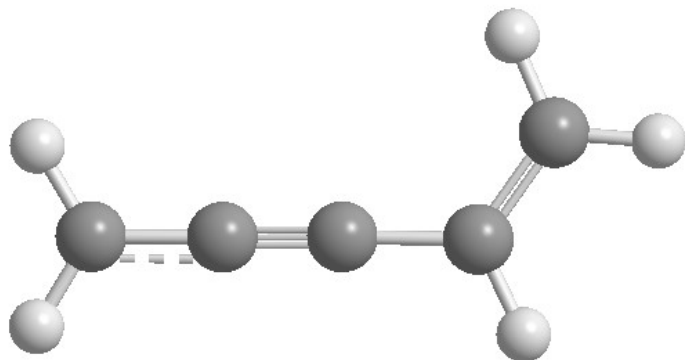
Geometries

C	-2.565278	0.177938	-0.000114
H	-2.959343	1.182951	0.000036
H	-3.264706	-0.644358	-0.000283
C	-1.230748	-0.045076	-0.000056
C	-0.013963	-0.238563	0.000004
C	1.362824	-0.487708	0.000114
H	1.666950	-1.527923	0.000328
C	2.307045	0.470212	0.000035
H	3.354539	0.211491	0.000163
H	2.043281	1.517021	-0.000140

Frequencies

141.9540	178.9855	285.4053
328.9317	447.5005	534.8473
670.4722	740.4732	761.2372
939.4596	1010.5888	1041.3602
1074.9957	1305.0046	1319.2864
1452.2257	1499.7240	1612.6632
2035.6161	3162.5869	3165.4798
3175.6041	3256.6314	3271.3957

Picture



i25

T1 diagnostic: 0.01510417

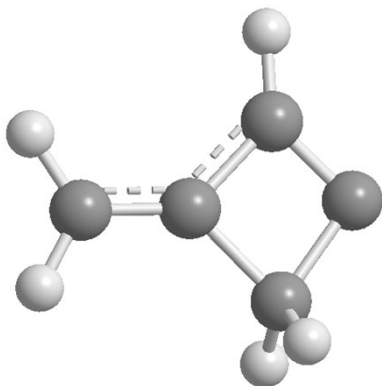
Geometries

C	-1.785190	0.005980	-0.000160
H	-2.364146	0.917815	-0.000093
C	-0.456843	0.036638	-0.000014
C	0.613430	-1.072679	0.000278
H	0.645649	-1.689991	-0.894173
C	1.523036	0.144762	-0.000679
C	0.578449	1.090180	0.000385
H	0.551856	2.165954	0.000408
H	-2.316891	-0.933757	-0.000199
H	0.646242	-1.689306	0.895192

Frequencies

201.7711	348.3160	462.0991
692.5683	724.4030	833.8807
848.0185	889.2603	918.5022
1007.9113	1008.5534	1068.6897
1138.8390	1160.3458	1223.2476
1452.2205	1482.3571	1606.8241
1738.3252	3091.9829	3147.3859
3165.8020	3255.6969	3264.2808

Picture



i17

T1 diagnostic: 0.01312925

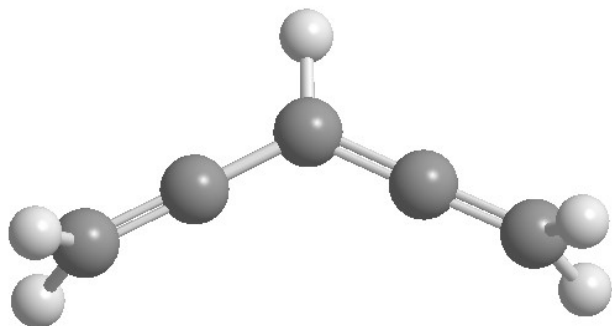
Geometries

C	-2.365318	-0.439535	-0.000006
H	-2.877101	-0.696978	0.922691
C	-1.204111	0.138946	0.000161
C	0.000000	0.758593	-0.000215
C	1.204093	0.138906	0.000405
C	2.365326	-0.439521	-0.000074
H	2.877328	-0.697039	0.922480
H	2.876220	-0.697635	-0.923089
H	-2.876407	-0.697738	-0.922885
H	0.000015	1.845053	-0.000823

Frequencies

110.4076	133.2468	155.3784
351.5282	452.1887	506.8807
613.7116	888.3018	901.5547
903.2749	955.8266	983.0701
987.0645	1034.7715	1334.4953
1451.8838	1466.1106	1862.2402
1939.2981	3088.8227	3092.9366
3130.6487	3152.2295	3152.2879

Picture



i16

T1 diagnostic: 0.01483925

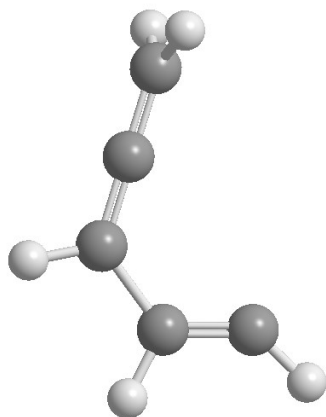
Geometries

C	-2.151457	-0.464890	0.000116
H	-2.628112	-0.759543	0.925929
C	-1.042663	0.215584	-0.000038
C	0.074510	0.896763	-0.000257
C	1.429106	0.314440	0.000234
C	1.748860	-0.955388	-0.000162
H	2.651231	-1.540061	0.000099
H	-2.627806	-0.760483	-0.925556
H	0.013453	1.978082	-0.000836
H	2.241099	1.042949	0.001006

Frequencies

38.8138	148.4728	326.4063
386.7109	516.8107	633.9158
688.9846	841.7768	869.2278
879.7008	911.6468	930.4014
1016.7895	1155.9420	1283.4100
1380.1352	1486.0567	1722.3633
2054.4825	3067.2759	3141.7878
3168.8011	3218.0873	3279.4311

Picture



i23

T1 diagnostic: 0.01512980

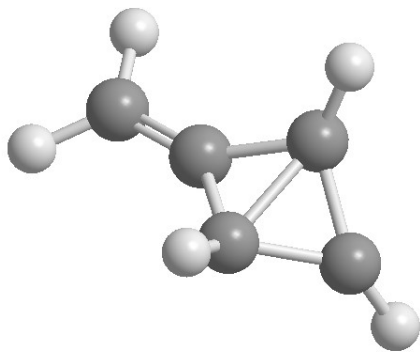
Geometries

C	-1.911459	0.000001	0.171913
H	-2.457279	-0.927495	0.243414
C	-0.596609	0.000001	0.010946
C	0.579412	-0.811731	-0.265587
H	0.725722	-1.479390	-1.100745
C	1.588947	0.000012	0.402430
H	2.024960	0.000005	1.390035
C	0.579402	0.811709	-0.265605
H	0.725713	1.479433	-1.100710
H	-2.457270	0.927501	0.243426

Frequencies

219.3869	347.6509	528.0416
671.1184	708.0398	743.8857
781.0352	834.8691	850.3024
889.6473	1010.3886	1019.6286
1040.9763	1115.7374	1165.9742
1179.8936	1321.6088	1466.6571
1802.5892	3177.3947	3192.7253
3211.8768	3217.4926	3268.2096

Picture



i19

T1 diagnostic: 0.01408456

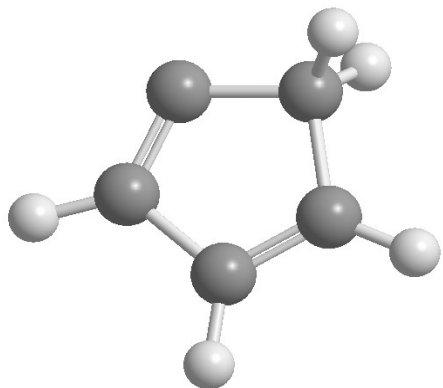
Geometries

C	-0.609013	0.976400	0.000272
C	0.732834	0.916699	-0.000352
C	1.179471	-0.497632	0.000435
C	-1.177466	-0.424298	-0.000111
C	0.073044	-1.231460	-0.000412
H	-1.216699	1.866705	0.000044
H	1.407774	1.759121	-0.000745
H	2.204970	-0.827232	0.000454
H	-1.795333	-0.618822	-0.878637
H	-1.793927	-0.618026	0.879904

Frequencies

310.3126	458.5937	681.8882
789.1292	805.7976	837.3961
913.8240	940.3577	955.3404
967.0270	1003.6152	1119.5848
1125.0960	1222.4795	1255.1360
1350.5681	1423.4338	1628.9937
1659.5505	3064.9699	3099.7447
3214.5511	3242.0781	3249.2337

Picture



i11

T1 diagnostic: 0.01558170

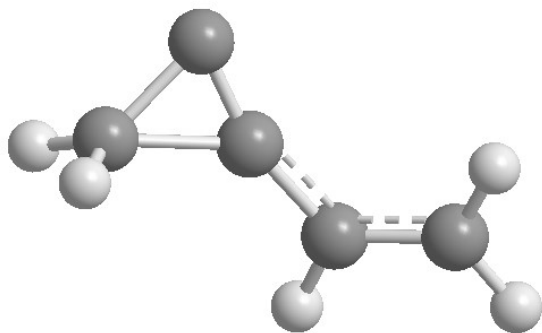
Geometries

C	2.106215	0.190351	0.169765
C	0.999213	-0.472431	-0.180157
C	-1.293354	0.927015	-0.219348
C	-0.308920	0.104832	-0.144369
C	-1.812910	-0.386317	0.223708
H	3.075549	-0.280005	0.103957
H	2.061826	1.211037	0.519594
H	1.064693	-1.499581	-0.515981
H	-2.333421	-1.029878	-0.477497
H	-2.010112	-0.582271	1.272338

Frequencies

73.0422	199.6527	282.9094
435.7246	639.9907	700.0958
750.9729	900.6140	960.3645
996.4950	1017.2421	1054.8013
1075.8098	1114.1267	1327.0105
1450.2924	1514.9786	1654.1810
1874.0093	3088.4375	3169.3887
3172.7755	3179.2073	3265.9112

Picture



i12

T1 diagnostic: 0.01642391

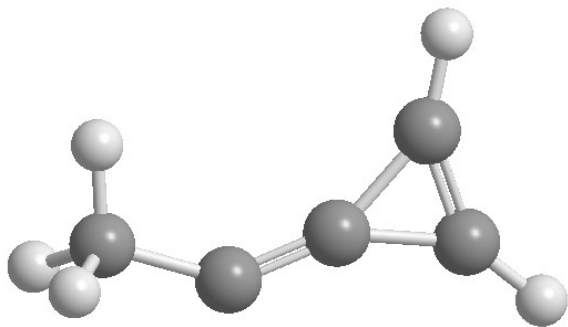
Geometries

C	-2.220220	0.140812	-0.000011
C	-0.884711	-0.472306	-0.000032
C	1.508077	0.770391	0.000183
C	0.371553	-0.170354	0.000051
C	1.783164	-0.509916	-0.000113
H	-2.799165	-0.142925	-0.879732
H	-2.136584	1.233927	-0.000459
H	1.860405	1.785857	-0.000610
H	2.526984	-1.286453	0.000123
H	-2.798815	-0.142172	0.880208

Frequencies

129.5649	161.7356	192.8901
383.7272	468.4123	623.2122
709.1342	775.3870	872.6424
951.8836	1041.4159	1048.0259
1061.6170	1177.4306	1407.9964
1472.8307	1499.7177	1617.7626
1872.7404	2996.0338	3069.6042
3090.9185	3250.0157	3294.1066

Picture



i13

T1 diagnostic: 0.01507129

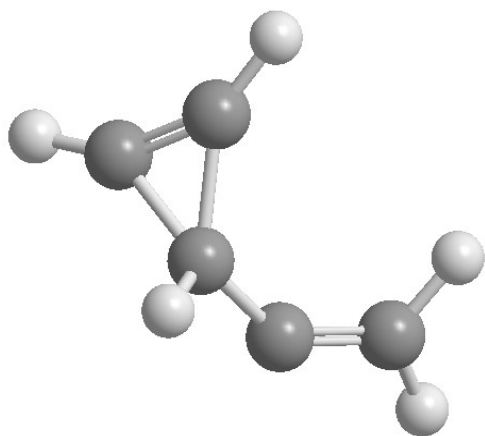
Geometries

C	2.005346	0.269606	-0.194308
C	0.995164	-0.512606	0.086794
C	-1.248156	0.772772	0.160261
C	-0.392810	-0.448171	0.498321
C	-1.494197	-0.289513	-0.526764
H	2.955846	-0.114012	-0.541772
H	1.930321	1.351667	-0.085615
H	-1.419888	1.809380	0.377703
H	-2.036457	-0.798896	-1.300313
H	-0.621908	-1.000660	1.404178

Frequencies

86.2085	194.7876	333.3899
494.5931	575.3843	645.1030
756.5109	844.8021	895.1246
900.7020	948.6193	1005.0511
1026.3692	1057.9347	1124.2240
1367.1673	1430.6961	1702.3674
1756.9999	3064.7666	3113.1674
3183.6056	3271.4564	3318.9050

Picture



i27

T1 diagnostic: 0.01590340

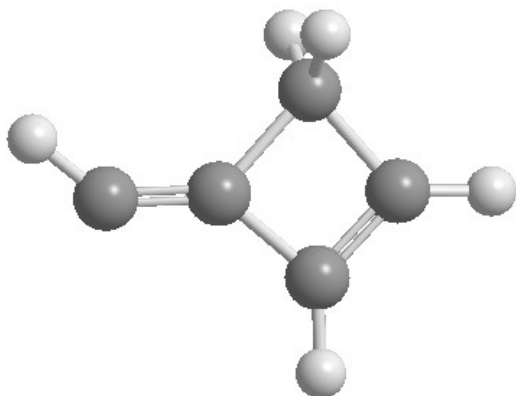
Geometry

H	0.000000	-2.772221	0.482730	0.000008
H	0.000000	0.577167	-2.111420	-0.000031
H	0.000000	0.375549	1.695812	0.892322
H	0.000000	0.375570	1.695780	-0.892372
C	0.000000	-0.624112	-0.104400	0.000002
C	0.000000	-1.922111	-0.174188	0.000010
C	0.000000	0.522655	-1.033634	-0.000015
C	0.000000	0.408996	1.072647	-0.000014
H	0.000000	2.514785	-0.037208	0.000039
C	0.000000	1.436097	-0.048040	0.000022

Frequencies

223.9067	336.7597	490.6766
657.1877	717.4695	770.7059
784.2269	875.2396	952.4197
969.8033	998.2265	1044.3756
1098.9767	1117.9547	1208.3090
1314.6679	1477.1348	1628.0753
1756.3134	3072.9102	3126.4600
3215.5698	3245.3620	3289.8652

Picture



i29

T1 diagnostic: 0.02039656

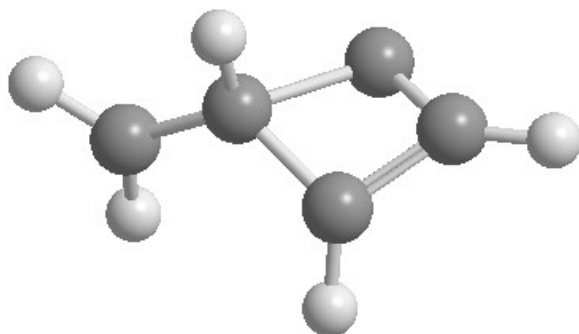
Geometry

H	0.000000	-2.693444	0.049576	-0.039402
H	0.000000	-0.346037	1.676888	-0.557880
H	0.000000	2.742113	-0.401181	0.317029
H	0.000000	1.998733	0.466841	-1.141128
C	0.000000	-1.626274	-0.040001	0.033388
C	0.000000	-0.661788	-0.903225	-0.388734
C	0.000000	-0.516353	0.834418	0.109206
C	0.000000	1.875710	0.013873	-0.169811
H	0.000000	0.530847	-0.524890	1.415670
C	0.000000	0.556670	-0.116271	0.416903

Frequencies

188.0048	280.7075	327.5705
467.5743	586.5467	626.9367
631.4626	794.0558	884.7181
958.7631	1040.4095	1069.3278
1144.4338	1176.6370	1250.4205
1309.6103	1399.8898	1473.8718
1494.7964	3104.1785	3180.6861
3196.9078	3290.2966	3296.6291

Picture



i33

T1 diagnostic: 0.01952476

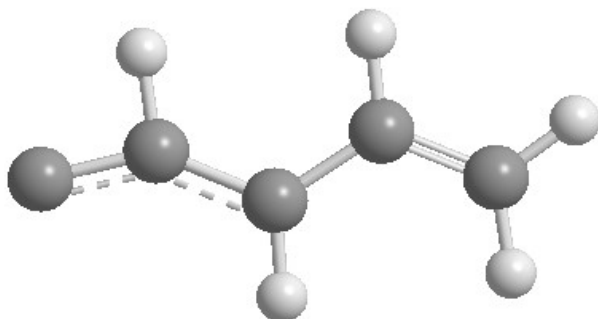
Geometry

H	-1.574279	1.272875	-0.000049
H	-0.030818	-1.465777	-0.000027
H	2.483877	-1.200045	-0.000001
H	3.192255	0.512339	0.000025
C	-1.417913	0.168280	-0.000015
C	-2.687663	-0.146980	0.000026
C	-0.110784	-0.384236	-0.000014
C	2.319160	-0.127663	0.000008
H	0.944443	1.473521	0.000013
C	1.061286	0.391780	0.000001

Frequencies

103.1060	145.9107	258.1364
304.9455	482.2741	576.3068
644.3333	768.9608	829.5313
862.4057	973.0980	995.6774
1138.4133	1211.9761	1303.8323
1335.6480	1472.9702	1538.8238
1696.0785	2939.3312	3157.5293
3165.7746	3201.9477	3258.8613

Picture



i26

T1 diagnostic: 0.01605158

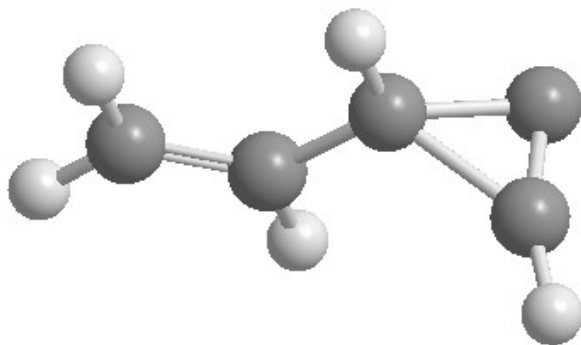
Geometry

H	2.021851	-0.958431	1.260126
H	0.136967	1.369398	0.614932
H	-2.281526	0.931936	0.694784
H	-2.970286	-0.564869	-0.136072
C	1.683656	-0.359676	0.441362
C	1.621234	0.286016	-0.656892
C	0.313047	0.445000	0.073421
C	-2.108072	0.030202	0.123256
H	-0.719133	-1.230835	-0.824527
C	-0.874510	-0.326074	-0.249353

Frequencies

143.4591	280.0759	310.0291
473.3748	584.9052	639.9430
687.0920	854.9390	905.6906
947.7796	966.6742	1044.7455
1047.1556	1181.1972	1321.8820
1348.7262	1467.3870	1673.5555
1742.8729	3124.0680	3161.4152
3177.3450	3254.8870	3357.3772

Picture



i32

T1 diagnostic: 0.01372530

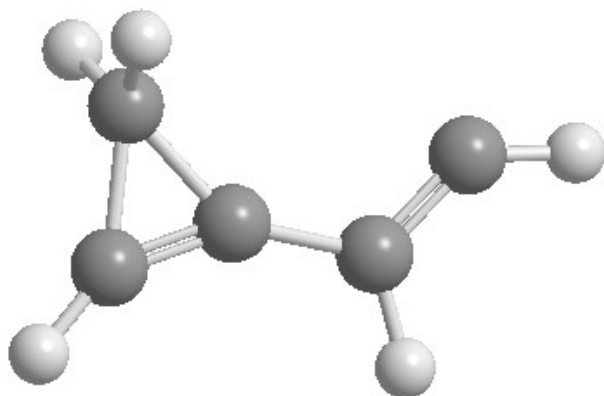
Geometry

H	1.443149	-1.529066	0.000001
H	-2.197857	-1.461769	-0.000001
H	-1.518278	1.408176	0.911454
H	-1.518278	1.408176	-0.911453
C	-0.274602	-0.220647	0.000000
C	1.141915	-0.480458	0.000001
C	-1.496723	-0.649699	-0.000001
C	-1.329188	0.847924	0.000000
H	3.141997	0.492224	-0.000001
C	2.066810	0.449924	-0.000001

Frequencies

149.2120	202.4338	308.4158
525.1605	655.9806	670.4281
757.6165	840.8842	869.7077
958.9046	1019.7798	1071.5394
1076.1912	1114.2581	1205.0829
1272.1199	1532.9189	1682.9044
1924.6329	3068.2241	3069.9964
3135.2720	3274.1201	3298.9405

Picture



i28

T1 diagnostic: 0.01769493

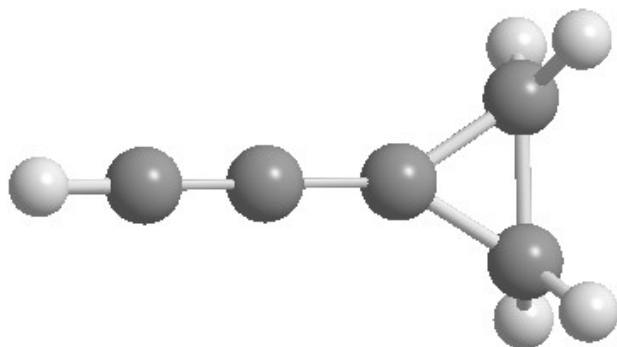
Geometry

H	-3.457096	0.000048	0.013110
H	1.694121	-1.273952	0.920965
H	1.694070	1.273976	0.920969
H	1.732146	1.272066	-0.899126
C	-1.176067	-0.000029	-0.004285
C	-2.397580	0.000004	0.004111
C	0.173776	-0.000012	-0.019797
C	1.416971	0.765555	0.005253
H	1.732183	-1.272032	-0.899130
C	1.416996	-0.765536	0.005254

Frequencies

49.2164	190.8851	383.1250
461.5615	536.7339	620.5544
644.9368	751.6876	850.3777
985.2205	1006.5026	1053.6011
1055.009	1084.9963	1164.5598
1454.9964	1466.1715	1542.1562
2038.286	3110.1162	3110.9370
3181.0838	3193.2829	3485.2632

Picture



i30

T1 diagnostic: 0.02168264

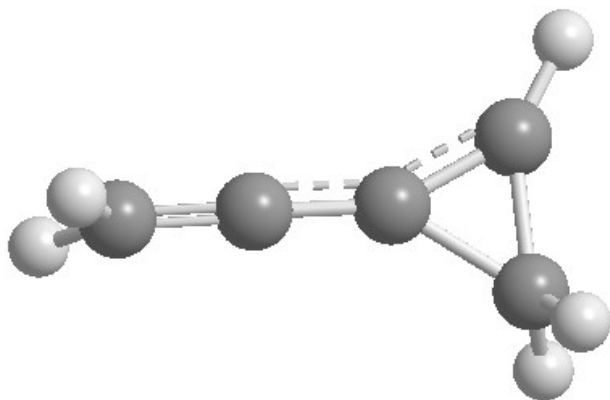
Geometry

C	-0.293911	0.103910	-0.000473
C	1.020068	0.037415	0.000197
C	-1.474535	0.766613	-0.001469
C	-1.581949	-0.707610	0.000451
C	2.319274	-0.047896	0.000135
H	-1.989273	1.706888	0.004778
H	-1.857623	-1.228641	-0.911816
H	-1.857583	-1.226809	0.913817
H	2.885437	-0.082148	0.924027
H	2.885354	-0.083883	-0.923862

Frequencies

173.6826	188.6445	220.4640
406.0061	498.7280	538.7845
663.6454	874.3734	943.1506
974.0768	999.0438	1011.3770
1034.2756	1064.9970	1110.4003
1402.9747	1491.5227	1531.7922
1940.2909	3074.7157	3114.6130
3146.5491	3183.9775	3301.9843

Picture



i31

T1 diagnostic: 0.01787859

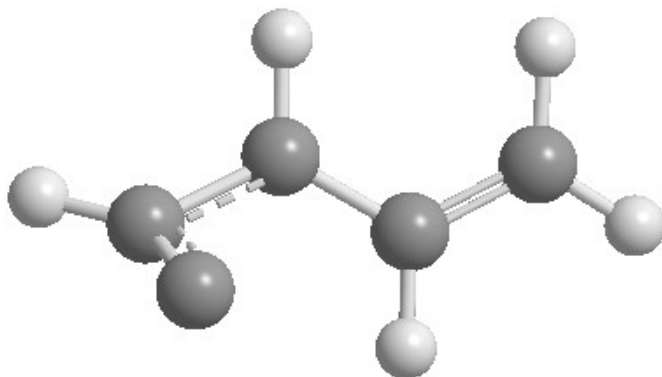
Geometry

C	1.630184	0.304383	0.222682
C	1.714873	-0.842164	-0.405268
C	0.217867	0.595993	-0.033119
C	-2.131525	-0.032425	-0.103395
C	-0.836595	-0.273895	0.262531
H	2.357382	1.009466	0.595259
H	-0.005611	1.508105	-0.577103
H	-2.395412	0.845100	-0.675938
H	-2.925118	-0.708805	0.170619
H	-0.600067	-1.165215	0.826576

Frequencies

152.5331	202.2818	284.3599
309.2266	522.8831	580.1511
704.8367	814.8298	877.0048
936.7041	1017.3396	1035.3048
1146.5421	1210.5333	1297.8422
1301.1542	1441.7991	1538.0056
1630.0368	3145.8426	3170.8843
3202.2841	3215.4252	3272.5307

Picture



PRODUCTS

p1

T1 diagnostic: 0.01355370

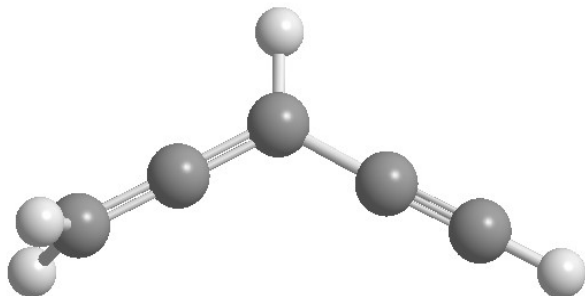
Geometries

C	2.379481	-0.465525	0.000103
C	1.301463	0.077775	0.000275
C	0.052925	0.760178	-0.000127
C	-1.109886	0.150466	-0.000070
C	-2.268191	-0.439307	0.000021
H	-2.765013	-0.696369	-0.926142
H	-2.765285	-0.695561	0.926262
H	3.320228	-0.953811	-0.000944
H	0.075322	1.844213	-0.000383

Frequencies

138.2842	296.2742	345.8787
353.5545	603.2085	613.4659
638.8172	671.4137	885.7588
888.9620	952.9534	1011.1392
1138.0006	1356.3913	1474.2810
2034.7922	2175.4317	3144.8882
3154.2597	3223.0162	3488.4259

Picture



p2

T1 diagnostic: 0.01292315

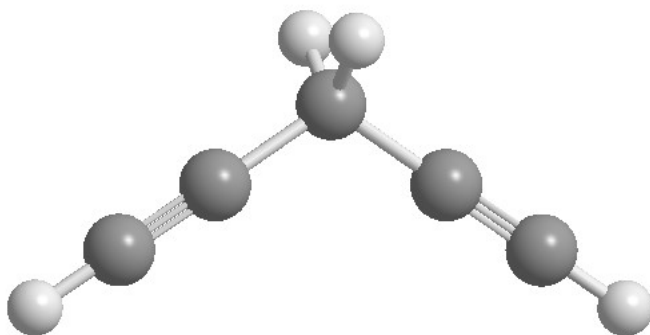
Geometries

C	-2.233165	-0.577439	-0.000072
C	-1.221477	0.074205	-0.000088
C	1.221758	0.074691	-0.000001
C	2.233002	-0.577642	-0.000023
H	3.120217	-1.157452	0.000107
C	-0.000018	0.880415	0.000044
H	-0.000110	1.534641	-0.874186
H	-3.120537	-1.157010	0.000506
H	-0.000171	1.534450	0.874417

Frequencies

135.1590	307.4838	326.6490
331.7157	563.1229	658.2849
660.2572	671.1304	673.0668
907.6602	943.0214	1002.5579
1251.5819	1346.4305	1470.5450
2196.6230	2199.1460	3049.8726
3080.3336	3490.0996	3491.0645

Picture



p3

T1 diagnostic: 0.01319528

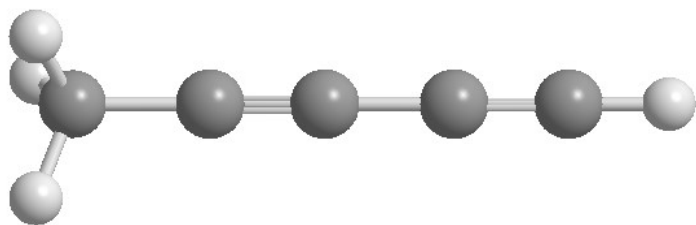
Geometries

C	-2.514000	-0.000100	0.000069
H	-2.899817	-0.988530	0.247379
C	-1.060794	0.000532	-0.000323
C	0.151289	-0.000326	0.000311
C	1.515924	0.000098	-0.000309
C	2.726678	-0.000092	0.000181
H	-2.900594	0.707891	0.732377
H	3.786744	0.000252	-0.000104
H	-2.900914	0.279711	-0.979224

Frequencies

145.6398	145.9198	337.6871
337.8996	516.2573	516.2733
636.0173	636.0220	676.8863
1057.8020	1058.1087	1179.5233
1424.1481	1489.0302	1489.1690
2126.5616	2311.4369	3052.1929
3119.3770	3119.4503	3485.0396

Picture



p4

T1 diagnostic: 0.01430064

Geometries

C	0.000000	0.000000	1.892449
H	0.000000	0.000000	2.952882
C	0.000000	0.000000	0.682678
C	0.000000	0.000000	-0.682678
C	0.000000	0.000000	-1.892449
H	0.000000	0.000000	-2.952882

Frequencies

235.0769	235.0769	514.8342
514.8342	647.0721	647.0721
652.7990	652.7990	907.6747
2068.6838	2239.9926	3481.5313
3482.3864		

Picture



p5

T1 diagnostic: 0.02241138

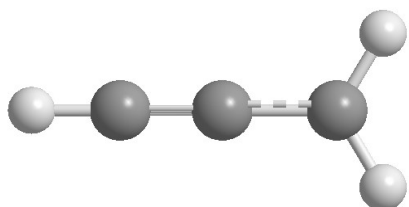
Geometries

C	1.253552	0.000020	-0.000017
H	1.803769	0.927723	-0.000024
H	1.803827	-0.927646	-0.000024
C	-0.118008	-0.000020	0.000012
C	-1.337289	-0.000069	0.000002
H	-2.397122	0.000336	0.000067

Frequencies

348.9451	405.9039	509.9718
638.5246	676.4915	1042.6059
1074.9223	1474.0782	2040.9431
3174.6147	3271.1819	3484.7045

Picture



p6

T1 diagnostic: 0.01588649

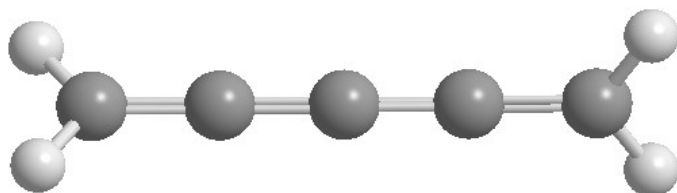
Geometries

C	-2.585155	-0.000067	0.000207
H	-3.144592	0.665645	-0.643673
C	-1.274098	-0.000027	-0.000055
C	0.000002	0.000177	-0.000457
C	1.274102	-0.000001	-0.000202
C	2.585149	-0.000037	0.000241
H	3.144249	0.644033	0.666046
H	-3.144306	-0.665748	0.644363
H	3.144642	-0.644200	-0.665144

Frequencies

149.8653	149.8761	333.7291
333.7413	528.2716	528.2774
700.5873	748.3674	854.4652
854.4693	1012.9088	1012.9184
1324.1270	1445.7756	1514.0314
1940.4868	2209.5899	3142.2861
3143.1021	3222.5105	3222.5272

Picture



p7

T1 diagnostic: 0.01200065

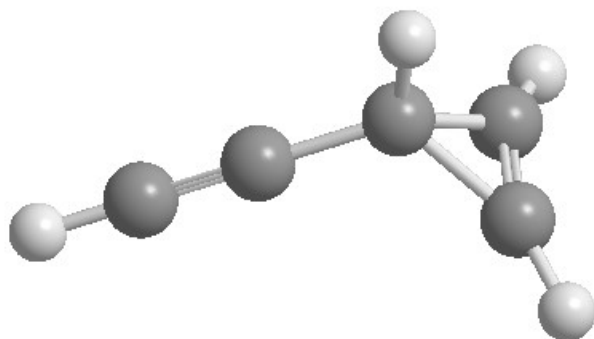
Geometries

C	1.403265	-0.644393	-0.236843
C	0.315647	0.000059	0.593127
C	-2.200711	-0.000177	-0.244099
C	-1.054614	0.000326	0.134558
C	1.403087	0.644261	-0.237208
H	1.794146	-1.584403	-0.575189
H	0.417948	0.000073	1.673407
H	-3.205701	-0.000655	-0.580274
H	1.793557	1.584527	-0.575152

Frequencies

202.8401	217.6552	526.2150
535.9857	620.0710	632.1997
666.5304	814.0772	849.7064
910.8663	966.9411	1017.8716
1057.0719	1165.2232	1376.9867
1710.9609	2174.1930	3116.5819
3277.6218	3324.6412	3489.6153

Picture



p8

T1 diagnostic: 0.01230353

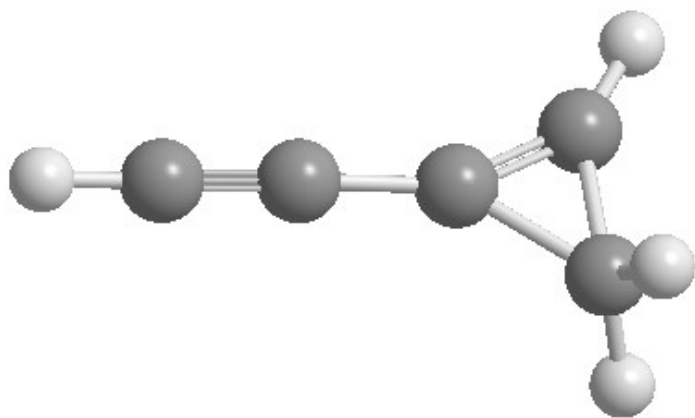
Geometries

C	-1.526255	-0.710272	0.000023
C	-0.248500	0.105786	-0.000051
C	2.344652	-0.067889	0.000036
C	1.139938	0.035073	-0.000092
C	-1.359984	0.778917	0.000077
H	-1.822811	-1.216764	-0.913134
H	-1.823045	-1.216857	0.913056
H	3.401909	-0.147124	0.000228
H	-1.855160	1.731050	-0.000100

Frequencies

191.2425	204.1444	464.3325
511.3852	636.4281	650.0415
653.5126	745.9727	958.8509
1011.6820	1011.8634	1073.4242
1105.8980	1157.7240	1531.0755
1787.0990	2174.5397	3078.1190
3152.0575	3293.9518	3484.0390

Picture



p9

T1 diagnostic: 0.01352481

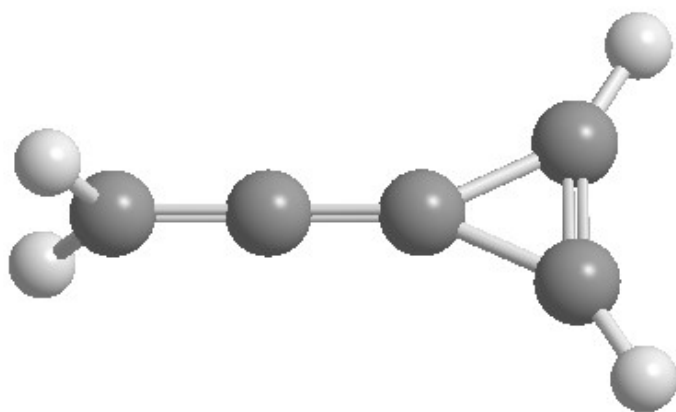
Geometries

C	2.293491	-0.000114	0.000164
C	0.983781	0.000190	-0.000504
C	-1.604099	0.654719	0.000118
C	-0.305748	0.000299	0.000218
C	-1.603956	-0.654986	-0.000150
H	2.863989	0.000144	-0.921583
H	2.863332	-0.000620	0.922259
H	-2.154068	1.577473	0.000011
H	-2.154064	-1.577645	0.000232

Frequencies

194.3601	196.5593	358.9437
542.6732	638.5665	639.5816
716.8701	857.6474	873.5937
897.1650	981.6659	1049.3758
1058.5812	1369.6421	1523.2975
1656.6643	2101.3351	3114.5431
3182.5531	3264.7458	3308.5414

Picture



p10

T1 diagnostic: 0.01188767

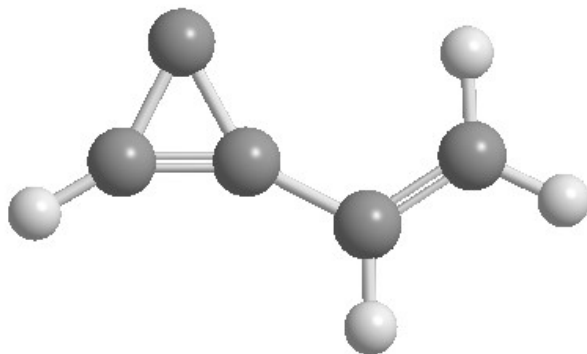
Geometry

C	-1.943649	-0.316283	0.000021
C	-0.954283	0.580233	-0.000029
C	1.298755	-0.981552	-0.000044
C	0.418412	0.139334	0.000008
C	1.730275	0.361744	0.000051
H	-2.980589	-0.014563	0.000015
H	-1.719166	-1.373409	0.000055
H	-1.159042	1.642385	-0.000080
H	2.561736	1.044729	-0.000029

Frequencies

100.0647	207.9696	368.4542
528.7622	713.4427	748.8952
903.6409	947.3325	1023.9557
1028.3639	1028.3922	1207.6530
1305.0367	1337.7429	1444.5507
1659.3946	1768.4728	3167.5831
3188.7072	3262.9390	3265.5419

Picture



p11

T1 diagnostic: 0.02427936

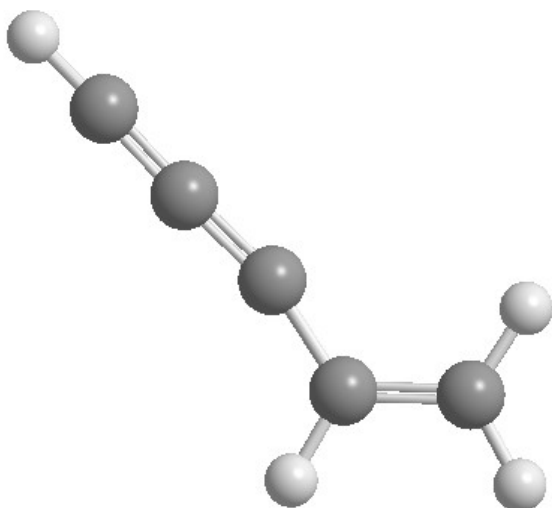
Geometry

C	1.794838	1.910498	0.000000
C	0.888913	1.051963	0.000000
C	0.000000	0.113146	0.000000
C	-1.158108	-0.646288	0.000000
C	-1.195468	-2.003615	0.000000
H	2.545845	2.663427	0.000000
H	-2.100382	-0.097055	0.000000
H	-2.141749	-2.529927	0.000000
H	-0.284761	-2.590673	0.000000

Frequencies

66.3665	144.3131	337.4583
404.3470	409.9853	451.5736
454.8875	617.9994	786.9940
889.0699	952.3927	1067.5286
1275.2863	1384.4886	1526.2893
1567.2667	1760.2690	3125.0370
3166.4166	3269.1780	3463.2873

Picture



CH₃

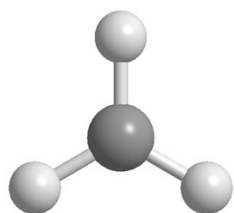
Geometries

C	0.000000	0.000000	0.000383
H	0.000000	1.075803	-0.000766
H	0.931673	-0.537902	-0.000766
H	-0.931673	-0.537902	-0.000766

Frequencies

514.5117	1427.7246	1427.7253
3139.8697	3321.1825	3321.2000

Picture





T1 diagnostic: 0.01376912

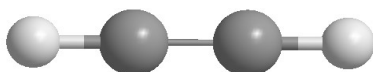
Geometries

C	0.000000	0.000000	0.601066
H	0.000000	0.000000	1.661284
C	0.000000	0.000000	-0.601066
H	0.000000	0.000000	-1.661284

Frequencies

628.6482 628.6482 762.4262
762.4262 2028.2071 3438.0702
3535.6603

Picture



Transition States

ts i4_i21

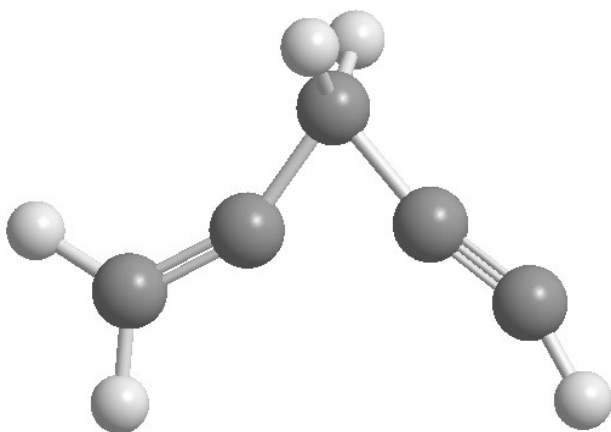
Geometries

C	2.028638	-0.654378	0.000000
C	1.032450	0.077695	0.000000
C	-0.789846	-0.015470	0.000000
C	-1.949875	-0.620290	0.000000
C	0.056650	1.171934	0.000000
H	2.568308	-1.574093	0.000000
H	-2.888128	-0.059110	0.000000
H	-2.036576	-1.703405	0.000000
H	0.044145	1.789832	0.902968
H	0.044145	1.789832	-0.902968

Frequencies

-682.7640	134.2351	190.2129
316.9608	355.2958	489.6954
508.9269	688.6036	853.3299
906.5767	937.8233	957.1382
1025.3346	1117.5589	1192.5472
1428.1971	1443.8847	1764.8748
1964.5463	3014.5281	3043.1163
3071.5310	3148.8735	3409.8888

Picture



ts i21_i22

T1 diagnostic: 0.02221998

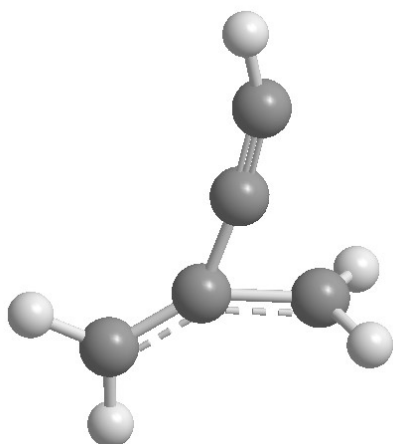
Geometries

C	0.565764	-1.965849	0.000000
C	0.222539	-0.764732	0.000000
C	0.000000	0.628643	0.000000
C	0.662279	1.776148	0.000000
H	0.128957	2.715385	0.000000
H	1.741507	1.793900	0.000000
C	-1.341818	0.058016	0.000000
H	-1.880230	-0.055165	0.928545
H	1.237413	-2.792318	0.000000
H	-1.880230	-0.055165	-0.928545

Frequencies

-671.1750	198.7764	243.3501
309.7393	379.0894	420.9459
618.4508	691.7729	777.5672
803.6824	852.3791	930.1959
959.0081	1031.0504	1176.6177
1431.2806	1466.3245	1721.8096
1986.0914	3154.9570	3168.7208
3263.5462	3264.5556	3411.3945

Picture



ts i4_i6

T1 diagnostic: 0.01284946

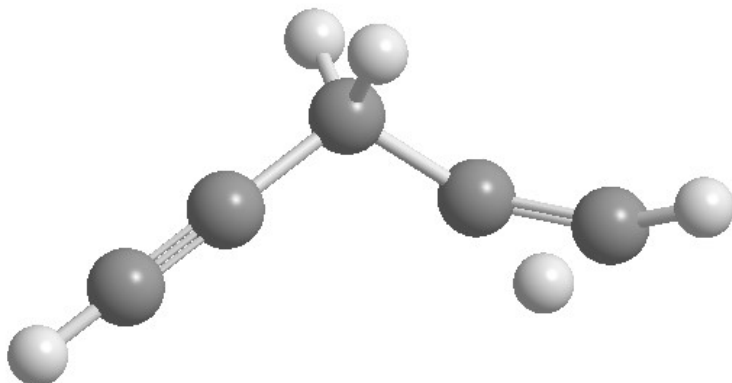
Geometries

C	-2.343629	-0.511657	0.054805
C	-1.304706	0.096472	0.032629
C	-0.043674	0.830923	0.007243
H	-0.096444	1.616871	-0.747534
C	1.139809	-0.044747	-0.279603
C	2.283988	-0.467223	0.142945
H	3.023621	-0.444297	0.937818
H	1.821365	-0.868916	-0.986646
H	-3.257808	-1.047416	0.075133
H	0.118535	1.321147	0.973116

Frequencies

-2082.8410	63.2656	183.7960
245.1564	327.5340	354.3511
491.7192	632.6427	655.1179
666.4169	823.0357	888.1964
942.3686	980.5818	1220.9121
1307.9306	1464.8719	1829.1844
2193.9781	2390.8604	3015.9541
3080.4548	3110.1388	3491.2537

Picture



ts i3_i4

T1 diagnostic: 0.01751347

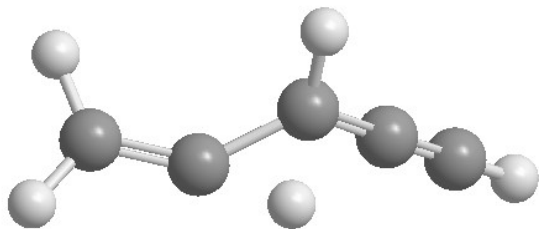
Geometries

C	2.488300	-0.363606	-0.080381
C	1.367983	0.085166	-0.032372
C	0.061439	0.639836	0.024488
H	-0.411520	0.387825	1.221404
C	-1.102660	-0.168087	0.246342
C	-2.354110	-0.286451	-0.165327
H	-2.629400	-0.000469	-1.177955
H	-3.124487	-0.724401	0.452288
H	3.467455	-0.766215	-0.130348
H	-0.067754	1.662106	-0.321892

Frequencies

-1956.7906	131.2005	210.9864
316.9679	380.5800	507.6693
591.1153	663.3064	682.5871
825.8092	874.3359	921.9520
1024.8999	1103.2911	1132.8212
1292.3507	1448.9358	1681.9956
2151.9226	2182.2224	3094.5810
3110.8876	3216.3021	3489.8059

Picture



ts i4_i16

T1 diagnostic: 0.02919094

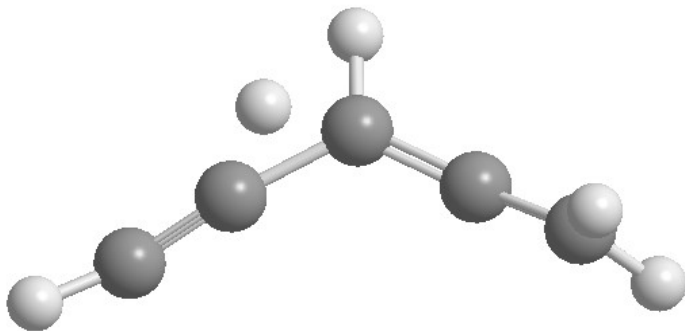
Geometries

C	-2.359856	-0.529603	-0.108710
C	-1.304775	0.085075	0.037428
C	-0.032815	0.761340	-0.047611
H	-0.086986	1.840726	-0.170518
C	1.164390	0.141943	-0.194089
C	2.291289	-0.457374	0.057692
H	2.626262	-0.645746	1.080049
H	2.953870	-0.801997	-0.733465
H	-3.280125	-1.005867	0.136607
H	-0.762418	0.604599	1.219075

Frequencies

-1683.4517	125.8667	179.0119
326.1496	358.9108	424.9094
558.6489	614.1086	644.6616
752.8356	895.5940	901.7555
954.3229	993.3136	1100.1426
1205.1365	1340.3387	1449.2925
1908.2200	2043.9155	3054.1323
3126.8127	3132.8399	3432.8557

Picture



ts i15_i18

T1 diagnostic: 0.01584469

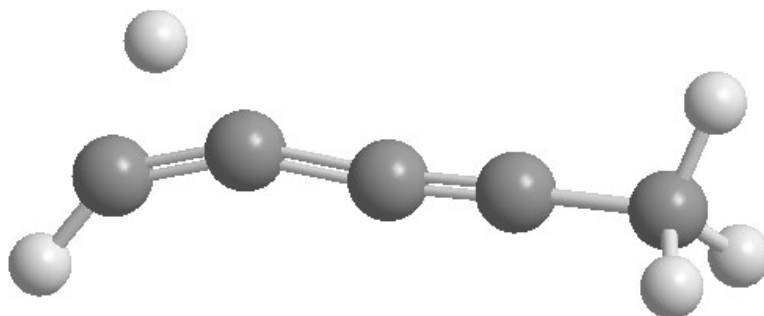
Geometries

C	2.581352	-0.053068	-0.000003
H	2.947692	-0.579955	-0.880862
H	3.013904	0.947472	-0.000382
C	1.129203	0.001427	0.000000
C	-0.086226	0.018871	0.000001
C	-1.450780	0.184392	0.000011
H	-2.320867	1.109027	-0.000043
C	-2.707046	-0.136815	0.000004
H	-3.387453	-0.986089	-0.000036
H	2.947710	-0.579290	0.881245

Frequencies

-2081.5899	20.6874	136.1712
142.1374	242.2544	294.0676
376.0636	484.0667	587.1020
657.9915	859.9018	1054.7597
1056.4046	1139.5849	1423.3010
1486.9618	1490.4661	1847.2970
2272.4608	2355.2436	3046.9908
3071.8858	3110.2893	3114.4816

Picture



ts i14_i18

T1 diagnostic: 0.01727809

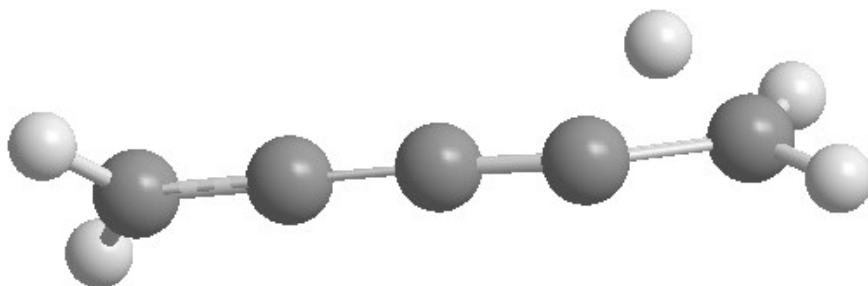
Geometries

C	-2.638145	0.087733	0.023331
H	-3.142474	1.008270	-0.242424
H	-3.258440	-0.752010	0.310927
C	-1.328878	-0.008924	-0.007552
C	-0.054029	-0.082376	-0.034614
C	1.216999	-0.268131	-0.134772
H	1.993458	-0.890491	0.635789
C	2.526999	0.228470	0.025828
H	3.340003	-0.264503	-0.485126
H	2.729776	1.158104	0.547513

Frequencies

-1843.1828	128.2744	154.2650
252.9760	354.7533	521.3830
522.9633	588.1550	754.1855
813.7477	849.8502	1014.1771
1039.0499	1054.4087	1244.9261
1459.2084	1470.5478	1762.5971
2174.2753	2226.4624	3105.2457
3129.8774	3204.1986	3236.3844

Picture



ts i3_i5

T1 diagnostic: 0.01737646

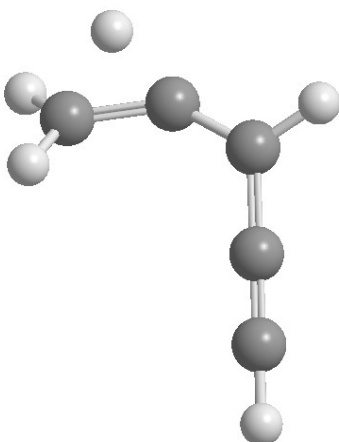
Geometries

C	2.209563	-0.567900	-0.029612
C	1.229154	0.139396	0.011200
C	0.069313	0.957416	0.050939
C	-1.152214	0.449982	-0.181223
C	-1.836462	-0.764975	0.031744
H	-2.269357	0.427074	0.455813
H	-2.645035	-1.037515	-0.631597
H	-1.477354	-1.510082	0.737166
H	3.072312	-1.182208	-0.066207
H	0.203310	2.019216	0.206540

Frequencies

-1847.9891	124.4423	273.8417
310.9324	415.6460	526.1754
590.1019	637.5045	664.9345
810.3131	881.4646	957.1466
1037.5335	1101.0151	1131.8039
1353.1778	1464.3121	1652.4091
2178.5838	2195.3070	3089.5648
3180.9872	3223.0992	3489.6013

Picture



ts i4_p2

T1 diagnostic: 0.01580473

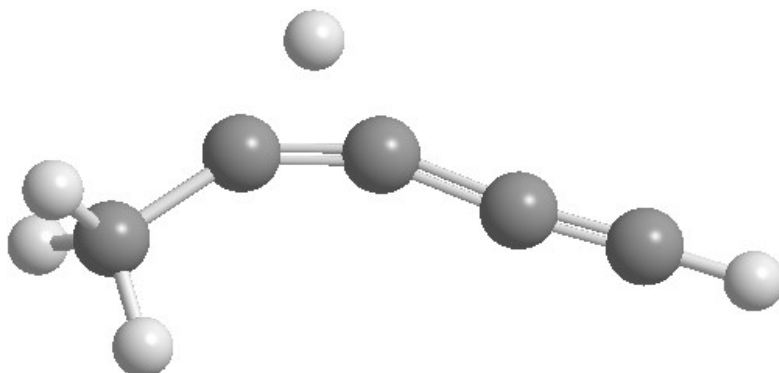
Geometries

C	2.625816	-0.315387	0.000001
C	1.451086	-0.008659	-0.000001
C	0.165461	0.484513	-0.000002
C	-1.131079	0.447172	0.000000
C	-2.324520	-0.437651	0.000001
H	-2.938974	-0.251969	-0.879255
H	-2.013523	-1.485670	0.000022
H	-2.938996	-0.251939	0.879234
H	3.643246	-0.612402	0.000002
H	-0.472339	1.582051	0.000007

Frequencies

-2087.0758	104.0345	130.4980
232.0448	277.4546	350.2460
503.6647	510.2599	561.6587
646.6399	714.8649	1027.5868
1031.1523	1067.2117	1395.6624
1477.8515	1487.1017	1889.4335
2159.7508	2342.7717	3026.1116
3109.3933	3128.1733	3486.0599

Picture



ts i22_i24

T1 diagnostic: 0.02498764

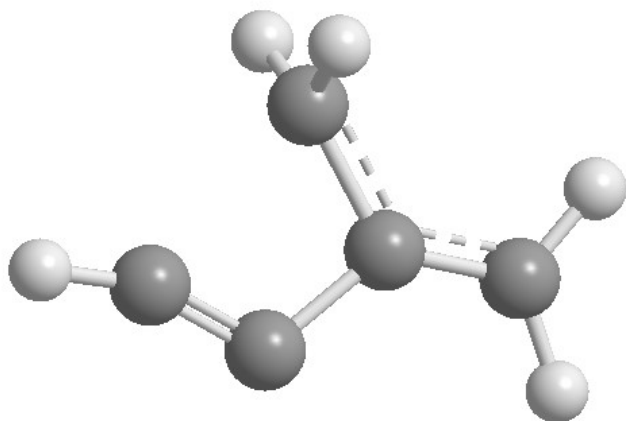
Geometries

C	1.828349	-0.307762	0.000086
H	2.196679	-1.322206	-0.000028
H	2.548779	0.496831	0.000237
C	0.524663	-0.053570	0.000046
C	-0.226140	1.248799	0.000160
H	-0.297627	1.801356	-0.926636
C	-1.732954	-0.363982	-0.000197
C	-0.620284	-0.948374	-0.000161
H	-0.297820	1.801076	0.927108
H	-2.791817	-0.227726	-0.000282

Frequencies

-807.1340	87.5769	351.7372
373.3330	535.1122	586.7392
637.5005	708.5402	750.7700
831.5249	913.7645	938.5019
961.5932	1038.7499	1244.9653
1417.4792	1451.9726	1734.2400
1798.5147	3137.0391	3172.2668
3251.6430	3263.7200	3395.3736

Picture



ts i22_i9

T1 diagnostic: 0.01296415

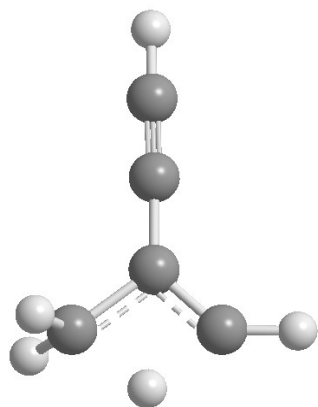
Geometries

C	-2.276940	-0.095910	-0.000116
C	-1.074465	0.016203	-0.000052
C	0.337920	0.107208	0.000022
C	1.175923	1.136099	0.000232
H	1.106008	2.217680	0.000429
C	1.353044	-1.002919	-0.000093
H	1.484499	-1.564563	0.918681
H	1.484606	-1.564285	-0.919021
H	-3.333552	-0.183617	-0.000181
H	2.165551	0.130698	0.000133

Frequencies

-2232.2978	183.3353	233.9933
466.0297	508.9108	521.4519
569.4931	655.9815	657.0943
713.5087	851.2901	965.7487
994.2517	1059.5631	1121.2612
1223.0656	1434.9058	1711.2916
1876.6144	2200.8361	3099.8970
3172.3971	3201.6370	3485.6507

Picture



ts i24_i25

T1 diagnostic: 0.02793113

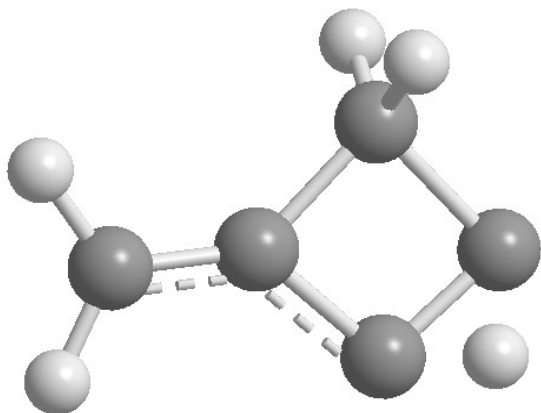
Geometries

C	-1.861601	-0.068530	0.006599
H	-2.376907	-1.017028	-0.023802
C	-0.541212	-0.017037	-0.020178
C	0.571759	0.998973	0.020943
H	0.668754	1.591057	0.925521
C	1.644098	-0.206182	-0.086972
C	0.561158	-1.042703	-0.091509
H	1.233386	-1.005831	0.939975
H	-2.454689	0.833643	0.055700
H	0.684238	1.611026	-0.870696

Frequencies

-846.9339	176.6176	346.1641
431.7800	473.6839	722.5461
726.9165	840.5928	857.5802
884.4198	942.3976	950.3800
1107.6386	1141.0638	1168.2433
1373.7435	1434.0959	1447.9427
1738.1777	2270.2115	3092.5080
3165.6096	3171.3399	3257.0225

Picture



ts i24_i14

T1 diagnostic: 0.02392986

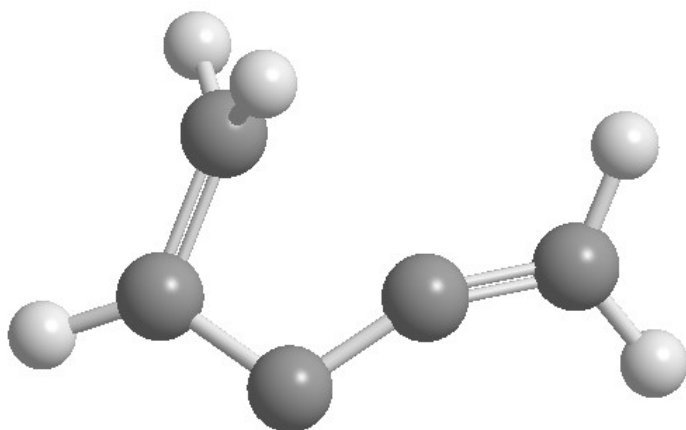
Geometries

C	1.973491	0.172627	-0.105332
H	2.290176	1.187314	0.077239
C	0.743169	-0.212421	0.124064
C	-1.042819	0.987142	0.032632
H	-1.305748	1.749020	-0.697871
C	-1.448653	-0.381680	-0.119685
C	-0.312408	-1.064522	0.167643
H	2.702101	-0.529609	-0.489582
H	-0.776197	1.342235	1.014709
H	-2.387009	-0.755832	-0.500427

Frequencies

-748.9935	221.3643	267.5173
541.1420	555.1971	640.4035
722.1193	853.0132	862.7648
893.5591	986.3764	1005.8466
1043.2380	1169.3659	1299.0259
1431.6830	1478.0892	1542.4086
1908.0525	3101.8079	3156.5836
3216.5311	3241.7632	3249.1054

Picture



ts i25_p5

T1 diagnostic: 0.02160105

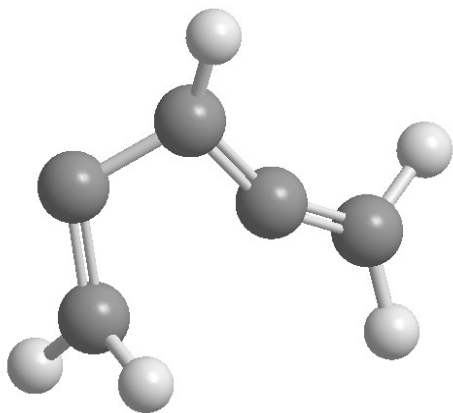
Geometries

C	1.844863	-0.323589	-0.080710
H	2.599882	0.283010	-0.567852
C	0.649497	0.183869	0.132360
C	-1.124663	-1.003578	0.053986
H	-0.939691	-1.260837	1.088990
C	-1.375000	0.318726	-0.267958
C	-0.338404	1.146704	0.083763
H	-0.298318	2.196953	0.320581
H	2.112595	-1.323592	0.219461
H	-1.412222	-1.828329	-0.589827

Frequencies

-684.7212	250.1191	295.8160
442.7249	636.4076	644.8283
698.8477	803.6778	880.6055
932.7947	979.8239	1012.9617
1064.7861	1162.8712	1292.5533
1438.8503	1474.1960	1531.3666
1788.5530	3122.4645	3137.8588
3205.1699	3240.9122	3245.3289

Picture



ts i23_i25

T1 diagnostic: 0.01910441

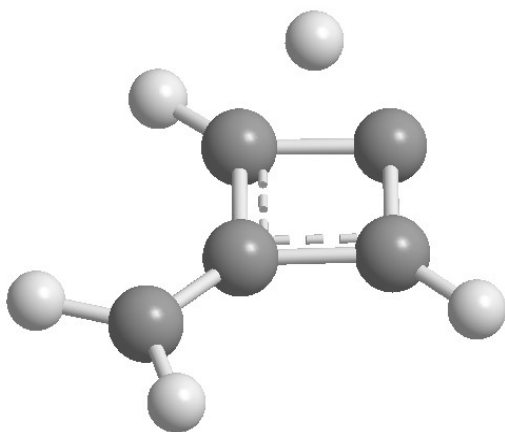
Geometries

C	1.854763	-0.058849	0.017517
H	2.463177	0.833920	0.030353
C	0.527768	0.018587	-0.020950
C	-0.614584	-0.955113	-0.057416
H	-1.400458	-0.749287	0.934771
C	-1.634087	0.080481	-0.067474
C	-0.508269	1.052030	-0.005668
H	-0.486242	2.130412	0.015214
H	2.359287	-1.013628	0.033128
H	-0.689312	-2.024236	-0.209519

Frequencies

-1123.2304	199.7324	339.4666
454.2843	670.8965	722.0309
724.4830	833.2122	870.9338
921.6650	944.3692	948.6894
1078.9839	1171.9772	1212.6830
1278.5224	1306.2873	1458.2248
1761.7943	2097.4955	3167.7462
3193.3311	3230.8055	3258.0052

Picture



ts i14_p5

T1 diagnostic: 0.03070841

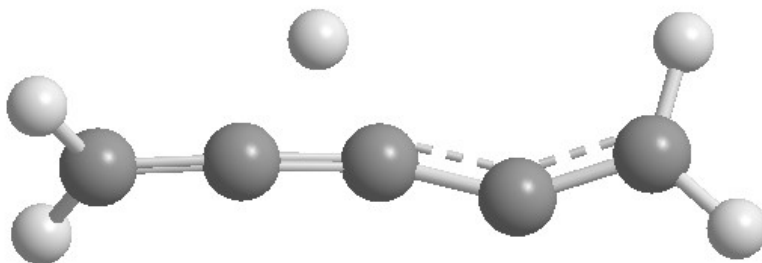
Geometries

C	2.573286	0.090962	0.046736
H	3.367531	-0.532208	0.437059
C	1.317863	-0.314679	0.043801
C	0.033472	-0.035724	-0.173818
C	-1.249494	0.016324	-0.000422
C	-2.582404	-0.019841	0.068547
H	-3.123071	-0.774312	-0.482431
H	-3.134224	0.691527	0.660614
H	2.865637	1.063713	-0.341715
H	-0.532213	1.129026	-0.182594

Frequencies

-1584.0371	122.9523	144.0991
287.0716	374.2411	430.3184
524.2606	597.9555	679.1658
728.4104	774.4557	882.5586
1014.0675	1024.7323	1274.0400
1444.7887	1479.9644	1782.7352
2005.7241	2094.2398	3090.4438
3174.8782	3187.1865	3269.0391

Picture



ts i16_i17

T1 diagnostic: 0.01551145

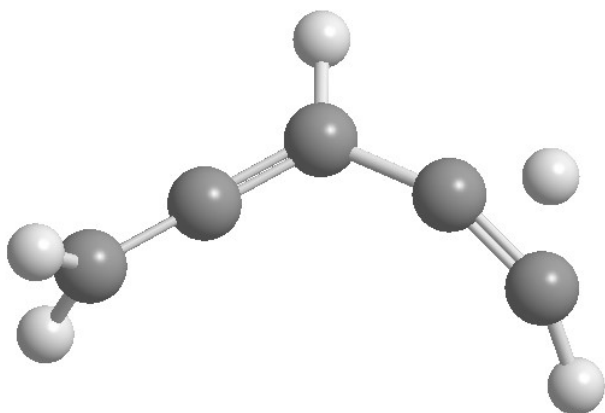
Geometries

C	2.201315	-0.638900	-0.023922
H	2.533453	-1.474219	-0.635982
C	1.277734	0.249777	0.132700
C	-0.005818	0.850986	-0.138367
C	-1.131522	0.178581	-0.059320
C	-2.237875	-0.496216	0.065365
H	-2.695062	-0.987865	-0.783425
H	-2.736080	-0.585437	1.022564
H	2.300367	0.270714	0.894316
H	-0.025686	1.911439	-0.356205

Frequencies

-2071.7331	76.0032	183.4007
260.4560	299.3581	328.9528
504.3496	628.0099	650.9631
827.1044	878.0731	881.0676
916.2515	1013.1705	1112.9183
1336.7376	1471.6333	1852.8240
2016.8932	2364.8677	3084.5622
3136.6014	3169.4722	3212.4268

Picture



ts i16_i23

T1 diagnostic: 0.02096196

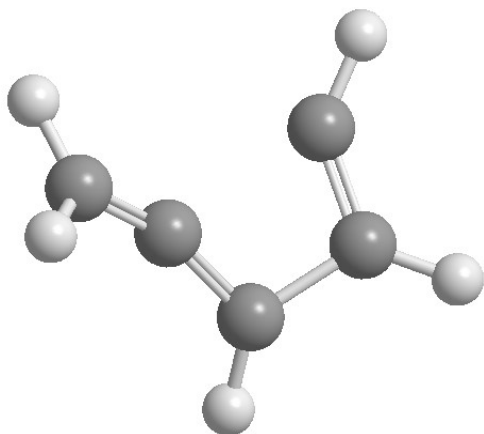
Geometries

C	-1.949234	0.247242	0.106612
H	-2.593323	-0.279308	0.799424
C	-0.730694	-0.177663	-0.124446
C	0.328146	-1.018497	-0.128878
C	1.454864	-0.171704	0.198887
C	1.029308	1.048135	-0.135480
H	-2.330144	1.145208	-0.355504
H	2.385368	-0.470113	0.665877
H	1.404778	2.060424	-0.076180
H	0.338981	-2.021288	-0.533785

Frequencies

-747.4630	254.6559	281.4673
477.2601	612.7561	669.4027
737.3195	790.6413	857.2000
872.8668	923.6459	1001.9618
1040.1628	1062.9328	1235.4344
1343.8067	1456.2592	1574.6926
1899.2251	3149.4693	3166.6463
3195.7818	3211.6302	3237.7101

Picture



ts i5_i8

T1 diagnostic: 0.02458066

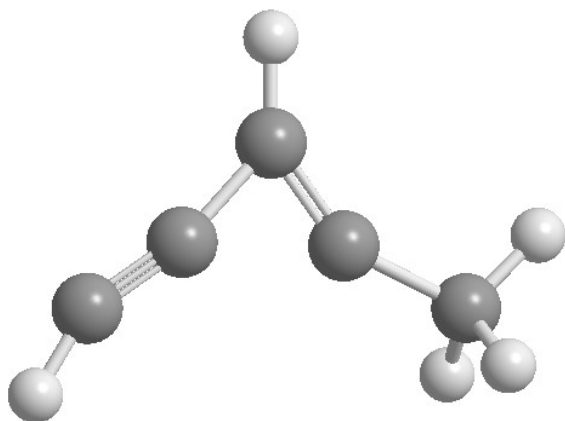
Geometries

C	-2.132526	-0.600499	-0.000103
H	-2.696969	-1.501494	-0.000108
C	-1.099405	0.099410	-0.000045
C	0.663351	0.098209	-0.000001
C	-0.128838	1.135095	0.000019
H	-0.131390	2.217125	0.000083
C	1.996909	-0.511539	0.000082
H	2.124868	-1.144678	0.877841
H	2.125016	-1.144613	-0.877703
H	2.781531	0.249601	0.000176

Frequencies

-714.0594	127.7343	184.2951
224.9359	390.0926	427.9499
522.7332	524.9373	778.8800
875.5947	953.4707	1044.4800
1050.3421	1176.5266	1405.3917
1476.9562	1482.7508	1788.3346
1892.6730	3024.1203	3098.4217
3114.4149	3172.1820	3428.0105

Picture



ts i8_i9

T1 diagnostic: 0.02313588

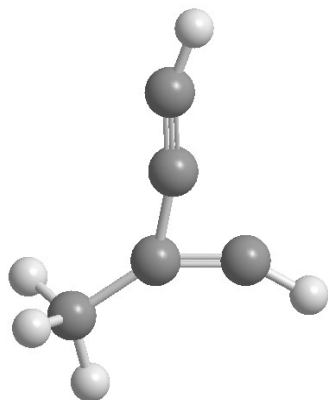
Geometries

C	-2.016670	-0.619484	0.000163
H	-3.078746	-0.656691	0.000355
C	-0.876797	-0.116614	0.000059
C	0.519705	0.159234	-0.000065
C	0.055897	1.379443	-0.000084
H	0.240452	2.439830	-0.000125
C	1.758048	-0.660988	-0.000074
H	1.779076	-1.304040	0.878839
H	1.778955	-1.304216	-0.878862
H	2.639162	-0.024423	-0.000198

Frequencies

-753.6499	139.8414	226.6035
248.6633	422.3045	461.7775
522.8837	552.0443	638.8610
740.6529	786.8235	987.5164
1052.9524	1199.8603	1411.2888
1489.0064	1494.8522	1726.7346
1918.1187	3059.7120	3125.1107
3151.1862	3260.2945	3435.9789

Picture



ts i18_p3

T1 diagnostic: 0.01368186

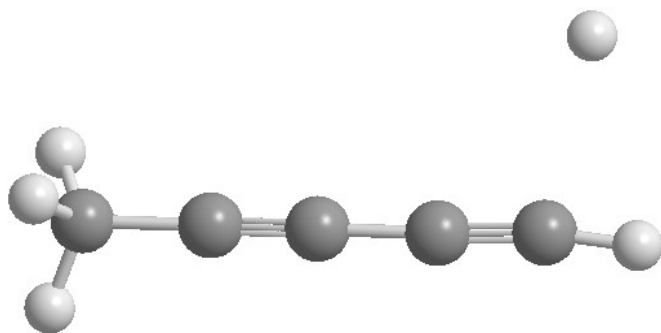
Geometries

C	-2.601988	0.061611	-0.000070
H	-2.980921	0.324724	0.991993
H	-3.041656	-0.898881	-0.285432
C	-1.151608	-0.011250	0.000259
C	0.057199	-0.071353	0.000173
C	1.416395	-0.142968	0.000036
C	2.628659	-0.158025	-0.000120
H	3.678488	-0.319348	-0.000268
H	-2.955222	0.817440	-0.707949
H	3.207372	2.007970	-0.000019

Frequencies

-348.9190	17.3520	132.0410
148.1799	233.6316	336.8443
352.7779	526.8409	538.4429
632.5779	681.1456	697.1524
1046.1448	1047.4767	1184.8677
1413.6468	1472.3485	1472.7095
2137.6532	2333.7805	3021.0495
3080.1231	3081.2009	3472.9798

Picture



ts i18_p6

T1 diagnostic: 0.01813766

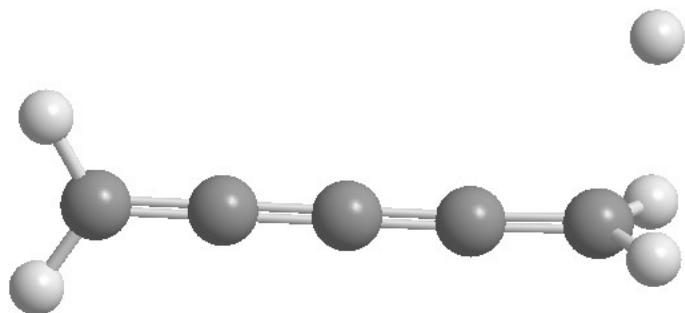
Geometries

C	2.487519	-0.145299	0.000000
H	3.042211	-0.221663	-0.925031
H	3.083457	1.877199	0.000001
C	1.176424	-0.121585	0.000001
C	-0.090639	-0.060943	0.000001
C	-1.362640	-0.001193	0.000000
C	-2.664352	0.060850	0.000000
H	-3.267207	-0.837694	-0.000033
H	3.042212	-0.221731	0.925025
H	-3.178544	1.012919	0.000032

Frequencies

-694.5692	137.0386	151.1984
264.0875	311.1520	357.4741
366.6638	553.7887	557.8947
785.3298	798.1798	882.1672
901.5274	1014.4905	1024.3452
1337.3719	1444.4420	1527.4249
1994.7230	2391.1036	3145.7451
3151.4978	3223.8217	3232.7034

Picture



ts i6_p2

T1 diagnostic: 0.01622289

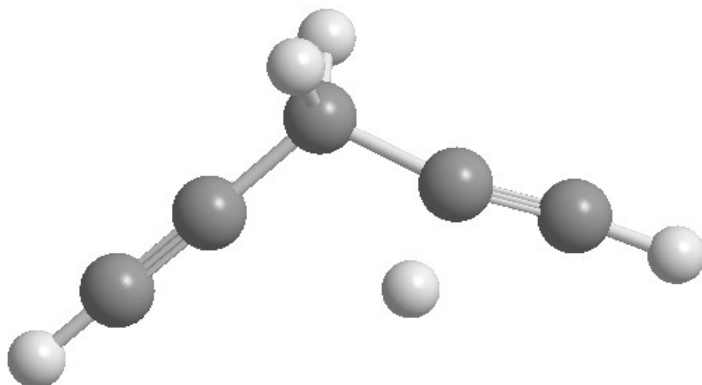
Geometries

C	-2.282775	-0.544728	-0.067137
C	-1.259398	0.087525	-0.036464
C	-0.024190	0.868840	-0.009080
H	0.045651	1.470795	-0.916773
C	1.189546	0.036321	0.082398
C	2.245729	-0.495618	-0.191259
H	3.155614	-1.034776	-0.274120
H	-3.180917	-1.106999	-0.090349
H	-0.052746	1.561695	0.832597
H	0.818933	-0.604755	1.777906

Frequencies

-855.7037	102.2611	171.9114
318.9862	354.9092	416.8832
520.2883	569.4926	657.5445
661.9715	674.2243	682.7544
911.0033	949.2636	1002.9928
1248.8411	1343.7192	1471.0770
2139.7196	2198.9650	3058.6997
3094.5989	3478.9451	3490.9363

Picture



ts i3_p1

T1 diagnostic: 0.01707830

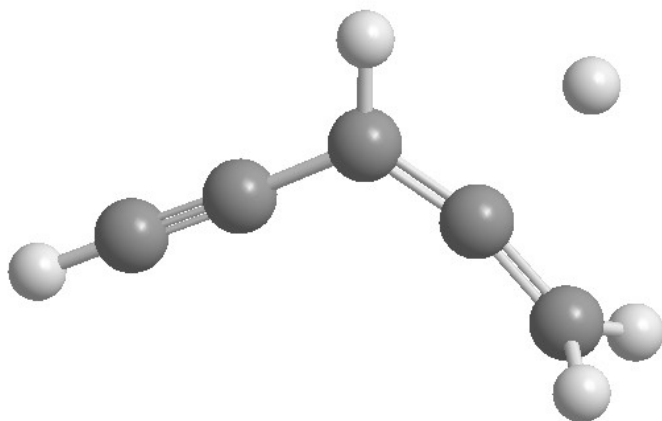
Geometries

C	1.104389	0.088590	0.000000
C	0.000000	0.814234	0.000000
C	-1.294776	0.215118	0.000000
C	1.974226	-0.901539	0.000000
C	-2.411438	-0.250098	0.000000
H	2.331960	1.547606	0.000000
H	0.053752	1.896662	0.000000
H	2.382773	-1.284779	0.928928
H	2.382773	-1.284779	-0.928928
H	-3.385662	-0.672544	0.000000

Frequencies

-924.3869	95.3518	150.8665
283.0914	360.1403	388.9960
548.3642	594.4698	632.0588
632.5458	683.0897	875.0433
880.5204	963.0874	1015.1830
1134.7664	1358.9554	1470.2997
1977.8610	2179.9645	3143.9253
3189.2392	3229.1710	3495.5619

Picture



ts i5_p3

T1 diagnostic: 0.01732475

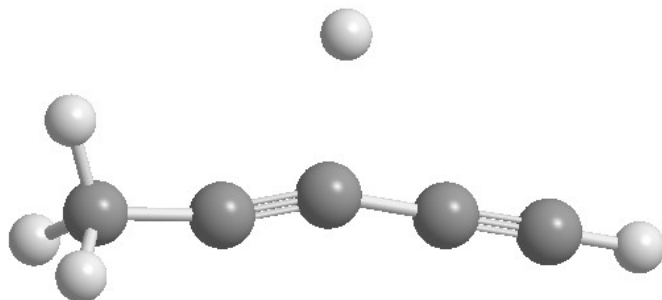
Geometries

C	2.704893	-0.159419	0.000003
C	1.506741	-0.014471	-0.000001
C	0.139365	0.167505	-0.000006
C	-1.055239	-0.093515	-0.000004
C	-2.504126	-0.117425	0.000003
H	-2.896060	0.902111	0.000082
H	-2.886172	-0.628764	-0.882693
H	-2.886161	-0.628895	0.882627
H	3.755933	-0.296527	0.000007
H	0.162650	1.956024	0.000006

Frequencies

-1038.4136	91.6988	138.7393
165.3440	313.2104	348.5632
533.7056	535.4446	576.1682
652.2279	659.9454	727.4113
1045.4896	1060.3141	1172.4265
1418.8185	1480.2539	1485.6591
2131.6789	2340.3431	3039.3237
3103.9625	3122.4627	3491.5208

Picture



ts i7_p3

T1 diagnostic: 0.01651544

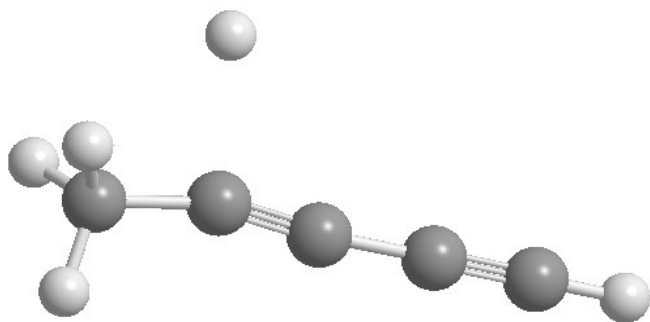
Geometries

C	2.754172	-0.045341	-0.000009
C	1.545301	-0.037044	-0.000006
C	0.182871	-0.039461	-0.000003
C	-1.029601	0.084391	0.000007
C	-2.469533	-0.166435	-0.000004
H	-2.657113	-1.239307	-0.000066
H	-2.937471	0.270921	0.879996
H	-2.937475	0.271024	-0.879951
H	3.814317	-0.048125	-0.000012
H	-1.181516	1.968834	0.000118

Frequencies

-844.1659	137.2327	142.9277
173.2395	362.5131	396.9164
479.7443	525.5927	572.4204
650.1482	658.6927	695.6921
1055.5988	1067.5073	1173.4548
1421.8556	1486.2757	1491.8128
2146.1265	2374.8209	3059.0395
3131.2699	3131.5696	3490.4828

Picture



ts i15_p3

T1 diagnostic: 0.01740758

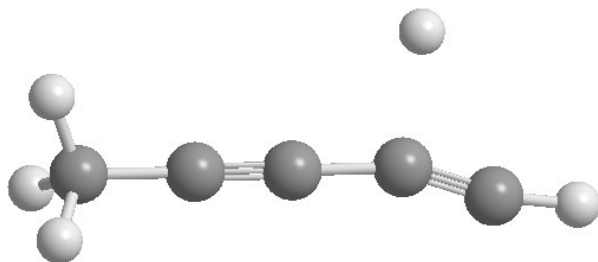
Geometries

C	-2.553264	-0.065443	0.000060
H	-2.918703	-0.592744	0.880481
H	-2.978523	0.937424	0.003407
C	-1.101250	-0.008693	-0.000105
C	0.106779	0.030083	-0.000082
C	1.484836	0.094503	-0.000012
H	1.558960	1.860736	0.000078
C	2.653987	-0.260973	0.000046
H	3.710935	-0.355184	0.000106
H	-2.919198	-0.587101	-0.883512

Frequencies

-1127.0485	12.5531	148.2890
157.9671	350.5728	354.0362
501.5871	532.1614	571.4611
625.3958	658.4621	723.9185
1058.7289	1059.9447	1176.2384
1424.1406	1489.2021	1489.4892
2086.5422	2383.2118	3053.9948
3121.1787	3121.9533	3473.0523

Picture



ts i16_p1

T1 diagnostic: 0.01325162

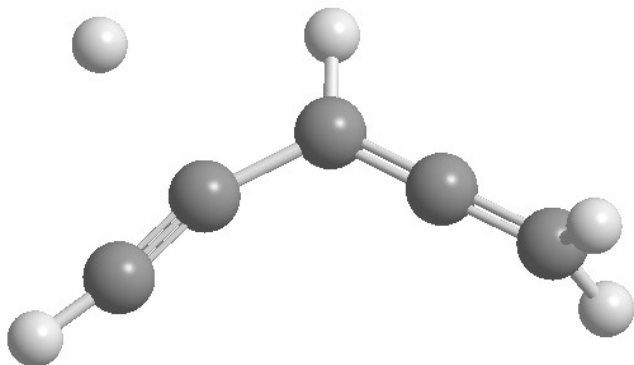
Geometries

C	2.266139	-0.449712	0.029828
C	1.126751	0.168971	-0.012888
C	-0.017259	0.805781	-0.053343
C	-1.277142	0.113696	0.000918
C	-2.127684	-0.752216	-0.010005
H	2.750718	-0.791892	-0.878943
H	2.760250	-0.644890	0.976161
H	-0.026285	1.887558	-0.131915
H	-2.964017	-1.409495	0.005328
H	-2.345495	1.639599	0.302306

Frequencies

-850.1180	40.5544	152.0312
326.2564	370.7973	405.3522
536.8729	614.5898	641.1131
673.1278	687.1721	894.1780
902.9041	957.9484	1013.5390
1140.0000	1347.6332	1472.3106
2074.9596	2139.7756	3148.7453
3189.7489	3232.9097	3472.1616

Picture



ts i17_p6

T1 diagnostic: 0.01911124

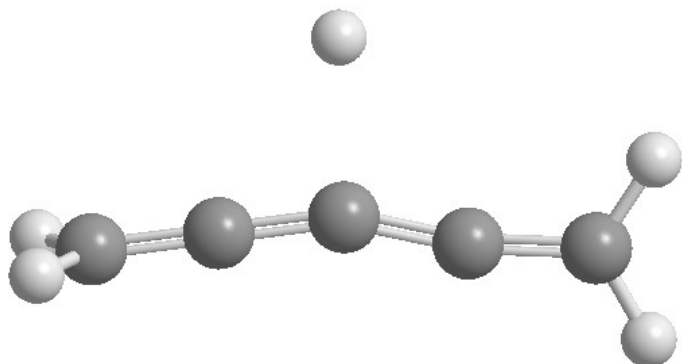
Geometries

C	2.563150	-0.139787	-0.000040
H	3.149826	0.772105	-0.000224
C	1.263032	-0.091978	0.000048
C	0.002093	0.175391	0.000079
C	-1.267312	0.008051	0.000003
C	-2.557098	-0.160532	-0.000035
H	-3.110026	-0.234719	-0.926703
H	-3.110118	-0.234454	0.926600
H	3.096873	-1.080866	0.000068
H	-0.049737	2.031058	-0.000072

Frequencies

-1029.5411	152.3266	158.2507
254.1352	324.5298	361.8258
497.9987	556.9792	577.2201
735.9734	805.2055	880.5638
885.1548	1001.7879	1013.5455
1337.1724	1438.3401	1528.8917
2013.5058	2330.8666	3130.5640
3150.4561	3211.4359	3229.5692

Picture



ts i17_p1

T1 diagnostic: 0.01388495

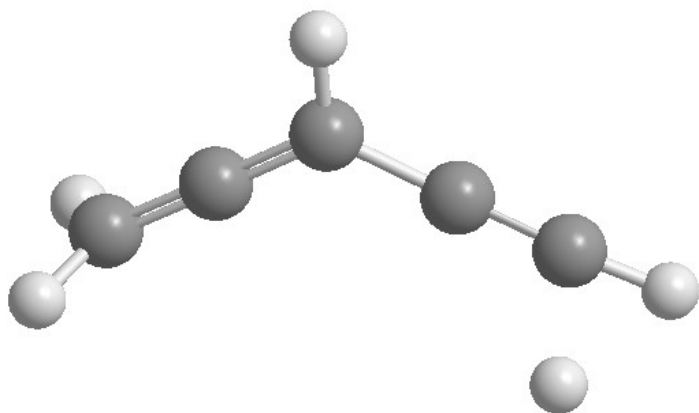
Geometries

C	-2.344543	-0.458770	-0.044864
H	-2.787200	-0.950300	0.816951
C	-1.196000	0.140589	0.035697
C	-0.040997	0.764367	0.121846
C	1.215760	0.147692	-0.112849
C	2.307230	-0.350101	-0.256256
H	2.821920	-1.072399	1.829400
H	3.249652	-0.764582	-0.517875
H	-2.899206	-0.495409	-0.978304
H	-0.033865	1.820021	0.388386

Frequencies

-296.7828	59.8533	141.3162
200.0166	310.1157	359.5917
365.0488	606.6565	632.9142
681.4379	685.8594	882.7980
883.7699	954.5227	1000.8610
1137.7811	1351.9082	1462.0597
2035.3060	2175.9421	3111.0644
3115.9454	3183.3737	3473.6753

Picture



ts i14_p6

T1 diagnostic: 0.01844492

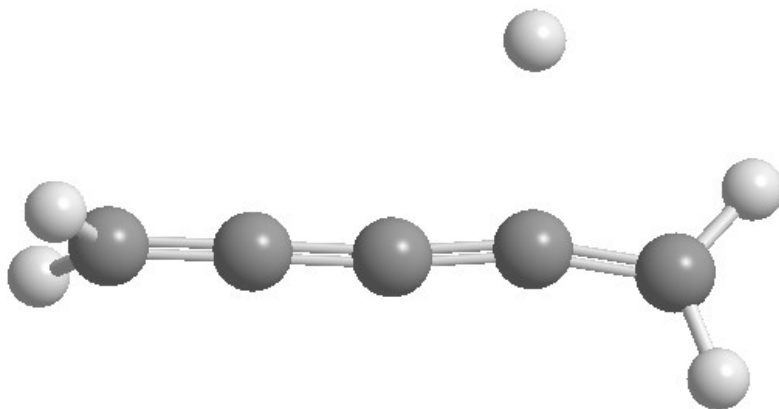
Geometries

C	-2.611300	-0.022949	0.000031
H	-3.169672	-0.013886	-0.926259
H	-3.169651	-0.013766	0.926333
C	-1.305778	-0.042131	0.000018
C	-0.038194	-0.066797	0.000006
C	1.240403	0.037523	-0.000018
H	1.267634	2.044559	-0.000205
C	2.533470	-0.157063	-0.000012
H	3.238649	0.659236	-0.000069
H	2.921432	-1.167635	0.000047

Frequencies

-922.9292	147.3689	151.0926
245.7289	356.0059	413.0314
465.7142	556.5635	572.4855
770.3624	789.8493	886.3274
898.0016	1019.7187	1020.9228
1344.6124	1448.1739	1537.0166
2008.6272	2320.0424	3150.4316
3156.0925	3231.0196	3247.5919

Picture



ts i4_p1

T1 diagnostic: 0.01881087

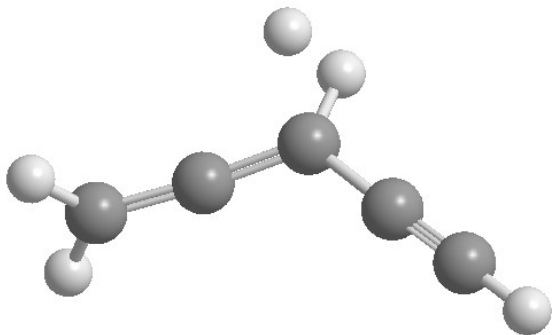
Geometries

C	2.364407	-0.518315	0.066665
C	1.300321	0.036081	-0.041576
C	0.050412	0.720068	-0.190007
H	0.139847	1.660796	1.383401
C	-1.112963	0.083404	-0.122643
C	-2.266037	-0.473470	0.081142
H	-2.765671	-1.047117	-0.688847
H	-2.762935	-0.382332	1.040832
H	3.296604	-1.012847	0.166061
H	0.075319	1.694895	-0.662932

Frequencies

-1007.7540	135.3910	228.4748
306.8188	347.8146	456.4978
499.3027	589.3505	634.2926
648.6982	678.6041	891.0297
947.2245	970.1377	998.5289
1127.8925	1350.4274	1462.6591
1993.8668	2210.9490	3125.6171
3156.8046	3204.0594	3490.5878

Picture



ts i4_p2

T1 diagnostic: 0.01590452

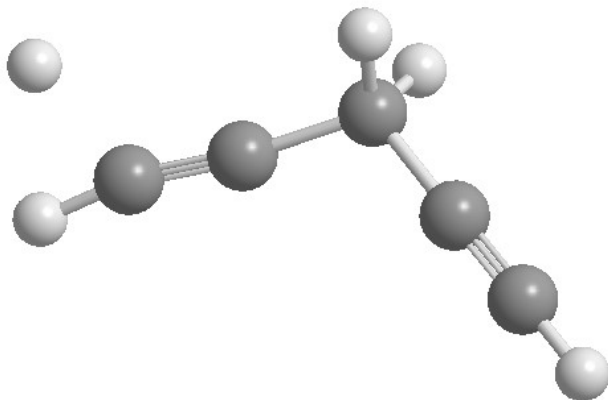
Geometries

C	2.335280	-0.561825	0.069890
C	1.316479	0.076132	0.016721
C	0.084924	0.863810	-0.046999
H	0.007234	1.489823	0.846576
C	-1.118464	0.042895	-0.152223
C	-2.172471	-0.552415	-0.093856
H	-2.993823	-1.195864	-0.289809
H	-3.051550	0.077102	1.463062
H	3.229790	-1.128497	0.117272
H	0.133867	1.545849	-0.898302

Frequencies

-765.6252	58.4791	135.8888
241.1774	315.7839	335.1131
457.8571	575.5637	661.4167
666.3277	675.2410	835.4970
908.5266	938.3521	1005.8432
1245.4677	1343.5789	1464.2734
2165.1872	2199.1480	3036.5213
3073.6189	3462.5980	3490.3188

Picture



ts i9_p4

T1 diagnostic: 0.01837190

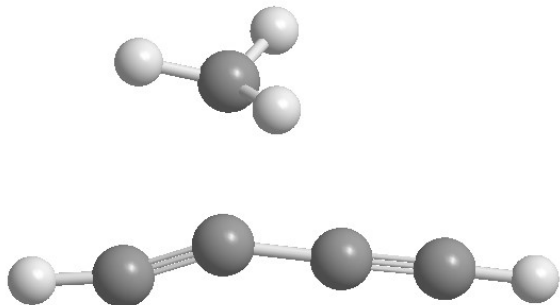
Geometries

C	2.163877	0.017291	0.000069
C	0.990538	-0.264267	0.000025
C	-0.364132	-0.556117	-0.000012
C	-1.310431	-1.340641	-0.000040
C	-1.070846	1.537361	-0.000031
H	3.199127	0.244709	0.000096
H	-2.287406	-1.757270	-0.000065
H	-2.143585	1.427085	-0.000026
H	-0.611084	1.861870	0.920233
H	-0.611089	1.861840	-0.920307

Frequencies

-653.2117	92.3512	157.8948
244.2719	271.1698	468.0147
487.1336	536.5857	574.9852
576.1628	649.5853	661.5000
684.5715	866.8183	930.2515
1434.5666	1439.0810	1981.5785
2277.4538	3115.9683	3281.2300
3282.8221	3457.5561	3491.6118

Picture



ts i7_p4

T1 diagnostic: 0.01752857

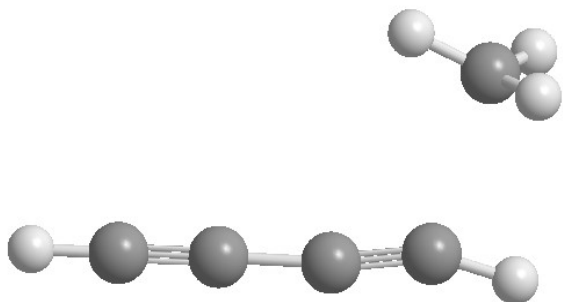
Geometries

C	2.570526	-0.472643	-0.000001
C	1.471044	0.030331	0.000001
C	0.239776	0.611559	0.000005
C	-0.926447	0.972920	0.000007
C	-2.400874	-0.802412	-0.000004
H	3.532808	-0.917430	-0.000001
H	-1.741674	1.654637	0.000022
H	-1.697751	-1.618241	0.000322
H	-2.909077	-0.578652	0.924512
H	-2.908461	-0.578846	-0.924904

Frequencies

-527.1545	45.4405	90.7136
240.3142	285.2703	447.3365
486.7091	513.0236	534.3165
636.0572	658.0346	666.8696
719.9057	834.9256	915.9905
1430.4088	1438.4911	2046.0588
2312.3417	3121.1539	3286.0720
3295.9448	3437.9842	3491.2955

Picture



ts i16_p5

T1 diagnostic: 0.01941648

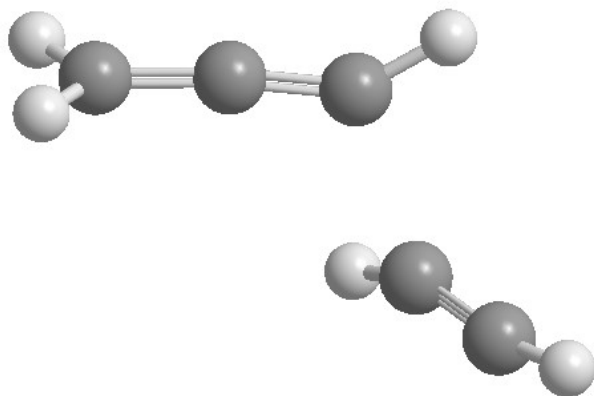
Geometries

C	-2.325168	-0.440529	0.167677
C	-1.232053	0.302507	0.017359
C	-0.132156	0.890968	-0.142182
C	1.469508	-0.433652	-0.412419
C	2.418492	-0.241025	0.339576
H	-2.645434	-0.765234	1.146937
H	-2.935529	-0.711404	-0.681467
H	0.317808	1.858368	-0.179108
H	1.000776	-0.980150	-1.198611
H	3.070645	0.128803	1.092192

Frequencies

-750.3178	23.0189	131.0840
250.5556	321.2804	396.7144
486.7191	558.1810	649.3702
713.6988	758.3494	779.5842
803.1368	896.6339	1037.1073
1162.5929	1478.7822	1828.4307
1962.4301	3159.6648	3245.5991
3365.8915	3373.6068	3469.9728

Picture



ts i2_i3

T1 diagnostic: 0.01886575

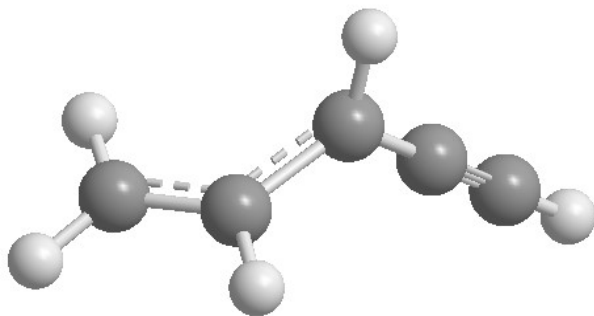
Geometries

C	-1.173263	0.265832	0.397283
C	-2.039343	-0.563635	-0.176912
H	-1.377289	0.634007	1.399037
H	-1.871501	-0.955803	-1.169923
H	-2.936954	-0.874086	0.337701
C	0.070577	0.742865	-0.240132
C	2.342709	-0.466376	0.090426
C	1.277805	0.105695	-0.065298
H	0.046669	1.654875	-0.822638
H	3.268166	-0.965281	0.223621

Frequencies

-205.9614	172.5542	317.4602
381.9529	474.7755	504.6432
603.0420	642.6214	689.7026
934.8869	968.1410	1011.4217
1062.7918	1142.9866	1323.5165
1356.8981	1461.4688	1685.8789
2046.5426	3125.2747	3162.6589
3173.8448	3251.4489	3485.1351

Picture



ts i10_i12

T1 diagnostic: 0.01425934

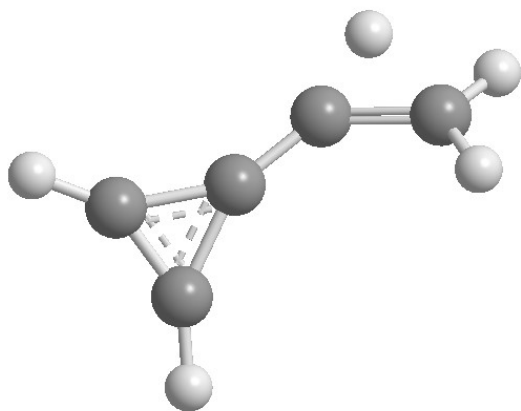
Geometries

C	-2.183810	0.218611	0.094683
C	-0.929031	-0.398487	-0.241353
C	1.498749	0.761926	-0.049030
C	0.350747	-0.135811	-0.047579
C	1.726850	-0.527150	0.104286
H	-3.023617	0.079212	-0.571081
H	-2.268548	0.981484	0.862790
H	-1.842495	-1.017090	0.422308
H	1.905896	1.753705	-0.130720
H	2.447738	-1.311850	0.250669

Frequencies

-1954.7089	161.6020	227.8687
361.0961	391.7386	525.1827
632.2057	744.4072	817.0462
839.9792	896.2884	966.1573
1038.2031	1059.5102	1072.4808
1249.4872	1462.6734	1586.3718
1810.6381	2202.8767	3091.1381
3215.0934	3247.5975	3289.7639

Picture



ts i10_i13

T1 diagnostic: 0.02671607

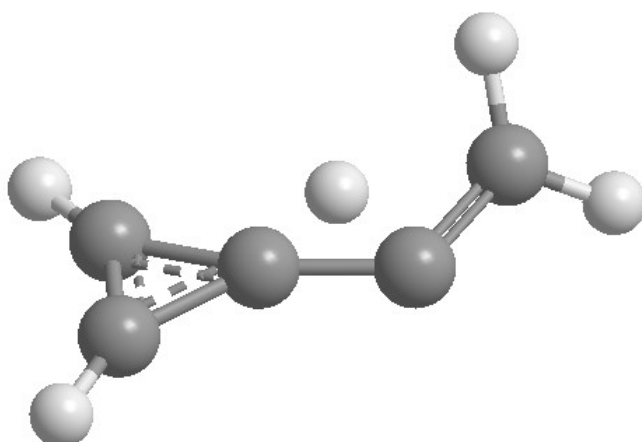
Geometries

C	2.143885	0.239922	-0.014310
C	1.009528	-0.563298	-0.138085
C	-1.387338	0.808205	-0.050147
C	-0.302835	-0.173177	0.033872
C	-1.706167	-0.472546	-0.003038
H	3.004779	0.032736	-0.630676
H	2.271777	0.963765	0.782488
H	0.396965	-0.637188	1.057024
H	-1.731498	1.822183	-0.149258
H	-2.484460	-1.216126	-0.029330

Frequencies

-1375.1904	186.7236	287.2656
422.1596	464.9455	548.7104
615.5553	646.6831	744.1127
839.5573	917.3098	964.0903
989.5611	1039.6923	1096.3970
1267.4929	1473.4221	1570.8701
1680.1714	1933.8307	3125.0068
3235.3625	3241.7157	3284.5634

Picture



ts i1_i2

T1 diagnostic: 0.02692907

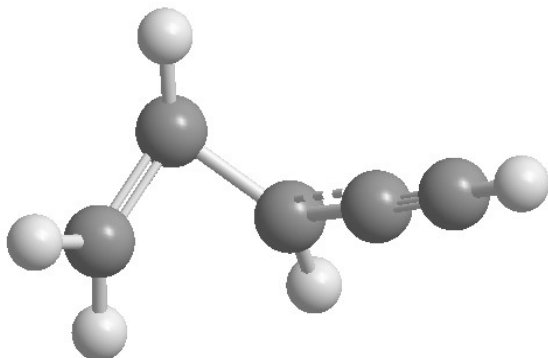
Geometries

C	-1.718473	-0.492460	-0.364056
C	-0.140547	0.669135	-0.152317
C	2.270871	-0.319331	0.001855
C	1.145357	0.123718	-0.091146
C	-1.226717	0.192294	0.726251
H	-2.014222	0.034256	-1.261535
H	-1.883698	-1.567620	-0.377650
H	-0.320744	1.497001	-0.824119
H	3.254012	-0.707631	0.074722
H	-1.018284	-0.296144	1.665061

Frequencies

-1043.4202	172.0304	210.3151
446.8276	509.2650	531.8574
665.6640	674.1642	717.3420
812.6538	962.8617	997.4077
1048.6699	1140.3042	1253.9657
1343.5534	1368.3165	1534.8172
2138.1148	3096.9546	3179.4165
3196.0259	3222.6038	3490.0517

Picture



ts i11_i14

T1 diagnostic: 0.02606897

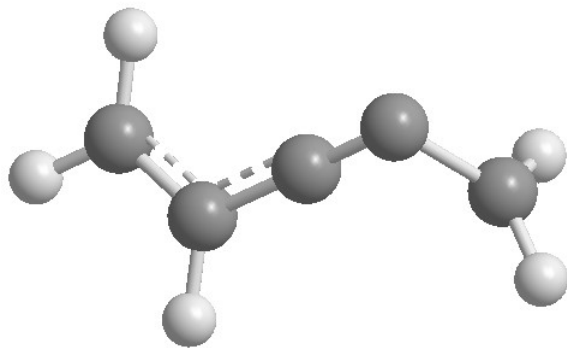
Geometries

C	-2.173350	-0.154614	0.284817
C	-1.099489	0.443688	-0.243953
C	1.291618	-0.740008	-0.353832
C	0.176249	-0.169153	-0.264484
C	2.090907	0.291305	0.340059
H	-3.150002	0.299886	0.213818
H	-2.095119	-1.116596	0.768650
H	-1.191397	1.406022	-0.731247
H	2.660560	0.999793	-0.239968
H	2.060350	0.383587	1.413099

Frequencies

-589.9383	84.4822	195.3701
245.6608	312.1805	497.6836
575.4250	697.5540	874.9070
985.4902	990.4175	1012.9882
1088.7257	1120.4654	1327.3914
1440.4842	1455.4493	1673.7017
1935.4278	3165.9611	3171.9315
3181.0078	3270.4678	3283.8650

Picture



ts i13_i16

T1 diagnostic: 0.02051995

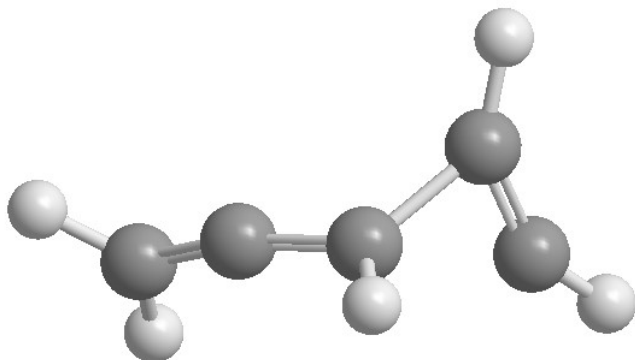
Geometries

C	2.138960	0.289953	-0.178427
C	1.009232	-0.291791	0.104846
C	-1.589922	0.753617	0.108678
C	-0.281143	-0.506412	0.475442
C	-1.429647	-0.382381	-0.473314
H	2.980592	-0.252477	-0.592247
H	2.284039	1.354105	-0.005139
H	-2.063982	1.712238	0.204980
H	-0.463602	-0.982482	1.429540
H	-1.821923	-1.009300	-1.260488

Frequencies

-739.5154	145.8352	202.2710
362.8557	429.9493	537.7785
621.3779	700.2608	832.9095
892.8502	896.5668	946.0401
997.0064	1090.7046	1171.1774
1320.3937	1453.2262	1712.0264
1862.6670	3085.8299	3170.4446
3171.2242	3191.2083	3298.1734

Picture



ts i12_i15

T1 diagnostic: 0.02380206

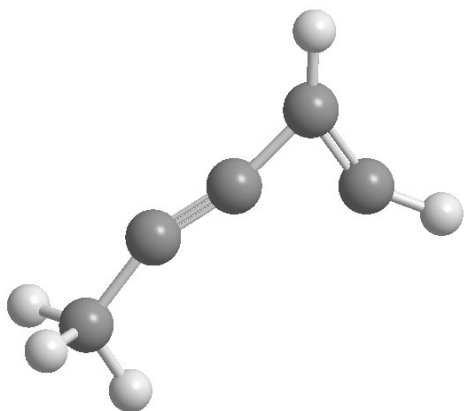
Geometries

C	2.299375	0.162098	0.000014
C	0.921764	-0.313448	0.000015
C	-1.729042	0.766009	-0.000060
C	-0.327028	-0.267922	0.000011
C	-1.721316	-0.538721	0.000019
H	2.842125	-0.181641	-0.880642
H	2.842049	-0.181426	0.880801
H	2.327603	1.255977	-0.000119
H	-2.315017	1.669902	-0.000114
H	-2.359275	-1.410908	0.000073

Frequencies

-718.4295	76.7569	143.7093
191.5862	380.6430	404.1702
530.7364	714.2761	789.0151
862.8847	1028.1759	1064.3354
1087.789	1254.6315	1416.9465
1481.1871	1492.8355	1649.3838
2001.6525	3016.3112	3080.3666
3102.7429	3185.0913	3252.1711

Picture



ts il_p7

T1 diagnostic: 0.01382931

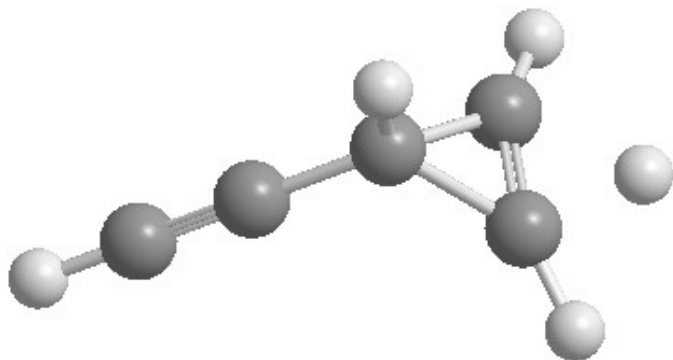
Geometries

C	1.349872	-0.380441	-0.516493
C	0.265737	-0.174631	0.524654
C	-2.278441	0.006804	-0.188683
C	-1.124373	-0.074791	0.131811
C	1.269923	0.811528	-0.014502
H	1.673155	-1.029702	-1.310828
H	0.417857	-0.600910	1.514654
H	-3.300028	0.081601	-0.473534
H	1.576498	1.842119	0.009605
H	2.736212	-1.423924	0.639378

Frequencies

-616.5486	186.5758	198.2671
248.5444	348.3348	536.1560
542.2296	666.3986	670.1151
706.0412	846.6387	878.9085
917.7373	953.4875	1024.8979
1053.7815	1174.1107	1378.8478
1676.5224	2243.1993	3116.1642
3282.4620	3326.0220	3485.7641

Picture



ts i1_p8

T1 diagnostic: 0.01615710

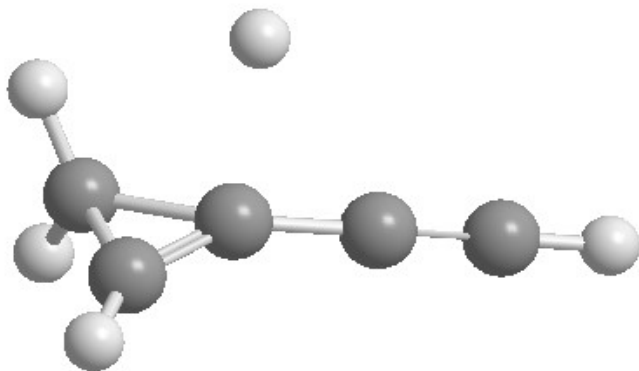
Geometries

C	1.529997	-0.690532	-0.131651
C	0.247320	0.093976	0.113722
C	-2.345514	-0.062505	-0.105696
C	-1.147722	0.028558	0.006774
C	1.340444	0.785442	-0.081752
H	1.969248	-1.216241	0.709221
H	1.686763	-1.165081	-1.095796
H	-3.398525	-0.133886	-0.205466
H	1.794801	1.748093	-0.218174
H	0.200562	-0.162517	2.001836

Frequencies

-943.6713	186.1818	229.5677
316.4004	461.2348	491.4509
513.0436	642.2301	660.1815
671.3160	737.8497	948.9295
1002.2534	1031.8016	1075.7561
1098.0491	1161.1577	1521.9348
1752.1995	2226.6426	3080.9658
3156.9525	3293.6895	3487.9571

Picture



ts i10_p9

T1 diagnostic: 0.01559292

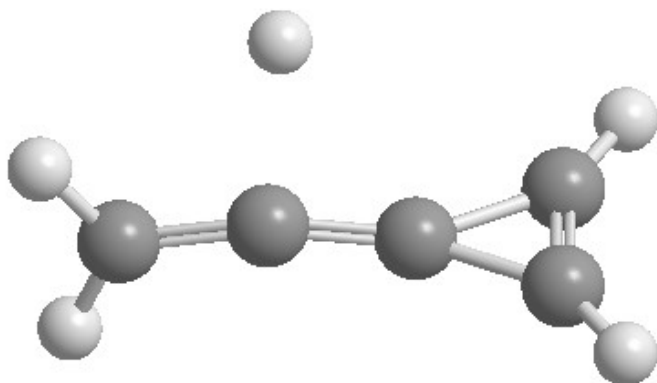
Geometries

C	-2.256407	0.000570	0.157083
C	-0.961216	-0.000545	-0.047384
C	1.622043	0.656593	0.040938
C	0.334938	-0.000097	0.076339
C	1.622494	-0.655988	0.043140
H	-2.959858	-0.000741	-0.664945
H	-2.668025	0.002677	1.159701
H	-0.884028	-0.006049	-2.160441
H	2.169857	1.580297	0.019707
H	2.170942	-1.579387	0.025287

Frequencies

-309.3236	106.3621	197.7339
231.7335	337.4205	456.3595
534.5494	663.5997	664.2071
727.5308	881.3269	883.8997
911.0040	982.2293	1047.1006
1065.2920	1368.2371	1511.8017
1654.3263	2047.9126	3125.3160
3202.7373	3268.1643	3311.2685

Picture



ts i16_i19

T1 diagnostic: 0.02304596

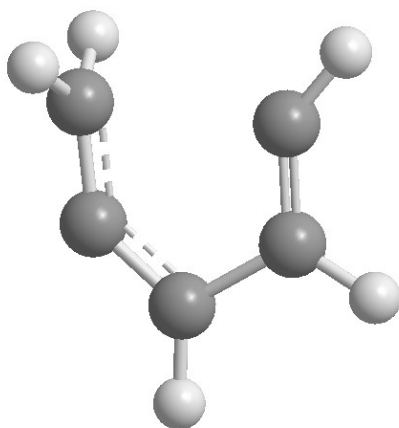
Geometries

C	1.503895	-0.464967	0.000035
C	0.916348	0.731515	0.000344
C	-0.325773	1.172860	-0.000316
C	-1.268334	0.025020	0.000494
C	-0.761882	-1.195062	-0.000309
H	1.867689	-0.904827	-0.921911
H	1.870570	-0.904304	0.921070
H	-0.656463	2.198549	-0.001631
H	-2.339623	0.200806	0.001259
H	-1.127687	-2.206425	-0.000278

Frequencies

-516.7104	259.0309	412.0885
531.1483	537.8356	670.5616
682.6664	827.3157	864.4459
877.6546	892.2048	980.6439
1003.4833	1119.2294	1218.8557
1318.4068	1471.6783	1626.1214
1812.8336	3126.2844	3143.8322
3203.0307	3235.2028	3277.6301

Picture



ts i2_i26

T1 diagnostic: 0.02496451

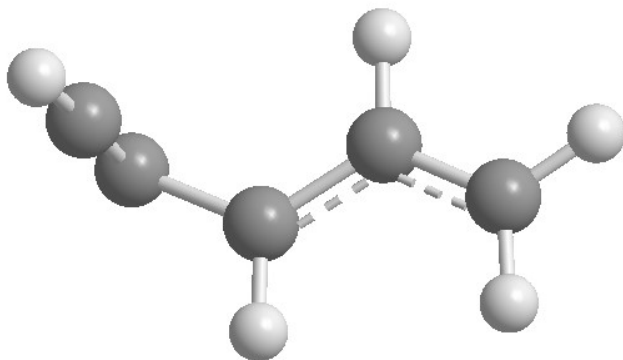
Geometry

C	-1.914845	0.448484	0.345831
C	-1.574433	-0.379726	-0.525538
C	-0.199298	-0.541733	0.046831
C	2.161195	0.068347	0.171034
C	0.901522	0.268172	-0.293007
H	-2.265114	1.146761	1.071846
H	-0.060125	-1.366318	0.732461
H	2.382411	-0.726607	0.869094
H	2.980633	0.689852	-0.152862
H	0.717346	1.075053	-0.991448

Frequencies

-540.0456	172.2925	181.8204
307.1668	514.2437	584.9689
611.5855	772.9987	846.9418
861.9288	919.8062	1020.1003
1079.2028	1194.7462	1294.4555
1310.2078	1445.1077	1559.0496
1791.1534	3166.7671	3176.9853
3188.5389	3265.2190	3415.5042

Picture



ts i26_i11

T1 diagnostic: 0.01713153

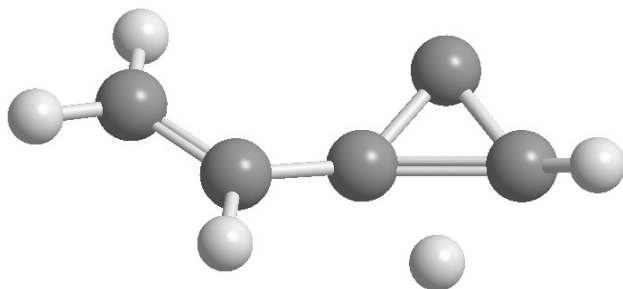
Geometry

C	-2.039955	0.302526	0.035813
C	-1.005114	-0.553595	0.047278
C	1.188129	0.946235	0.065818
C	0.330486	-0.121365	-0.226451
C	1.928091	-0.216095	0.004953
H	-3.047472	-0.049493	0.192299
H	-1.886253	1.357949	-0.130845
H	-1.171205	-1.610782	0.202774
H	2.600029	-0.729180	0.683051
H	1.095077	-1.114728	-0.511750

Frequencies

-1049.8406	141.4145	207.3997
278.6593	509.3009	625.0063
667.4253	716.1102	836.6230
933.0980	993.9990	1008.7216
1052.6738	1084.5635	1231.8492
1332.9762	1437.8799	1503.0949
1610.3938	2074.9269	3166.3054
3176.2113	3193.3054	3275.3672

Picture



ts i3_i27

T1 diagnostic: 0.01928282

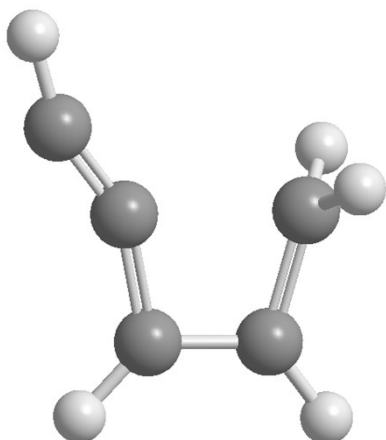
Geometry

C	-0.776093	-0.183286	-0.000022
C	-1.994824	0.055253	-0.000008
C	0.385167	-1.051586	-0.000079
C	0.743033	1.127952	0.000091
C	1.412195	-0.198422	-0.000003
H	-2.893332	0.623672	0.000030
H	0.358498	-2.132101	-0.000164
H	0.722778	1.708830	0.914439
H	0.722790	1.708964	-0.914172
H	2.472402	-0.408831	-0.000006

Frequencies

-772.9821	209.0868	290.1797
384.6357	521.9081	627.1501
651.8737	702.2964	771.3533
826.6283	955.8483	995.8478
1051.0702	1053.2206	1116.3505
1346.8890	1458.8070	1668.2784
1944.2604	3120.6194	3191.1548
3210.5740	3217.9852	3438.3643

Picture



ts i22_i28

T1 diagnostic: 0.02130402

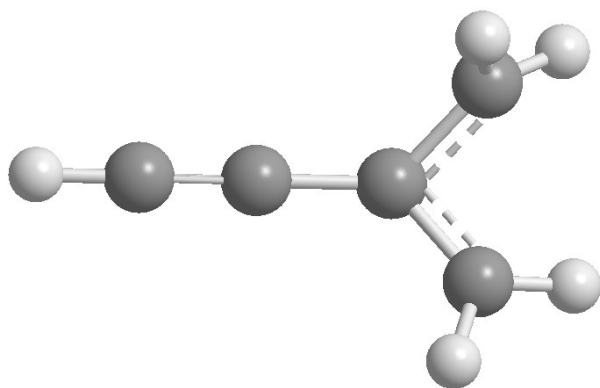
Geometry

C	-1.069167	0.009633	-0.084774
C	-2.270113	0.040856	0.041639
C	0.315881	-0.021749	-0.264863
C	1.297411	1.006789	0.086170
C	1.204520	-1.027286	0.062370
H	-3.326864	0.070735	0.153386
H	1.251441	1.463735	1.066734
H	2.066848	1.326396	-0.607369
H	0.953818	-1.840611	0.745428
H	2.183570	-1.069715	-0.401435

Frequencies

-999.5114	185.7387	209.3078
459.7152	548.3447	592.4644
606.6782	630.1529	687.5910
695.2653	813.0317	928.9764
963.8638	1045.4757	1277.1222
1418.9186	1443.0009	1540.1011
2152.3692	3101.5966	3150.0362
3217.7868	3265.4027	3480.5839

Picture



ts i10_i29

T1 diagnostic: 0.02815775

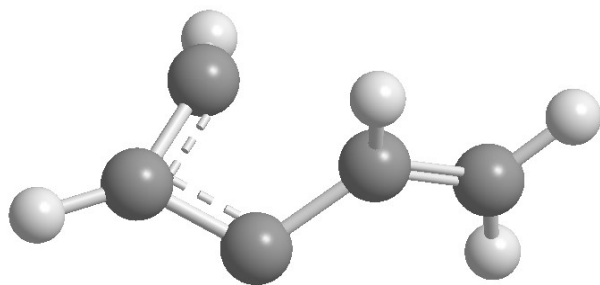
Geometry

C	-1.651532	-0.241497	0.021916
C	-0.418913	-0.812412	-0.167193
C	-0.944236	0.908670	-0.038688
C	1.957797	0.004030	-0.176896
C	0.711386	-0.094911	0.401353
H	-2.667516	-0.589684	-0.024162
H	-0.753814	1.637984	-0.813727
H	2.755903	0.522386	0.329868
H	2.145202	-0.396796	-1.160804
H	0.593208	0.242832	1.425869

Frequencies

-678.2539	228.4654	307.1963
474.5672	507.2519	533.8377
616.2877	757.3659	803.8439
888.2948	940.2319	980.2344
1091.4200	1152.7705	1180.4362
1267.5343	1387.7930	1493.2025
1546.1222	3137.2224	3176.7871
3179.3220	3271.4888	3278.8417

Picture



ts i29_i31

T1 diagnostic: 0.01939651

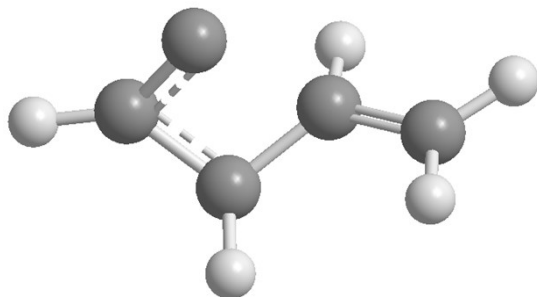
Geometry

C	-1.637310	0.011946	0.066133
C	-0.790223	-0.927434	-0.419068
C	-0.464208	0.810151	0.090074
C	1.903339	-0.002100	-0.159177
C	0.598444	-0.101177	0.416006
H	-2.695561	0.192335	0.052173
H	-0.285752	1.652705	-0.573569
H	2.730344	-0.557883	0.249887
H	2.068743	0.579451	-1.052820
H	0.521975	-0.614922	1.360524

Frequencies

-245.1127	319.9510	336.2429
362.2691	554.6089	627.8110
671.7263	791.3182	894.2474
945.0888	1005.0123	1049.4213
1150.9068	1206.9774	1254.8715
1321.5295	1421.3929	1496.5824
1499.7264	3114.1345	3180.3889
3217.9267	3288.5423	3292.2906

Picture



ts i29_i30

T1 diagnostic: 0.02684554

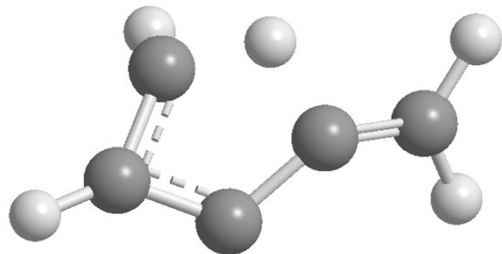
Geometry

C	1.643413	-0.263327	-0.001941
C	0.427527	-0.843263	0.094440
C	0.891519	0.924258	0.062259
C	-1.984089	-0.007627	0.103106
C	-0.683168	-0.122898	-0.331369
H	2.668944	-0.560672	-0.087669
H	0.657373	1.510606	0.941965
H	-2.414681	-0.764324	0.742226
H	-2.618718	0.787847	-0.252836
H	-0.064130	0.903689	-0.902659

Frequencies

-1459.7293	196.4741	293.7663
509.5945	525.7112	553.2648
578.0466	685.4901	727.4511
856.5511	967.6858	1043.9021
1069.1777	1126.6808	1194.3346
1281.0761	1404.4362	1492.5456
1530.5694	1922.4589	3167.5620
3169.3157	3268.8508	3311.5015

Picture



ts i31_i33

T1 diagnostic: 0.02010529

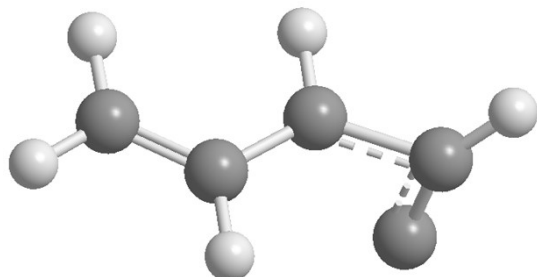
Geometry

C	1.688886	0.258471	0.339717
C	1.626213	-0.709267	-0.514295
C	0.267640	0.460775	-0.129003
C	-2.127462	0.040338	-0.068416
C	-0.856187	-0.294953	0.266222
H	2.290860	0.937696	0.915523
H	0.083772	1.354136	-0.717244
H	-2.334597	0.916556	-0.666135
H	-2.967377	-0.555615	0.252022
H	-0.667194	-1.184962	0.850483

Frequencies

-359.1631	178.0359	252.8069
296.3683	478.3374	592.1781
664.4845	817.2003	904.0376
920.5963	994.6866	1028.2385
1066.1074	1214.2377	1301.3404
1311.5181	1445.2635	1558.1708
1673.2099	3138.6095	3169.2325
3201.0543	3268.8062	3274.5277

Picture



ts i33_i16

T1 diagnostic: 0.02358839

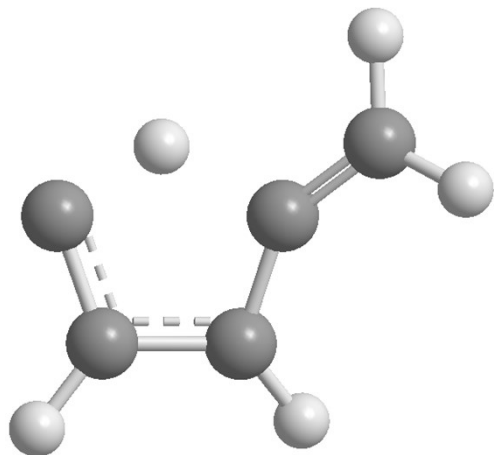
Geometry

C	1.500218	0.178565	0.160060
C	1.227221	-1.150002	-0.030091
C	0.350636	0.949039	-0.120929
C	-1.989092	-0.161453	0.110806
C	-0.708285	0.033743	-0.140714
H	2.479148	0.548656	0.439217
H	0.287860	1.997037	-0.393751
H	-2.489560	-1.084940	-0.154524
H	-2.570525	0.601173	0.621330
H	0.008880	-1.161275	-0.387064

Frequencies

-1258.8043	212.7251	284.6816
462.5362	508.0913	682.2782
745.4025	767.9988	865.9490
874.8737	937.7480	981.4520
1042.4108	1101.8657	1195.5201
1343.4698	1420.9942	1458.3992
1758.4450	1967.8499	3147.6620
3194.0963	3229.4672	3242.7114

Picture



ts i30_i32

T1 diagnostic: 0.01711198

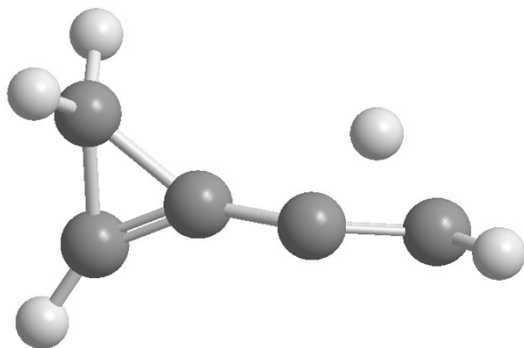
Geometry

C	-0.276931	-0.115597	-0.003586
C	1.072984	-0.022103	0.273240
C	-1.403442	-0.786596	-0.048508
C	-1.561692	0.692187	-0.030994
C	2.292200	-0.070774	-0.260658
H	1.662075	1.063272	0.051476
H	-1.893637	-1.730558	0.081457
H	-1.890170	1.194540	0.876676
H	-1.796663	1.226301	-0.946842
H	3.179689	0.063745	0.360273

Frequencies

-995.3089	141.9522	165.4104
338.2834	401.9353	610.2416
623.3587	731.6608	939.2789
965.0297	992.4894	1024.4896
1074.8326	1101.1422	1149.1888
1264.8072	1517.0249	1612.9380
1768.9726	2271.9832	3059.3814
3068.7980	3130.9289	3309.0770

Picture



ts i32_i1

T1 diagnostic: 0.01390449

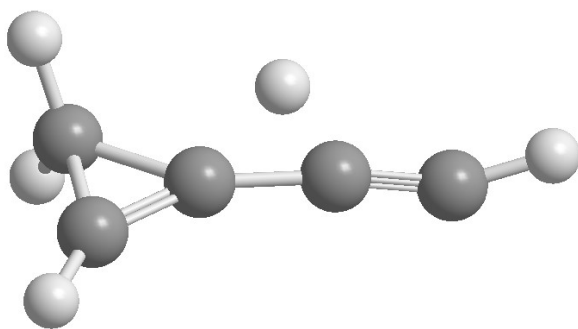
Geometry

C	-0.262989	-0.107536	0.045849
C	1.136201	-0.030791	0.035367
C	-1.421388	-0.773040	-0.042264
C	-1.530874	0.714017	-0.044551
C	2.354106	0.053928	-0.173658
H	0.516131	-0.038192	1.231525
H	-1.928175	-1.711758	-0.165175
H	-1.878805	1.235732	0.848590
H	-1.732286	1.244195	-0.976626
H	3.372799	0.130555	0.137232

Frequencies

-1869.9098	186.5982	226.6440
337.8426	455.3763	490.7980
565.4470	621.4371	668.7144
755.0737	964.1637	990.0516
1025.6036	1062.1249	1082.8262
1143.6054	1497.1373	1586.7547
1667.2162	2074.3457	3058.6658
3131.3784	3316.2477	3414.0840

Picture



ts i10_i2

T1 diagnostic: 0.01751694

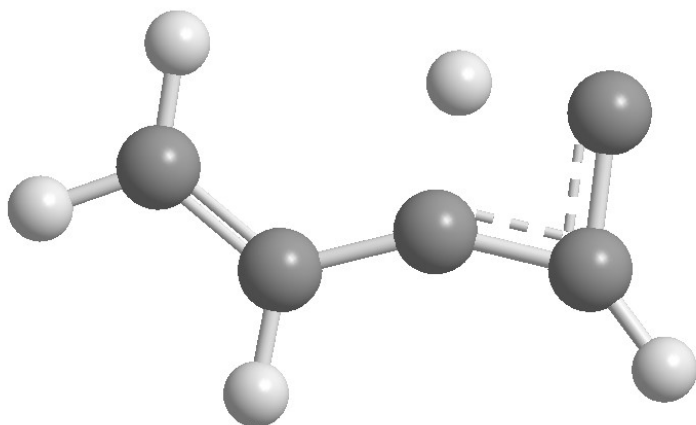
Geometry

C	1.639240	-0.472147	0.000095
C	1.784321	0.875514	-0.000170
C	0.298006	-0.168075	0.000136
C	-2.099841	0.348719	0.000036
C	-1.036250	-0.517912	-0.000094
H	2.294025	-1.320658	0.000095
H	-1.953115	1.418725	0.000291
H	-3.111366	-0.021479	-0.000127
H	-1.224438	-1.585913	-0.000351
H	0.482042	1.112737	0.000077

Frequencies

-656.1013	94.0761	267.5654
272.4187	548.9586	565.1989
658.7730	748.0923	780.7342
921.2701	936.8764	1005.6681
1061.4375	1173.5581	1234.6519
1394.6773	1403.9469	1535.7713
1629.3009	2217.6799	3157.6711
3174.9349	3277.8708	3317.1968

Picture



ts i30_i14

T1 diagnostic: 0.01361473

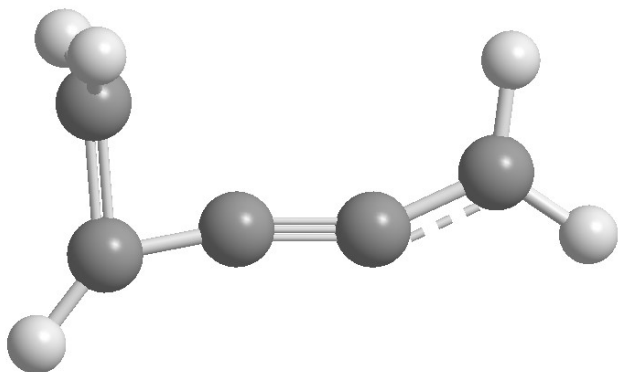
Geometry

C	2.279531	0.239299	0.000062
C	1.106102	-0.343349	-0.000061
C	-0.218438	-0.379792	-0.000081
C	-1.482986	-0.661802	-0.000002
C	-1.659130	0.793930	0.000001
H	2.374368	1.325507	0.000205
H	3.203166	-0.333253	0.000100
H	-2.110285	-1.543598	0.000282
H	-1.808350	1.330856	-0.930731
H	-1.809370	1.330767	0.930632

Frequencies

-732.4614	151.6608	172.5730
276.8421	345.1963	493.7912
569.2902	767.3543	785.6001
823.7509	913.1008	1008.6304
1050.6624	1074.2220	1227.0598
1435.9197	1466.4924	1720.9477
1992.9305	3099.2581	3130.4150
3186.3901	3206.2925	3237.9621

Picture



ts i31_i26

T1 diagnostic: 0.02010529

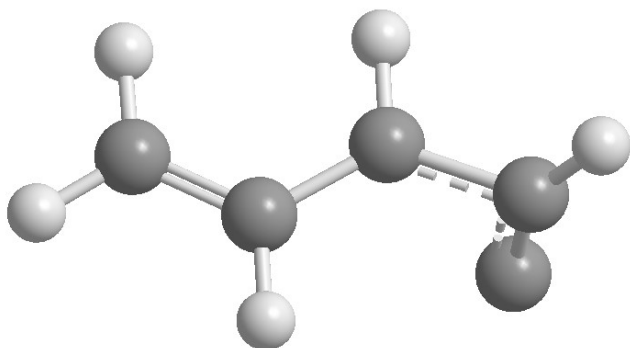
Geometry

C	1.688886	0.258471	0.339717
C	1.626213	-0.709267	-0.514295
C	0.267640	0.460775	-0.129003
C	-2.127462	0.040338	-0.068416
C	-0.856187	-0.294953	0.266222
H	2.290860	0.937696	0.915523
H	0.083772	1.354136	-0.717244
H	-2.334597	0.916556	-0.666135
H	-2.967377	-0.555615	0.252022
H	-0.667194	-1.184962	0.850483

Frequencies

-359.1631	178.0359	252.8069
296.3683	478.3374	592.1781
664.4845	817.2003	904.0376
920.5963	994.6866	1028.2385
1066.1074	1214.2377	1301.3404
1311.5181	1445.2635	1558.1708
1673.2099	3138.6095	3169.2325
3201.0543	3268.8062	3274.5277

Picture



ts i31_i16

T1 diagnostic: 0.02358839

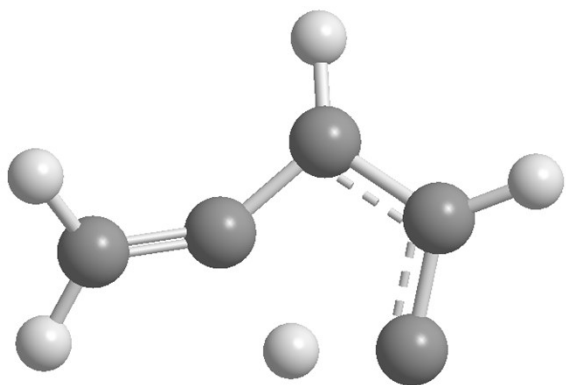
Geometry

C	1.500218	0.178565	0.160060
C	1.227221	-1.150002	-0.030091
C	0.350636	0.949039	-0.120929
C	-1.989092	-0.161453	0.110806
C	-0.708285	0.033743	-0.140714
H	2.479148	0.548656	0.439217
H	0.287860	1.997037	-0.393751
H	-2.489560	-1.084940	-0.154524
H	-2.570525	0.601173	0.621330
H	0.008880	-1.161275	-0.387064

Frequencies

-1258.8043	212.7251	284.6816
462.5362	508.0913	682.2782
745.4025	767.9988	865.9490
874.8737	937.7480	981.4520
1042.4108	1101.8657	1195.5201
1343.4698	1420.9942	1458.3992
1758.445	1967.8499	3147.6620
3194.0963	3229.4672	3242.7114

Picture



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