Supporting Information

Gas Phase Formation of Methyltriacetylene ($CH_3(C{\equiv}C)_3H$) - An Interstellar Molecule

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Experimental Procedures

Experimental: The reactions of 1-propynyl (CH_3CC; X^2A_1) with diacetylene (HCCCCH; $X^1\Sigma_g^+$) was studied under single collision conditions exploiting a universal crossed molecular beams machine at the University of Hawaii[1]. In the primary source chamber, the pulsed 1-propynyl molecular beam was produced by photodissociation of 1-bromopropyne (CH_3CCBr; 1717 CheMall, 95 %) seeded at a level of 0.5% in helium (99.9999 %; AirGas) at 193 nm (Complex 110, Coherent, Inc.) at 30 Hz and 20 mJ per pulse. This gas mixture - stored in a teflon-lined sample cylinder [2] - was regulated to 760 Torr and introduced into a piezoelectric pulsed valve operating at 60 Hz operated at pulse widths of 80 μs and peak voltages of -400 V. The pulsed 1-propynyl beam passes through a skimmer and is velocity selected by a four-slot chopper wheel rotating at 120 Hz. On-axis ($\Theta = 0°$) characterization of the primary beam determines a peak velocity v_p of 1769 ± 9 m s^{-1} and speed ratio S of 7.0 ± 0.3. The primary beam crosses perpendicularly the secondary supersonic beam of the hydrocarbon reactant generated in the secondary source chamber. A pulsed valve in the secondary source operated at a repetition rate of 60 Hz, a pulse width of 80 μs, and a peak voltage of -400 V, generated a pulsed molecular beam of diacetylene seeded in argon (99.9999%, AirGas) at fractions of 5% at 550 Torr. The diacetylene velocity distributions were determined to be v_p = 630 ± 15 m s^{-1} with S = 23.2 ± 0.3 resulting in a nominal collision energies E_C of 37.4 ± 0.4 kJ mol^{-1} and center-of-mass angles Θ_{CM} of 24.8 ± 0.5°. Diacetylene was produced using the procedure described previously.[3]

The machine operates a triply differentially pumped detector rotatable in the plane defined by both sources; this detector comprises of a Brink-type ionizer [4], a quadrupole mass spectrometer (QMS), and a Daly-type ion counter.[5] The neutral products formed in the reactive scattering process enter the detector and are ionized through electron impact at an electron energy of 80 eV at a current of 2.0 mA (ion flight constant = 5.88 ± 0.21 μs amu$^{-1/2}$) and then filtered according to mass-to-charge (*m/z*) ratios using the QMS (Extrel; QC 150) equipped with a 2.1 MHz oscillator. The ions are then accelerated by a negative 22.5 kV potential onto an aluminum coated stainless-steel target thus generating a cascade of secondary electrons that is directed toward an aluminum coated scintillator. The resulting signal is collected by a photomultiplier tube (PMT, Burle, Model 8850) operated at a negative potential of 1.35 kV. The signal output is discriminated at 1.6 mV (Advanced Research Instruments, Model F-100TD) and recorded by a multichannel scaler (MCS, SRS 430).

Time-of-flight (TOF) spectra were recorded at laboratory angles between $0° \le \Theta \le 69°$ with respect to the 1-propynyl radical beam ($\Theta = 0°$). The TOF spectra were then integrated and normalized to obtain the product angular distribution in the laboratory frame (LAB). To obtain the information on the reaction dynamics, a forward-convolution method is used to transform the LAB data into the center-of-mass frame (CM).[6-9] This represents an iterative method whereby user defined CM translational energy $P(E_T)$ and angular $T(\theta)$ flux distributions are varied until a suitable fit of the laboratory-frame TOF spectra and angular distributions are achieved. The CM functions comprise the reactive differential cross section $I(\theta,u)$, which is taken to be separable into its CM scattering angle θ and CM velocity u components, $I(u,\theta) \sim P(u)\times T(\theta)$. The differential cross section is plotted as a flux contour map that serves as an image of the reaction. Errors of the $P(E_T)$ and $T(\theta)$ functions are determined within the 1σ error limits of the accompanying LAB angular distribution while maintaining a good fit of the laboratory TOF spectra.

Reactive scattering signal was observed at mass to charge ratios (*m/z)* of 88 ($C_7H_4^+$), and 87 ($C_7H_3^+$) formally connected to the hydrogen loss reaction product, and the molecular hydrogen loss product, respectively. The time-of-flight spectra (TOF) recorded at these mass-to-charge ratios exhibited identical patterns after scaling with signal at m/z = 87 collected at a level of about 90 % of m/z = 88. These findings suggest that signal at m/z = 88 and 87 originate from the same reaction channel forming the heavy product (C_7H_4; 88 amu) along with atomic hydrogen (H; 1 amu); signal at m/z = 87 can be attributed to dissociative electron impact ionization of the C_7H_4 product in the electron impact ionizer. Therefore, having evidenced the hydrogen atom loss channel, the TOF spectra of the nascent C_7H_4 reaction product were collected at the best signal-to-noise ratio at *m/z* = 88 at distinct laboratory angles from 9.75° to 39.75° in 5° intervals with up to 2.9 × 10^6 TOFs per angle (Figure 1).

Theoretical: Geometries of the reactants, intermediates, transition states, and products of the 1-propynyl radical (CH_3CC; X^2A_1) reactions with diacetylene (HCCCCH; $X^1\Sigma_g^+$) were optimized using the density functional B3LYP/6-311G(d,p) level of theory.[10-11] Vibrational frequencies were computed at the same theoretical level and were utilized for the evaluation of zero-point vibrational energy corrections (ZPE) and in calculations of rate constants. The refinement of single-point energies was carried out employing the explicitly-correlated coupled clusters CCSD(T)-F12 method[12-13] with Dunning's correlation-consistent cc-pVTZ-f12 basis set.[14-15] The expected accuracy of this CCSD(T)-F12/cc-pVTZ-f12// B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p)) approach for relative energies is within 4 kJ mol-1 or better.[16] The GAUSSIAN 09[17] and MOLPRO 2010[15] program packages were employed for the electronic structure calculations. Rice-Ramsperger-Kassel-Marcus (RRKM) theory[18-20] was utilized to compute internal energy dependent rate constants for all unimolecular reaction steps on the C_7H_5 PES ensuing initial association of the 1-propynyl radical with diacetylene. For each intermediate or transition state, the numbers and densities of states were calculated within the harmonic approximation using B3LYP/6-311G(d,p) computed frequencies. Finally, RRKM rate constants were used to evaluate product branching ratios by solving first-order kinetic equations within steady-state approximation.[21]

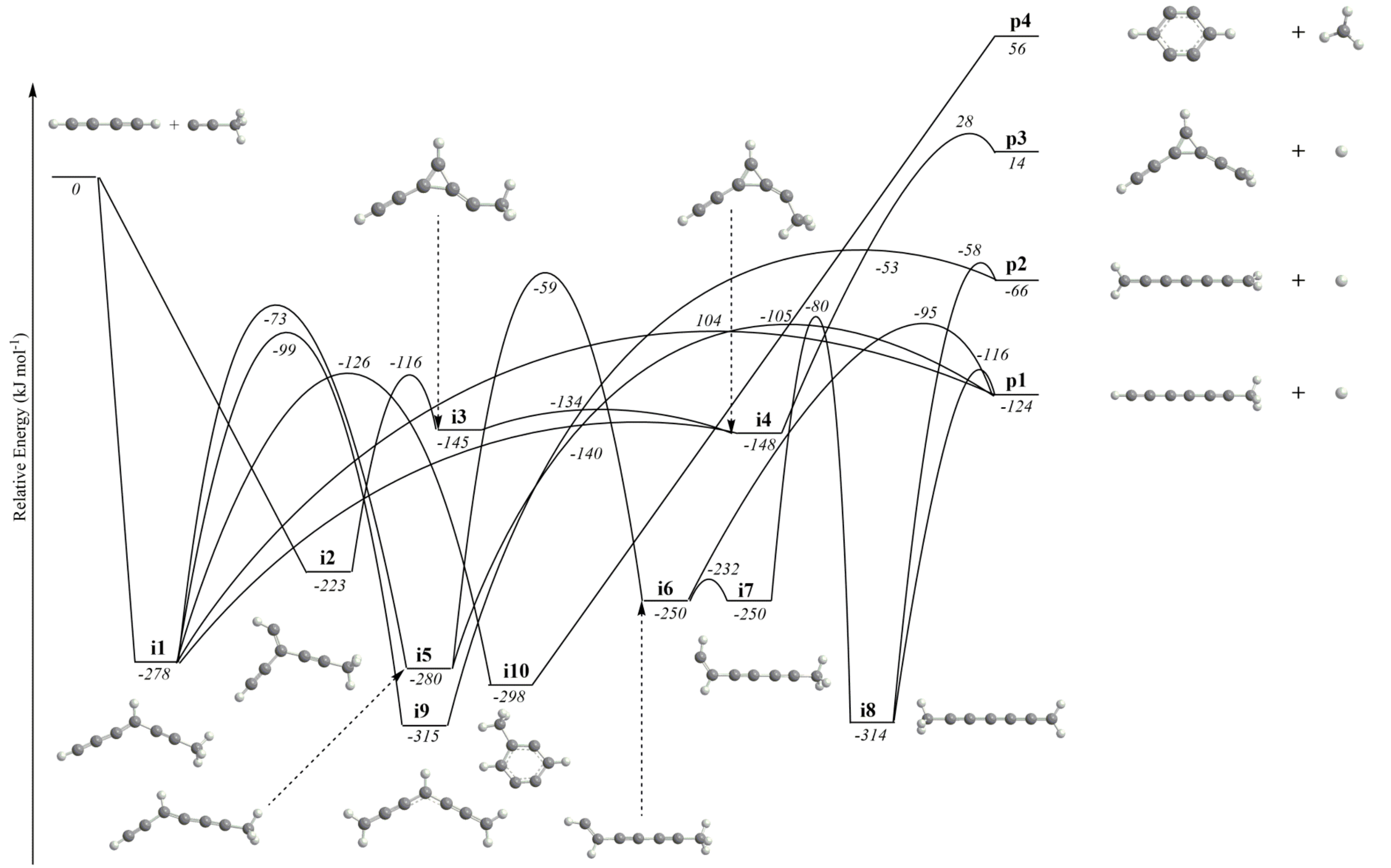

Figure S1. Schematic representation of the potential energy surface of the reaction of the 1-propynyl radical with diacetylene. All potential products are included in this PES. Energies calculated at the CCSD(T)-F12/cc-pVTZ-f12//B3LYP/6-311G(d,p) + ZPE(B3LYP/6-311G(d,p) level are shown in kJ mol^{-1} and are relative to the energy of the separated reactants. . The geometries of the transition states, reactants, intermediates, and products and their point groups and the symmetries of their electronic wave functions are compiled in the Supporting Information.

Optimized Cartesian coordinates (in Å) and calculated vibrational frequencies (in cm^{-1}) of the reactants, products, intermediates, and transition states in the 1-propynyl plus diacetylene reaction; point groups and electronic ground states are also given.

Reactants

C_4H_2, $D_{\infty h}$, $^1\Sigma_g^+$

C	0.000000	0.000000	0.682599
C	0.000000	0.000000	-0.682594
C	0.000000	0.000000	-1.889128
C	0.000000	0.000000	1.889123
H	0.000000	0.000000	-2.951424
H	0.000000	0.000000	2.951423

Frequencies:

235.4017	235.4017	526.9751
526.9751	661.6801	661.6801
661.9824	661.9824	916.8738
2110.6131	2284.9415	3476.6882
3478.5891		

C_3H_3, C_{3v}, $^2A_1$

H	0.000000	1.021621	-1.512622
C	0.000000	0.000000	-1.133496
C	0.000000	0.000000	0.336404
H	0.884750	-0.510811	-1.512622
H	-0.884750	-0.510811	-1.512622
C	0.000000	0.000000	1.553404

Frequencies:

125.	125.	934.
1009.	1009.	1410.
1479.	1479.	2190.
3054.	3133.	3133.

Intermediates

i1, C_1, ^2A

C	1.065779	0.431318	-0.011844
C	2.178298	-0.037989	-0.005882
C	3.516978	-0.608929	0.004512
H	3.584776	-1.470765	-0.666024
H	4.263958	0.123539	-0.314724
H	3.792718	-0.948926	1.007735
C	-2.578731	-0.181104	0.001030
C	-1.362749	0.314010	0.000857
C	-0.234227	1.000944	0.003617
C	-3.696846	-0.703061	0.000021
H	-0.284916	2.094439	0.018880
H	-4.687542	-1.089421	0.000270

Frequencies:

16.9601	33.1692	155.8254
195.1383	199.9585	239.5419
322.9392	387.6291	392.3330
492.3148	502.1028	564.7772
761.0747	790.1962	924.1747
1056.2134	1063.2680	1205.8193
1335.7553	1429.2927	1493.2768
1493.4445	1775.2299	1984.6189
2326.2520	3025.7314	3045.8332
3078.9014	3085.6590	3458.2123

i2, C_1, ^2A

C	0.588934	0.239174	0.003163
C	1.755982	-0.060658	0.000494
C	3.167717	-0.415289	-0.001367
C	-1.758267	-0.510741	0.000598
C	-0.805679	0.565777	0.000813
C	-1.243286	1.823447	-0.001239
C	-2.565977	-1.403380	-0.000489
H	3.303386	-1.491808	-0.137432
H	3.701664	0.093847	-0.808996
H	3.646691	-0.135004	0.941437
H	-2.213613	2.299832	-0.003621
H	-3.274677	-2.196844	-0.003218

Frequencies:

9.1256	87.8113	143.4763
198.6817	276.5457	312.7649
380.3582	451.1555	546.5839
585.5431	631.2393	651.1470
662.0628	667.0239	863.8363
1000.4976	1058.3508	1062.5012
1261.5207	1428.8386	1493.5633
1493.9333	1588.8052	2198.7378
2343.9427	3029.2842	3084.1912
3088.9119	3242.9336	3466.6772

i3, C_s, $^2A'$

C	0.586744	0.239928	-0.000173
C	1.630704	-0.520007	0.000165
C	3.099433	-0.535140	0.000180
C	-2.133071	-0.217630	-0.000177
C	-0.892056	0.402617	-0.000269
C	-0.150625	1.493154	-0.000179
C	-3.186055	-0.806618	0.000015
H	3.506502	-1.044184	-0.880437
H	3.504647	0.488704	-0.002240
H	3.506471	-1.040510	0.882747
H	-0.127719	2.573690	0.000390
H	-4.120352	-1.315517	0.002161

Frequencies:

91.0580	109.4764	141.6417

191.2408	228.8648	354.3406
363.1309	508.8800	578.1514
607.5042	623.1086	636.9899
724.7684	755.1910	951.1125
995.4194	1038.4786	1059.9148
1161.5298	1416.8495	1477.7789
1499.7935	1699.7411	1881.3870
2198.5717	2964.2051	3035.2914
3055.0517	3231.5053	3466.2181

i4, C_s, $^2A'$

C	0.670198	0.678977	-0.000465
C	1.862669	0.189618	0.000140
C	2.648911	-1.049603	0.000037
C	-0.316410	1.717122	0.000172
H	1.990062	-1.931239	0.000044
H	3.294166	-1.128125	-0.881705
H	3.294201	-1.128163	0.881756
H	-0.505175	2.781973	-0.000074
C	-1.928640	-0.349408	-0.000013
C	-0.846913	0.510335	0.000139
C	-2.829491	-1.154579	-0.000003
H	-3.635200	-1.849217	-0.000062

Frequencies:

84.7527	107.7129	183.8574
200.6332	208.8622	367.6492
404.5045	491.1747	497.8228
570.4074	602.7210	616.7733
746.1006	765.9679	911.4653
1011.1464	1035.7289	1061.1096
1193.2966	1416.9707	1478.0458
1498.8104	1709.2787	1886.2263
2184.4088	2970.5812	3037.7256
3056.1576	3222.7098	3465.8821

i5, C_1, ^2A

C	-1.055638	0.155566	-0.000297
C	-2.268735	-0.076172	0.000139
C	-3.696662	-0.324183	-0.000119
C	2.644392	-0.050056	-0.001361
C	1.490997	0.779786	0.000271
C	0.245858	0.336957	-0.000341
C	3.650228	-0.714428	0.000716
H	-4.269499	0.601392	-0.129007
H	-3.980083	-1.004794	-0.810145
H	-4.015664	-0.782578	0.941860
H	1.676214	1.858600	0.002237
H	4.526398	-1.317444	0.001013

Frequencies:

24.6765	30.7555	125.5764
144.0345	240.2784	295.2120
351.1830	374.2092	477.2877

525.7535	577.2768	645.0432
729.4263	779.2371	965.6809
1034.9688	1045.7712	1158.0007
1349.1549	1423.2551	1479.8116
1485.2992	1827.6293	2082.2822
2197.6819	3008.6362	3046.5052
3058.7468	3070.6437	3466.4883

i6, C_1, ^2A

C	1.159737	-0.049332	-0.000185
C	2.367882	0.032437	-0.000134
C	3.817416	0.129676	0.000147
C	-2.819006	-0.356260	0.000107
C	-1.409283	-0.212209	-0.000032
C	-0.197505	-0.139888	-0.000135
C	-3.696496	0.631029	0.000030
H	4.143145	1.173229	-0.047069
H	4.242499	-0.311923	0.906765
H	4.248388	-0.393791	-0.858850
H	-3.195759	-1.387317	0.000282
H	-4.774743	0.707092	0.000094

Frequencies:

14.6345	79.5359	98.0124
188.8375	241.8283	336.1844
381.6029	471.0878	567.2273
600.4497	606.3214	666.4074
817.4082	848.7623	998.8809
1054.9299	1055.8084	1267.6083
1306.3951	1427.8950	1490.0375
1490.2633	1632.4584	2251.8107
2346.2656	3014.8176	3024.1037
3080.2539	3081.8150	3240.0020

i7, C_s, $^2A'$

C	-1.128585	-0.068265	0.000065
C	-2.335520	0.031532	0.000122
C	-3.783494	0.149323	-0.000077
C	2.851681	-0.409926	-0.000047
C	1.437419	-0.280663	-0.000005
C	0.226813	-0.180317	0.000015
C	3.678417	0.621680	0.000006
H	-4.094275	1.198497	-0.002577
H	-4.218433	-0.329588	-0.882713
H	-4.218326	-0.325340	0.884904
H	3.256792	-1.423634	-0.000048
H	3.593855	1.699880	-0.000045

Frequencies:

8.1170	79.5490	99.3777
181.1229	246.3651	328.0192
387.6033	460.9416	573.3242
603.3389	606.7628	689.5843
867.9538	887.5925	987.8669

1054.7581	1055.6266	1274.9963
1304.0858	1427.8184	1489.9720
1490.0067	1611.4865	2245.0214
2342.6059	3024.3009	3080.7632
3081.7786	3092.0111	3235.6214

i8, C_s, $^2A'$

C	-1.211207	-0.000193	-0.000004
C	-2.433993	-0.001012	0.000014
C	-3.884343	0.000978	-0.000025
C	2.671681	0.000109	-0.000001
C	1.374881	0.000027	-0.000002
C	0.122180	0.000025	-0.000004
C	3.981850	0.000155	0.000000
H	-4.283281	1.020837	-0.015047
H	-4.279074	-0.523939	-0.875967
H	-4.278867	-0.497780	0.891149
H	4.557499	-0.924590	-0.000005
H	4.557432	0.924942	0.000000

Frequencies:

5.2107	74.8472	79.3800
169.2017	203.8291	245.8307
350.2162	433.0485	523.3713
540.9471	671.8278	749.2967
853.1629	939.4070	998.6573
1044.3664	1048.3613	1292.9888
1423.8507	1462.7332	1483.6940
1486.6690	1866.8566	2004.1041
2201.5540	3015.7048	3069.0334
3074.9203	3081.0282	3144.4765

i9, C_{2v}, $^2B_1$

C	-1.207201	0.436715	-0.003413
C	-2.322728	-0.117049	-0.001177
C	2.323718	-0.114134	-0.000681
C	1.210805	0.444901	-0.004716
C	-0.000248	1.074700	0.001207
C	3.513167	-0.720075	0.002349
H	-0.004823	2.165501	0.009737
H	4.437558	-0.151877	0.014146
C	-3.515408	-0.716870	0.002183
H	3.593510	-1.802091	-0.006918
H	-4.435794	-0.142392	0.009609
H	-3.603080	-1.798259	-0.001088

Frequencies:

67.7410	174.3476	194.9314
202.1207	310.6131	383.5353
398.8220	408.3762	499.7314
529.2594	538.4328	793.8701
794.7368	843.1463	846.1131
890.4090	1039.6600	1040.3754
1306.1223	1373.9989	1443.8115

1516.6858	1586.7844	1897.1573
2165.2069	3101.8476	3130.4244

i10, C_s, $^2A'$

C	0.119960	-1.100378	-0.000021
C	-0.811885	-0.065415	-0.000041
C	-2.298370	-0.338186	0.000022
C	1.089290	1.264653	0.000031
C	1.839498	0.254947	0.000025
C	1.501428	-1.092998	0.000000
C	-0.297228	1.255014	-0.000030
H	-2.866837	0.593798	-0.000193
H	-2.596671	-0.913281	-0.880571
H	-2.596638	-0.912794	0.880958
H	2.151684	-1.957397	-0.000027
H	-0.947698	2.123851	-0.000080

Frequencies:

44.7443	228.0453	329.0273
377.9542	461.8788	467.7346
587.2497	629.0201	636.7130
818.8369	857.9688	882.0181
1005.0942	1036.0164	1064.3765
1203.1736	1234.9866	1299.3847
1337.0581	1380.7806	1428.9025
1484.2687	1502.8994	1515.2337
1832.3831	3038.5243	3091.1349
3111.4161	3173.3498	3211.2221

Transition states

i1-i5, C_1, ^2A

C	-1.121502	0.124109	-0.000153
C	-2.327635	-0.054319	-0.000153
C	-3.757422	-0.305968	-0.000303
C	2.732407	-0.134180	0.000051
C	1.483071	0.401474	0.000044
C	0.187491	0.485488	0.000070
C	3.907083	-0.454929	-0.000032
H	-4.042153	-0.965135	-0.826834
H	-4.069389	-0.792761	0.929409
H	-4.333248	0.620486	-0.099273
H	0.912189	1.571003	-0.000343
H	4.911638	-0.803636	-0.000097

Frequencies:

2166.7370*i*	30.7065	65.7473
133.7782	179.4640	203.5530
302.4288	319.0306	422.7015
426.8480	467.4408	504.9228
524.4157	552.2882	625.0096

918.5122	1048.8415	1050.8844
1259.2649	1426.1919	1484.8599
1490.4136	1927.6621	2127.5531
2208.6715	2250.7245	3015.1798
3066.4993	3074.6259	3465.0316

i1-i9, C_s, $^2A'$

C	-0.394879	-1.358875	-0.000006
C	0.820029	-1.203505	-0.000005
C	-0.595258	1.354116	0.000003
C	-1.617296	0.532438	0.000008
C	-1.720401	-0.806185	-0.000001
C	0.581535	1.846661	-0.000006
H	-2.631879	-1.389756	-0.000003
H	1.034684	2.825216	-0.000015
C	2.063085	-0.540443	0.000005
H	1.456716	0.780266	-0.000004
H	2.659778	-0.580475	0.910430
H	2.659807	-0.580491	-0.910399

Frequencies:

1941.6252*i*	142.1173	231.5409
262.9811	396.8915	402.5324
478.9982	489.2567	522.2428
573.3698	616.4711	631.4258
837.0788	842.0769	877.2258
989.8234	1032.3644	1068.3436
1170.5447	1216.3873	1316.5913
1385.8623	1473.4876	1609.7534
1884.0135	2150.9758	3082.4587
3151.8664	3202.7149	3266.4124

i1-i4, C_s, $^2A'$

C	0.728533	0.708381	-0.000011
C	1.864752	0.147433	-0.000005
C	2.723429	-1.035186	0.000010
C	-0.303316	1.677158	0.000011
H	2.123401	-1.956746	-0.001171
H	3.372664	-1.068884	-0.881310
H	3.371039	-1.070049	0.882479
H	-0.462661	2.749528	0.000039
C	-1.995901	-0.327391	-0.000008
C	-0.922468	0.518483	-0.000014
C	-2.882068	-1.155205	0.000007
H	-3.682219	-1.855888	0.000025

Frequencies:

523.3263*i*	79.0613	84.7514
186.8452	191.9693	203.9943
378.3146	388.2790	479.4667
504.8925	544.9863	617.6451
720.5008	760.2831	838.3174
1023.5026	1062.2163	1071.8301
1244.9596	1420.0288	1480.7964

1494.7300	1761.1637	1931.7538
2146.4950	2979.5490	3042.2825
3061.5947	3182.6404	3465.7071

i1-i10, C_s, $^2A'$

C	-0.004877	-1.165356	-0.000763
C	0.972083	-0.371925	-0.000980
C	2.430400	-0.140265	0.000631
C	-1.247649	1.242838	0.000336
C	-1.932670	0.110465	0.000351
C	-1.421699	-1.148428	0.000193
C	-0.000800	1.487397	-0.000228
H	2.744160	0.450158	-0.864501
H	2.750119	0.392281	0.900636
H	2.965880	-1.091395	-0.032510
H	-2.020492	-2.052469	0.000957
H	0.791610	2.213073	-0.001823

Frequencies:

663.0328*i*	8.4973	151.0288
239.0487	322.4324	391.8447
427.5116	480.2970	519.1383
581.2996	671.9872	743.1912
749.6689	867.1167	1045.1186
1063.9994	1097.9312	1173.8427
1281.7518	1424.6944	1498.8291
1501.4314	1528.1678	1681.9786
1967.6819	3034.9630	3087.3792
3105.6189	3179.9531	3317.3562

i1-p1, C_1, ^2A

C	1.127576	0.076271	0.000064
C	2.332862	-0.038302	0.000027
C	3.777370	-0.184067	-0.000090
C	-2.785657	-0.091619	0.000004
C	-1.439729	0.007270	0.000063
C	-0.227880	0.221200	0.000069
C	-3.993235	-0.195552	-0.000068
H	4.271185	0.791600	-0.037230
H	4.120846	-0.699519	0.901919
H	4.114402	-0.763698	-0.864788
H	-5.053355	-0.281506	-0.000136
H	-0.200914	2.181917	-0.000178

Frequencies:

763.8169*i*	13.7365	81.6720
97.7214	194.2062	203.2292
350.3699	351.4654	421.2428
481.1197	495.9267	508.1606
540.0244	571.5621	586.1670
607.4013	950.6914	1054.1970
1055.2827	1309.6736	1426.5612
1487.2378	1487.8620	2101.3253
2205.2047	2321.6930	3026.2094

3084.1057	3084.8133	3466.0517

i2-i3, C_s, $^2A'$

C	0.546200	0.152009	0.000018
C	1.680628	-0.364454	0.000031
C	3.125017	-0.548430	-0.000014
C	-2.058211	-0.296340	-0.000003
C	-0.855860	0.441111	0.000008
C	-0.364309	1.659352	-0.000003
C	-3.071283	-0.946281	-0.000009
H	3.465000	-1.099987	-0.883018
H	3.644346	0.420190	-0.000715
H	3.465204	-1.098843	0.883618
H	-0.617826	2.713022	-0.000039
H	-3.969817	-1.516184	-0.000012

Frequencies:

688.5395*i*	83.4886	90.8143
129.9190	180.6322	242.2365
352.2951	352.8924	468.2758
516.6810	614.0408	638.7890
659.8759	683.3316	802.7040
893.5548	1031.5222	1064.2893
1251.0281	1424.5697	1485.0254
1493.0265	1707.1584	2018.7588
2215.0789	2987.2576	3043.3856
3064.1268	3194.9646	3465.1310

i5-p1, C_s, $^2A'$

C	1.150700	-0.003459	-0.000007
C	2.364374	-0.044934	0.000030
C	3.814427	-0.091032	0.000007
C	-2.763348	-0.055129	-0.000003
C	-1.418698	0.176499	-0.000012
C	-0.197340	0.030318	-0.000015
C	-3.956282	-0.247487	0.000009
H	4.239639	0.916870	-0.033207
H	4.192611	-0.584377	0.900580
H	4.190752	-0.641786	-0.867472
H	-1.581720	2.149625	0.000019
H	-5.004278	-0.428985	0.000020

Frequencies:

731.0964*i*	12.8318	79.5577
89.0777	213.2537	215.7935
324.1267	346.4300	433.3086
485.3104	489.3824	524.7477
564.9965	587.7518	598.4188
611.2400	945.4817	1050.8709
1052.3551	1315.4737	1425.7136
1485.4554	1485.9104	2108.3340
2237.0226	2288.2098	3024.5416
3082.0303	3083.6147	3468.1323

i5-i6, C_1, ^2A

C	-1.173757	-0.027410	-0.001251
C	-2.393263	-0.014521	-0.001076
C	-3.844172	-0.004098	0.000166
C	2.770944	0.026490	0.000205
C	1.407833	0.041535	-0.000372
C	0.165590	-0.060395	-0.000889
C	3.997623	-0.198243	0.000704
H	-4.231902	-0.048813	1.022932
H	-4.239665	0.905003	-0.464606
H	-4.249707	-0.862789	-0.544839
H	2.130540	1.269151	0.000314
H	5.005944	0.157297	0.001277

Frequencies:

1673.3736*i*	13.1061	71.4829
81.4212	202.7146	212.8781
307.3142	354.7452	429.7530
481.2853	506.3539	533.2315
576.8405	652.6115	703.0327
941.2242	1047.390	1049.3471
1270.3722	1336.9459	1425.8134
1483.5781	1488.7677	1916.1769
2169.9029	2228.7871	3017.6497
3070.9621	3076.4488	3384.4642

i9-p2, C_s, $^2A'$

C	-1.276427	-0.004462	-0.000036
C	-2.541073	-0.072801	-0.000007
C	2.545137	-0.055974	-0.000001
C	1.279688	0.054845	0.000000
C	0.002545	0.176756	-0.000013
C	3.852388	-0.177174	0.000008
C	-3.855668	-0.156661	0.000022
H	4.502661	0.693739	0.000390
H	4.333262	-1.151797	-0.000362
H	-4.422134	-0.191314	-0.926708
H	-4.422038	-0.192173	0.926777
H	-0.031290	2.254373	0.000070

Frequencies:

676.1884*i*	81.1843	84.2099
120.0900	198.8026	209.4785
335.2075	338.4487	387.6442
487.1224	489.2021	526.2456
542.4297	570.0517	591.6102
832.2819	848.2197	1017.4115
1017.6786	1057.7982	1391.4815
1452.8267	1553.8309	1889.6720
2090.4728	2167.7123	3114.3216
3115.5484	3187.8182	3190.1887

i3-i4, C_s, $^2A'$

C	-0.620464	0.494445	0.000052
C	-1.720215	-0.141630	0.000718
C	-3.026510	-0.776469	-0.000178
C	2.086972	-0.297816	-0.000026
C	0.933333	0.459100	-0.000099
C	0.289722	1.608363	-0.000133
C	3.042035	-1.039631	-0.000010
H	-3.181471	-1.398611	0.889324
H	-3.842443	-0.037550	-0.013313
H	-3.170950	-1.417715	-0.877907
H	0.387779	2.687006	-0.000071
H	3.897854	-1.671299	0.000023

Frequencies:

177.5715*i*	39.8941	105.8832
162.1455	188.6793	283.5667
330.8928	359.0940	491.9589
543.4288	579.0637	621.1727
681.3503	749.6798	868.0998
1007.0817	1017.6508	1053.5101
1195.8446	1425.7334	1485.1265
1487.7671	1741.6189	1940.9362
2173.6865	2959.7322	3015.3107
3043.6737	3196.2293	3464.9838

i4-p3, C_s, $^2A'$

C	-0.603977	0.537091	-0.000027
C	-1.757350	-0.034200	-0.000089
C	-2.906117	-0.681103	-0.000010
C	2.000624	-0.333202	-0.000005
C	0.864932	0.479835	-0.000010
C	0.295599	1.663478	0.000054
C	2.953689	-1.065058	-0.000012
H	-3.437510	-0.890295	0.924376
H	-3.437676	-0.890295	-0.924299
H	0.408040	2.735941	0.000167
H	3.801946	-1.709084	-0.000011
H	-2.419193	-2.647312	0.000369

Frequencies:

594.5374*i*	87.7467	179.5522
193.8927	204.0884	271.1106
330.2406	370.2918	456.3706
513.1402	596.7065	667.4443
681.2561	699.9287	752.0023
795.0656	798.6954	951.5540
1014.4546	1048.0755	1049.4278
1364.6260	1521.2654	1791.5220
2115.0929	2259.5792	3124.9193
3202.3272	3286.3186	3478.3217

i6-p1, C_1, ^2A

C	1.184012	-0.000528	-0.000155
C	2.395665	-0.020490	-0.000105
C	3.847106	-0.043064	0.000094
C	-2.754478	0.071489	0.000029
C	-1.387969	0.036133	-0.000071
C	-0.171305	0.021764	-0.000129
C	-3.923822	-0.297476	0.000100
H	4.225544	-1.037095	-0.256731
H	4.251595	0.667841	-0.726766
H	4.244157	0.222495	0.984570
H	-2.871464	1.924734	0.000170
H	-4.985081	-0.384949	0.000179

Frequencies:

903.2777*i*	19.7847	80.2361
84.5029	204.6815	214.1064
348.3428	361.4078	454.9110
511.5358	513.4597	524.6757
593.6112	616.9017	633.3652
646.6891	947.4316	1053.5283
1054.5698	1309.5423	1426.6511
1487.4787	1487.7608	2036.5458
2262.1985	2331.0389	3025.7253
3083.8773	3084.2592	3447.6292

i6-i7, C_s, $^2A'$

C	1.150049	-0.057388	-0.000217
C	2.357273	0.037228	-0.000149
C	3.805816	0.149770	0.000179
C	-2.834188	-0.396156	0.000142
C	-1.417332	-0.250685	-0.000077
C	-0.206317	-0.163736	-0.000188
C	-3.688569	0.597776	0.000064
H	4.121029	1.196473	-0.049537
H	4.235425	-0.285159	0.907920
H	4.242613	-0.371327	-0.857348
H	-3.199482	-1.432198	0.000422
H	-4.399972	1.391356	0.000017

Frequencies:

735.7153*i*	15.2514	78.9950
99.1656	185.7109	245.9310
334.7818	390.1143	473.6338
578.0483	600.5196	615.5885
637.0478	802.5317	958.6375
1054.9316	1055.9190	1277.2957
1297.1699	1427.9286	1490.2422
1490.4991	1621.6150	2247.4112
2345.3627	2992.5362	3023.6911
3079.7410	3081.0872	3429.6408

i7-i8, C_1, ^2A

C	-1.200899	-0.006923	-0.000164
C	-2.416054	-0.008798	-0.000372
C	-3.867641	-0.012243	-0.000406
C	2.721942	0.117418	0.000616
C	1.375948	-0.041238	0.000257
C	0.148537	-0.001571	0.000159
C	4.000907	-0.084363	0.000327
H	-4.261175	-0.712176	-0.744314
H	-4.258485	-0.313083	0.976745
H	-4.269743	0.979951	-0.228826
H	3.454802	1.141933	-0.002790
H	4.758156	-0.870321	-0.003313

Frequencies:

2153.1943*i*	7.9330	65.7158
77.8369	89.9036	195.4768
208.8072	313.4260	357.3454
446.8857	510.3992	524.1785
529.6350	606.0483	816.8792
926.9979	1051.5524	1052.5872
1295.0528	1425.9108	1486.2746
1489.1246	1875.2817	2171.8769
2262.5391	2294.3204	3020.4744
3064.7419	3075.5912	3078.3686

i8-p2, C_s, $^2A'$

C	-1.183052	-0.079892	-0.000277
C	-2.452074	-0.114262	-0.000074
C	-3.767688	-0.135775	0.000334
C	2.647989	0.022324	-0.000037
C	1.374016	-0.011165	-0.000259
C	0.097682	-0.044533	-0.000340
C	3.956212	0.057135	0.000301
H	-4.327313	-0.183105	-0.928210
H	-4.326635	-0.182540	0.929326
H	-4.418888	2.058669	0.000004
H	4.541796	-0.856833	0.000773
H	4.492524	1.000812	0.000216

Frequencies:

441.1988*i*	79.0636	87.7086
173.1045	211.3828	244.0414
275.9003	353.0812	353.7293
527.5423	534.7124	567.9909
635.3561	666.2860	690.8125
876.8846	883.3614	1019.6968
1024.0949	1068.9106	1397.6305
1455.6165	1578.8201	1934.2961
2184.2443	2226.2189	3146.2448
3148.1653	3232.4871	3233.6775

i8-p1, C_1, ^2A

C	1.221298	-0.017178	-0.000402
C	2.433248	0.016488	-0.000185
C	3.883963	0.058351	0.000463
C	-2.702439	-0.133511	0.000060
C	-1.350827	-0.087952	-0.000244
C	-0.131844	-0.055178	-0.000419
C	-3.916484	-0.124926	0.000372
H	4.251147	0.967942	-0.485202
H	4.277512	0.040938	1.021635
H	4.302339	-0.799753	-0.534990
H	-4.481926	2.120699	0.000009
H	-4.970569	-0.266378	0.000677

Frequencies:

301.9846*i*	45.1914	77.0297
81.5227	173.8808	207.4970
241.9301	357.2276	365.5683
521.9918	523.9362	534.2777
582.6013	680.9591	742.0540
749.0903	949.3667	1054.0728
1054.2547	1320.1684	1427.2001
1487.3457	1487.5003	2117.3704
2263.1048	2321.5361	3022.9872
3081.0535	3081.4788	3464.9423

Products

p1, C_{3v}, $^1A_1$

C	1.125017	-0.005659	-0.000214
C	2.336930	-0.003283	-0.001638
C	3.788415	0.005929	0.000061
C	-2.803763	-0.000370	0.001422
C	-1.448151	-0.002899	0.000886
C	-0.229855	-0.005656	0.001056
C	-4.013437	0.006362	-0.002007
H	4.174639	1.023876	-0.108924
H	4.183129	-0.403598	0.934899
H	4.188047	-0.593825	-0.823370
H	-5.076755	0.007008	0.000001

Frequencies:

79.9572	80.1694	206.0156
206.2027	350.2745	350.5636
468.1845	469.5160	522.5944
570.5666	570.7328	735.4928
737.4554	948.1193	1053.1609
1053.6704	1318.1406	1427.0196
1487.5555	1487.8469	2140.7471
2282.6422	2329.2833	3025.3224
3083.1049	3083.7067	3468.7152

p2, D_{2d}, $^{1}A_{1}$

C	1.278481	0.002501	0.000567
C	2.550099	0.003064	0.000789
C	-2.550120	-0.004135	-0.002259
C	-1.278454	-0.003558	-0.002368
C	-0.000049	0.000660	-0.000341
C	-3.862513	0.002122	0.001814
C	3.862533	-0.001395	0.000322
H	-4.422846	0.872332	0.333451
H	-4.437783	-0.860088	-0.324776
H	4.429300	-0.333099	0.866368
H	4.431461	0.325307	-0.866188

Frequencies:

81.5374	81.6114	211.2490
211.3030	342.0447	342.0965
520.4035	520.5636	561.3642
597.1460	679.0600	680.5076
839.1321	839.4380	1014.9570
1015.1738	1061.5524	1395.1921
1451.4318	1566.8564	1914.6380
2179.5548	2181.0783	3113.5620
3114.2132	3186.5522	3187.2309

p3, C_s, $^{1}A'$

C	-0.678862	0.434812	-0.000042
C	-1.807309	-0.190824	-0.002663
C	-2.948585	-0.830511	0.000982
C	1.974144	-0.294598	-0.000140
C	0.802976	0.447548	0.000248
C	0.163338	1.601572	0.000525
C	2.966334	-0.980531	0.000154
H	-3.450166	-1.112207	0.925770
H	-3.455439	-1.114066	-0.920338
H	0.226634	2.679460	0.000359
H	3.846753	-1.578002	-0.000171

Frequencies:

95.9885	176.8447	217.0161
231.3483	349.4351	430.4151
492.8004	584.9718	612.5400
617.6334	627.0814	664.9529
767.7060	785.4180	884.9350
996.9359	1025.1930	1047.7317
1364.5305	1523.5653	1755.1318
2101.5109	2205.1737	3084.1532
3145.6532	3248.8062	3464.3697

p4, D_{2h}, $^{1}A_{g}$

C_6H_2

C	-0.624041	1.109476	-0.000073
C	0.623780	1.109530	-0.000084

C	0.624057	-1.109499	-0.000026
C	-0.623772	-1.109483	-0.000014
C	-1.481248	-0.000127	0.000110
C	1.481228	0.000098	0.000083
H	-2.562761	-0.000274	0.000037
H	2.562742	0.000311	-0.000014

Frequencies:

235.6698	334.9972	416.9097
539.7314	576.9461	688.5956
830.5687	894.3903	980.8124
1098.3012	1215.4248	1293.0791
1311.2470	1345.6327	1854.9233
2040.3193	3214.0640	3217.0658

CH_3, D_{3h}, $^2A_1$’

C	-0.000001	-0.000043	-0.000331
H	0.935680	-0.541022	0.000662
H	-0.936539	-0.539527	0.000662
H	0.000865	1.080804	0.000662

Frequencies:

473.4215	1413.2446	1413.5537
3105.5661	3284.4381	3284.7686

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