

Supporting Information for

**Directed Gas-Phase Formation of the 1-Cyanovinyl Radical (H_2CCCN , X^2A')
in the Interstellar Medium**

Shane J. Goettl,^{a§} Ashleigh G. Hartwig,^{b§} Zhenghai Yang,^a Alexander M. Mebel,^{b*} Ralf I.
Kaiser^{a*}

^a Department of Chemistry, University of Hawaii at Manoa, Honolulu, Hawaii 96822, USA

Email: ralfk@hawaii.edu

^b Department of Chemistry and Biochemistry, Florida International University, Miami, Florida
33199, USA

Email: mebela@fiu.edu

[§] contributed equally

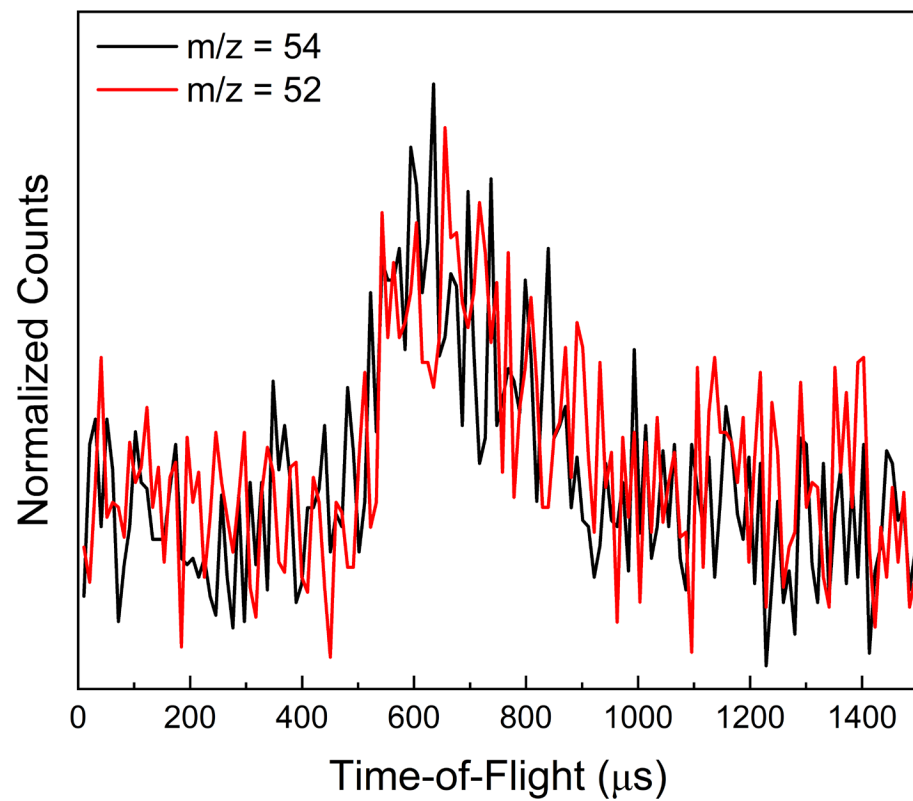


Fig. S1. Normalized time-of-flight (TOF) mass spectra for the reaction of ground-state atomic carbon with acetonitrile- d_3 (CD_3CN) at $m/z = 52$ and 54 .

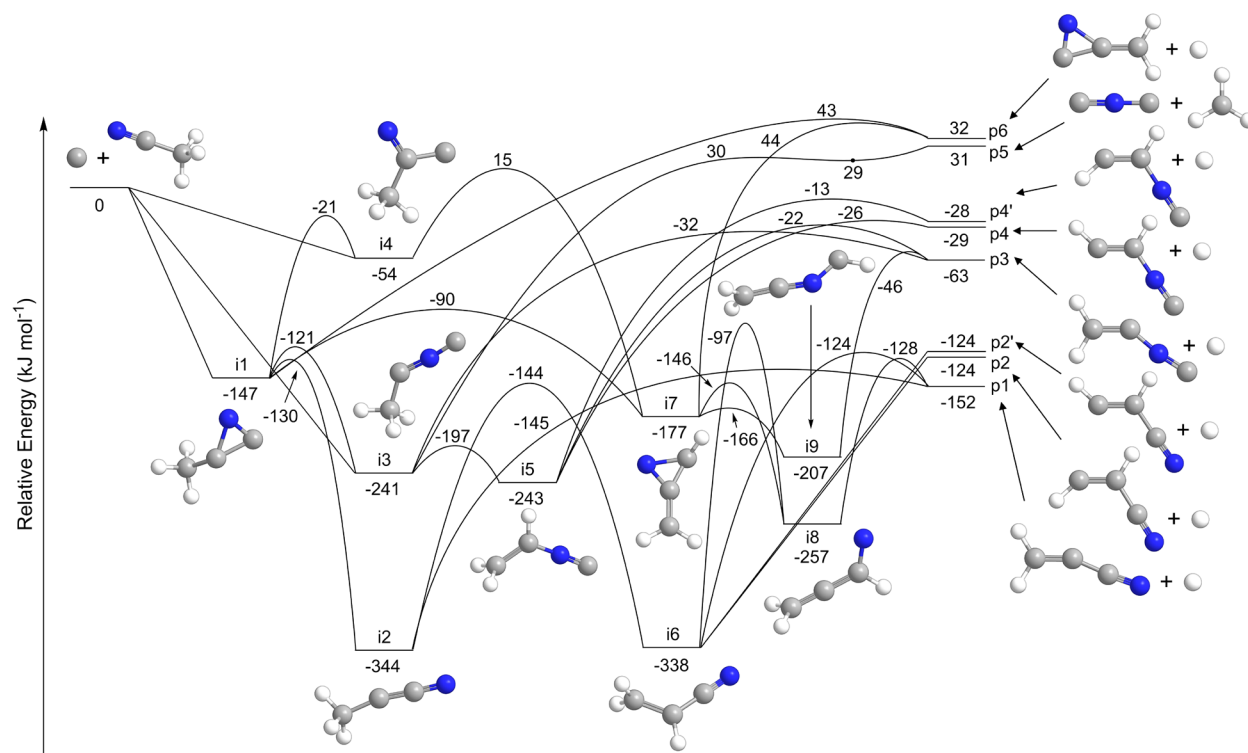


Fig. S2. Potential energy surface (PES) for the reaction of ground-state atomic carbon (C) with acetonitrile (CH_3CN) at the CCSD(T)-F12/cc-pVQZ-f12// ω B97XD/6-311G** + ZPE(ω B97XD/6-311G**) level of theory.

Table S1: Rate constants of unimolecular steps involved in the reaction of carbon with acetonitrile.

Reaction Step	k, s ⁻¹ (at 4 kJ mol ⁻¹)	k, s ⁻¹ (at 25 kJ mol ⁻¹)	k, s ⁻¹ (at 46 kJ mol ⁻¹)	Reaction Step	k, s ⁻¹ (at 0 kJ mol ⁻¹)	k, s ⁻¹ (at 25 kJ mol ⁻¹)	k, s ⁻¹ (at 46 kJ mol ⁻¹)
i4 → i7	0	7.72E8	7.79E9	i1 → p6	0	0	2.47E5
i7 → i4	0	9.72E5	2.05E7	i1 → i4	3.51E8	3.16E9	1.03E10
i3 → p3	2.96E11	4.90E12	2.41E13	i4 → i1	1.58E11	5.05E11	8.68E11
i3 → i5	1.60E13	1.91E13	2.18E13	i7 → i9	1.07E13	1.16E13	1.22E13
i5 → i3	4.66E12	5.54E12	6.27E12	i9 → i7	7.25E11	8.76E11	1.00E12
i3 → p5	0	0	5.96E6	i7 → i8	4.89E12	5.97E12	6.84E12
i1 → i3	3.04E12	3.69E12	4.19E12	i8 → i7	8.22E10	1.32E11	1.84E11
i3 → i1	2.25E10	3.99E10	5.93E10	i7 → p6	0	0	3.17E4
i1 → i7	5.63E11	9.42E11	1.32E12	i5 → p3	1.67E6	2.93E7	1.48E8
i7 → i1	9.76E10	1.90E11	2.94E11	i5 → p4	1.01E7	1.53E8	7.26E8
i1 → i2	3.05E12	3.45E12	3.76E12	i5 → p4'	6.20E5	2.61E7	1.79E8
i2 → i1	3.68E7	7.61E7	1.28E8	i2 → p1	7.75E9	1.63E10	2.76E10
i2 → i6	4.48E9	8.83E9	1.44E10	i9 → p3	1.70E9	1.09E10	3.35E10
i6 → i2	3.91E10	7.60E10	1.22E11	i8 → p1	2.24E11	4.38E11	6.97E11
i6 → i8	4.43E8	1.30E9	2.74E9	i6 → p2'	5.10E12	1.27E13	2.40E13
i8 → i6	1.23E10	3.04E10	5.66E10	i6 → p1	7.61E9	1.82E10	3.37E10

Table S2. Intermediate **i4** entrance channel branching ratios of reaction products and their yields.

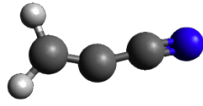
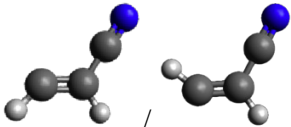
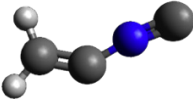
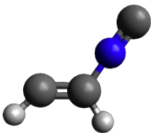
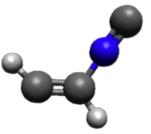
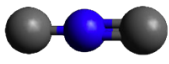
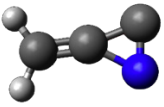
Products	Structure	Collision E: 4 kJ mol ⁻¹	Collision E: 25 kJ mol ⁻¹	Collision E: 46 kJ mol ⁻¹
P1	 +H	38.2%	38.3%	39.1%
P2' / P2	 + H	17.7%	15.7%	14.8%
P3	 +H	44.1%	45.9%	46.1%
P4	 + H	0	0	0
P4'	 + H	0	0	0
P5	 + CH ₃	0	0	0
P6	 + H	0	0	0

Table S3. Intermediate **i3** entrance channel branching ratios of reaction products and their yields.

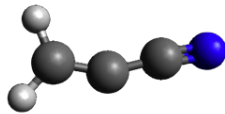
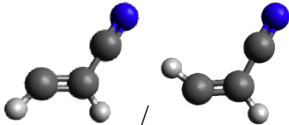
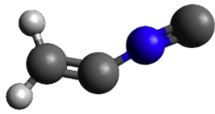
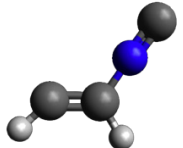
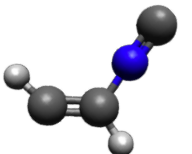
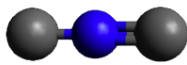
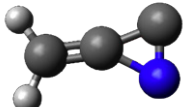
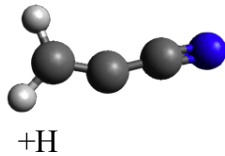
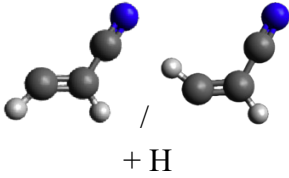
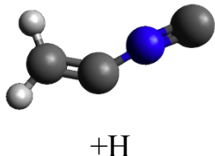
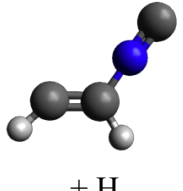
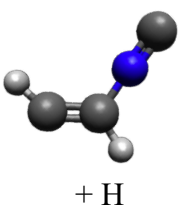
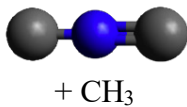
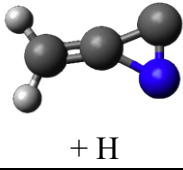
Products	Structure	Collision E: 4 kJ mol ⁻¹	Collision E: 25 kJ mol ⁻¹	Collision E: 46 kJ mol ⁻¹
P1	 +H	2.70%	0.3%	0.01%
P2' / P2	 + H	1.25%	0.1%	0
P3	 +H	96.0%	99.6%	99.9%
P4	 + H	0	0	0
P4'	 + H	0	0	0
P5	 + CH ₃	0	0	0
P6	 + H	0	0	0

Table S4. Intermediate **i1** entrance channel branching ratios of reaction products and their yields.

Products	Structure	Collision E: 4 kJ mol ⁻¹	Collision E: 25 kJ mol ⁻¹	Collision E: 46 kJ mol ⁻¹
P1	 +H	38.2%	38.2%	38.7%
P2' / P2	 + H	17.7%	15.8%	14.8%
P3	 +H	44.1%	46.0%	46.5%
P4	 + H	0	0	0
P4'	 + H	0	0	0
P5	 + CH ₃	0	0	0
P6	 + H	0	0	0

Data S1. Optimized Cartesian coordinates (Å) and vibrational frequencies (cm⁻¹) of reactants, products, intermediates, and transition states involved in the carbon (C,³P) plus acetonitrile (CH₃CN) reaction.

Reactants:

C

0 3

C,0,0.,0.,0.

CH₃CN

0 1

C,0,-3.78885834,2.2598366738,-1.8512122572

N,0,-4.6711100988,2.5321811055,-2.5349996435

C,0,-2.670542682,1.9167358158,-0.9843389099

H,0,-1.7530733792,2.3701359061,-1.3620443832

H,0,-2.5428920235,0.8338755986,-0.9512388961

H,0,-2.8562534766,2.2825049002,0.0264440899

Frequencies

1479.6916 1479.7910 2407.9731

3069.5957 3154.3957 3154.6853

Intermediates:

il

0 3

C,0,-6.7847562293,0.856337481,-1.133945604

N,0,-5.4264886786,0.4117559172,-0.5849943954

C,0,-8.1094596318,0.3681559377,-0.7012420099

H,0,-8.8739068726,1.1069363563,-0.956320386

H,0,-8.1298911578,0.1957667686,0.3807690999

H,0,-8.3561435704,-0.5660553234,-1.2126328132

C,0,-5.707993859,1.6074228603,-0.4736838983

Frequencies

104.9826 321.2338 358.4957

487.1488 760.4961 1011.1151

1060.3028 1225.4695 1396.4116

1460.0537 1469.7719 1812.6466

3026.0340 3107.7983 3123.5730

i2

0 3

C,0,-5.8890817377,2.5292803766,0.0178823812
C,0,-4.4692394633,2.2773577376,0.1658540082
H,0,-6.0668302311,3.3615806792,-0.6718459121
H,0,-6.3437299292,2.7845659387,0.9799146735
H,0,-6.4023653328,1.6447852061,-0.374884611
C,0,-3.2167343083,2.0007394981,-0.0053509585
N,0,-2.0477989976,1.7522605638,-0.1115595813

Frequencies

21.5084	46.9111	435.1741
438.7545	772.5439	1004.3663
1008.7695	1403.7855	1458.7599
1463.4065	1547.8245	1780.0947
3019.7662	3090.4029	3099.6399

i3

0 3

C,0,-6.0976143649,0.414630888,-0.0413307556
C,0,-4.7286855612,0.7452831373,-0.4726345955
H,0,-6.8254597702,0.8533314361,-0.7250134222
H,0,-6.2917351836,0.8046297375,0.9647097883
H,0,-6.2483596797,-0.6711936163,-0.0285158355
N,0,-3.5543306279,0.4753067938,-0.0154820101
C,0,-2.4158048125,0.2867516236,0.3182568305

Frequencies

82.0807	203.1320	392.8762
472.4593	852.0422	1004.6292
1055.7334	1391.9124	1403.9250
1464.8098	1469.5178	1827.5021
3015.7414	3081.4695	3138.1880

i4

0 3

C,0,-5.8137635892,-0.534976922,-0.0031110886
C,0,-4.3527265634,-0.1073785372,-0.0080687469
H,0,-6.456108192,0.3017649679,0.279590091
H,0,-5.9466251179,-1.346036817,0.713426482
H,0,-6.0897453235,-0.8770952906,-1.0009173923
C,0,-4.0430113966,1.194399947,0.321426723
N,0,-3.3493898175,-0.8798173482,-0.3023360682

Frequencies

112.6293	129.5412	347.3023
447.3455	840.8378	952.2360
1017.8839	1180.2831	1355.1892
1416.8484	1475.9171	1482.7422
3060.8372	3149.5128	3163.7888

i5

0 3

C,0,-6.1325125696,2.497322981,-0.2300132295
C,0,-4.9024583501,2.8007106969,0.4875824951
H,0,-6.5853413708,1.5126926629,-0.1655834606
H,0,-6.5924154769,3.2331323181,-0.8824044448
N,0,-3.6978404444,2.5711315918,-0.0723145336
H,0,-4.891924664,3.2173431745,1.4897838223
C,0,-2.6495571242,2.3629565748,-0.578180649

Frequencies

195.9203	296.6373	415.7116
426.3994	559.2571	573.5417
952.0521	997.6473	1183.6640
1377.2983	1438.0303	2066.6837
3126.8724	3176.1497	3229.5620

i6

0 3

C,0,-1.6414965116,0.2930885685,-0.0420387889
C,0,-0.4901802628,1.0578938096,-0.5028907893
C,0,0.7294468884,1.0299222239,0.1660018325
N,0,1.7463049868,1.0009954379,0.7297055616
H,0,-2.3433340242,0.72137278,0.6657438127
H,0,-1.8018495925,-0.7248338584,-0.3812799468
H,0,-0.5505029394,1.6805417821,-1.392938246

Frequencies

211.2359	315.4506	420.4609
520.4941	596.9558	615.8436
952.1579	963.8475	1152.3404
1354.7776	1428.3239	2185.1811
3135.7761	3148.8462	3241.3247

i7

0 3

C,0,-6.2293014256,2.5224890383,-0.4689494155
C,0,-4.9121791623,2.78956058,-0.1077170547
H,0,-6.5092767433,1.5197574127,-0.7680774937
H,0,-6.9769840589,3.3044011781,-0.4488508514
C,0,-3.8776250467,3.6306509557,0.2480046691
N,0,-3.7721751699,2.1431969527,0.0858891143
H,0,-3.2998183932,4.3856338825,-0.273048968

Frequencies

341.5349	359.2338	419.3404
732.7640	780.7451	819.4986
910.2813	991.5176	1063.4549
1235.5213	1459.5176	1664.7660
3165.4450	3184.4436	3280.5423

i8

0 3

C,0,-4.7154025676,0.8792654845,-0.3513232518
C,0,-3.5411710855,1.3981425613,-0.1812477741
H,0,-5.5062217731,1.0128038766,0.383930249
H,0,-4.9518052581,0.2883326093,-1.2337755473
C,0,-2.3077321571,1.9367709614,0.0017970435
N,0,-1.318675109,1.3311739621,0.612674126
H,0,-2.1206920496,2.9456205448,-0.3853548453

Frequencies

216.0616	216.9411	506.5190
579.1476	843.3136	913.7697
968.6328	981.8242	1177.6006
1330.1633	1434.9078	1922.4279
3052.2768	3108.9028	3186.0629

i9

0 3

C,0,-5.154099191,-0.2224129509,0.0074079569
C,0,-3.8504255728,-0.2756378614,-0.0743079237
N,0,-2.6313842945,-0.3411487577,-0.2506297734
C,0,-1.4932328426,-0.2758281741,0.3577104548
H,0,-5.7329489823,-1.1184440014,0.2007744118
H,0,-5.6766036168,0.7213719128,-0.1002769953
H,0,-0.5319765,-0.3864001674,-0.1406771311

Frequencies

167.9811	232.3030	464.2776
505.8558	661.0873	748.0012
963.5531	963.7162	1090.5954
1357.8529	1482.1426	1983.8664
3140.9230	3148.4119	3234.2064

Products:

p1

CH₂CCN

0 2

C,0,1.8032469346,-0.1532239957,-2.0547252891

C,0,0.9345621177,-0.0599449267,-1.0897960384

C,0,0.2541480262,-0.4589610126,0.0061547036

N,0,-0.3787210006,-0.7257732261,0.9500126837

H,0,1.9323228299,0.6442482871,-2.7822593627

H,0,2.4330910922,-1.035775126,-2.1683866971

Frequencies

133.2582 266.1552 455.7070

598.0799 878.7494 943.8837

968.3294 1428.6101 1826.5586

2169.4747 3098.5317 3187.7246

H

0 2

H 0. 0. 0.

p2'

CHCHCN

0 2

C,0,-4.1069818574,-0.070104431,-0.0085778368

C,0,-2.8888207389,0.4173955037,-0.0024701548

C,0,-2.6064920831,1.8213853208,0.0005378064

N,0,-2.3488925423,2.9430977453,0.0026722785

H,0,-4.5600641198,-1.0505315045,-0.0121800058

H,0,-2.0196929996,-0.2432717979,0.0007714928

Frequencies

242.0597 376.1859 563.8158

709.1750 790.7829 868.4300

1011.1068 1260.0918 1675.6603

2387.2771 3104.3407 3268.9445

p2

HCCHCN

0 2

C,0,-4.1206695934,0.0837670669,0.0036691383
C,0,-2.8658181756,0.4679437941,0.0005290107
C,0,-2.4971314117,1.8550196103,-0.0000355494
N,0,-2.2007806882,2.9677036272,-0.0004647258
H,0,-5.0999719253,0.5404983284,0.0061742975
H,0,-2.0503598488,-0.2513748605,-0.0017756054

Frequencies

229.5238	389.6552	547.0462
745.7489	848.3962	884.0728
988.3949	1260.7933	1662.2765
2377.5757	3159.5786	3264.845

p3

CH₂CNC

0 2

C,0,1.7188267474,0.0787400827,-0.0047322264
C,0,0.4736755201,0.4808829626,0.0421946676
N,0,-0.745094108,-0.0225895373,0.0127054782
C,0,-1.8928175005,-0.3170273574,-0.0000300068
H,0,2.5335105458,0.7907041643,0.0461149969
H,0,1.9643407952,-0.9782313148,-0.0957979096

Frequencies

215.7450	259.6602	451.6409
606.2343	901.4230	923.5853
1032.0247	1419.5083	1767.0047
2088.5396	3117.2414	3231.9208

H

0 2

H -2.17251 1.87876 -0.1192

p4'

CHCHNC

0 2

C,0,1.6395302655,0.3355251008,0.3076348086
C,0,0.457543143,0.8187189221,0.0118070408
N,0,-0.6958740661,0.0454575026,0.0235030897
C,0,-1.679294164,-0.59214541,0.028208771
H,0,2.0839756641,-0.6028130526,0.6014569643
H,0,0.3030824026,1.857784259,-0.2623437314

Frequencies

200.0232	285.5905	482.5304
731.4193	844.0670	882.8248
1014.0024	1298.3641	1667.5257
2227.1618	3180.3301	3282.3179

p4

HCCHNC

0 2

C,0,1.6444363487,-0.1947558578,0.0005332729
C,0,0.5711374999,0.5575094713,0.0001608763
N,0,-0.7175782199,0.0567690438,-0.0000234041
C,0,-1.8262785999,-0.3220799177,-0.000179074
H,0,2.7101496621,-0.0312053837,0.0007068077
H,0,0.6316615943,1.6459361367,-0.0000660476

Frequencies

204.9187	282.3871	516.6818
699.4338	785.4845	848.4196
1050.8096	1291.9070	1683.4114
2236.0991	3123.9740	3290.0252

p5

CNC

0 2

C,0,-9.9304491529,1.4622409238,0.
N,0,-8.68797,1.49723,0.
C,0,-7.4454908471,1.5322190762,0.

Frequencies

245.2384 408.9687 1319.8699
1462.7918

CH₃

0 2

C,0,-7.49944,3.3541909624,-0.0000050986
H,0,-7.49944,2.4781732654,-0.633328831
H,0,-7.49944,4.340681805,-0.4419712962
H,0,-7.49944,3.2436739672,1.0753052257

Frequencies

497.6761 1405.0952 1405.3461
3114.3935 3299.7241 3299.8701

p6**CyclicCH₂CCN**

0 2

C,0,1.7201648299,-1.1803200662,-2.0490889671
C,0,0.4986401731,-1.1487064985,-1.5955926291
H,0,2.4170420864,-0.3814081187,-1.8232930544
H,0,2.049846616,-2.0124287377,-2.6599308781
C,0,-0.8797823844,-1.4266909839,-1.2698717149
N,0,-0.4733047782,-0.3623919276,-0.7833254481

Frequencies

321.5922 375.8870 464.0428
578.5919 826.5973 842.1542
965.7993 1402.1605 1717.0267
1890.9795 3154.3002 3248.3281

Transition States:

TS1_2

0 3

C,0,0.0289600552,0.1048471293,0.2356268078
N,0,1.1936861162,-0.1219199527,-0.8495718491
C,0,-1.4123069052,-0.0574095879,0.1962962383
H,0,-1.862272411,0.6019045624,-0.5540622974
H,0,-1.8319184887,0.193529811,1.1745602589
H,0,-1.6855909645,-1.0908556678,-0.0444541533
C,0,1.358842598,0.2552037057,0.3651249947

Frequencies

-221.5286	148.2415	258.5078
567.3992	703.5441	1012.0749
1014.8552	1173.0689	1402.8765
1452.1881	1474.1007	1760.0066
3018.1334	3081.6860	3115.1803

TS1_3

0 3

C,0,-0.05701614,0.2799818002,-0.32089564
N,0,1.0803526964,-0.5388880332,-0.1808355147
C,0,-1.4311073929,-0.0090207271,0.1260552406
H,0,-2.1073175089,0.7800387336,-0.2074015038
H,0,-1.4868363526,-0.067377862,1.2203129296
H,0,-1.7769074407,-0.96524145,-0.2880830783
C,0,1.7381521385,0.1335875385,0.5879975665

Frequencies

-445.2260	126.0048	183.5635
378.1254	865.4445	1009.4357
1060.3908	1243.6463	1391.8567
1459.0888	1464.5670	1814.4855
3001.7161	3063.9906	3132.1440

TS1_4*0 3*

C,0,-0.1096664478,0.2874913642,-0.0195407764
 N,0,0.9550622213,-0.5666616078,0.1005099139
 C,0,-1.542988214,-0.0721580678,0.1793236743
 H,0,-2.1713420388,0.8032056296,0.0190529689
 H,0,-1.6903958094,-0.4449093471,1.194345853
 H,0,-1.8255902085,-0.8567020173,-0.5246384761
 C,0,0.7983324606,1.2056745735,-0.3103530449

Frequencies

<i>-712.7454</i>	<i>36.2184</i>	<i>342.9137</i>
<i>375.7776</i>	<i>795.1277</i>	<i>862.0247</i>
<i>1037.8382</i>	<i>1053.7091</i>	<i>1399.1494</i>
<i>1476.8528</i>	<i>1483.6321</i>	<i>1690.7151</i>
<i>3066.8788</i>	<i>3149.1965</i>	<i>3167.6720</i>

TS1_7*0 3*

C,0,-6.9235236615,0.5380114634,-0.4602885551
 C,0,-5.6993795136,0.4330121017,0.0236361979
 H,0,-7.7735565773,0.5165046397,0.2107649239
 H,0,-3.9440586665,2.2773101485,0.7349411779
 H,0,-7.0805968944,0.7067334935,-1.5175521374
 C,0,-4.2072673345,1.4018993532,0.1381598385
 N,0,-4.6037373523,0.1697188,0.6085085543

Frequencies

<i>-731.1690</i>	<i>314.8156</i>	<i>361.7248</i>
<i>410.0894</i>	<i>628.7840</i>	<i>690.7090</i>
<i>958.0149</i>	<i>1005.6431</i>	<i>1013.4990</i>
<i>1193.4629</i>	<i>1417.7359</i>	<i>1914.5494</i>
<i>3100.6830</i>	<i>3162.8190</i>	<i>3260.2668</i>

TS1_p6

0 3

C,0,-0.1212340299,-0.0875110443,-0.0934155143
 N,0,1.1530761698,0.2580418088,0.5922901107
 C,0,-1.3932469758,-0.3566280453,0.1006795028
 H,0,-2.3435086475,1.517639132,0.164146717
 H,0,-1.7750956808,-0.5097389375,1.1032634707
 H,0,-2.0257175991,-0.5974087885,-0.7453737456
 C,0,1.1642254936,0.2511580549,-0.6474282622

Frequencies

-529.9650	224.2464	247.8772
319.1302	449.4592	582.8847
588.7965	832.8386	865.0773
974.5867	1401.1401	1675.5117
1865.1257	3156.0343	3253.2441

TS2_6

0 3

C,0,1.7024930899,0.2344220303,-0.000755396
 C,0,0.3293952607,-0.172120104,-0.0064590672
 H,0,2.1804549327,0.5127888076,-0.9344693518
 H,0,1.2307093767,-1.0542167278,-0.022810661
 H,0,2.1823828021,0.4799075899,0.9411612876
 C,0,-0.9965225063,0.0218918296,-0.0011401724
 N,0,-2.17126848,0.0874013655,0.0016656567

Frequencies

-2044.9974	36.8750	193.5440
452.7451	532.3958	739.8058
806.3345	924.4583	1004.6298
1395.3835	1524.2014	2013.6551
2273.0325	3120.3845	3236.6415

TS2_p1

0 3

C,0,1.7191275553,0.4455528705,0.0750004854
 C,0,0.453758868,0.1945644616,0.3065130817
 H,0,2.0883753393,0.6042824962,-0.9378254311
 H,0,2.706519041,-1.5931801513,-0.1053210385
 H,0,2.4237403672,0.5950487812,0.8886472777
 C,0,-0.8289329553,-0.0614423269,-0.0180540174
 N,0,-1.9585482155,-0.2893361313,-0.2111103579

Frequencies

-460.2774	132.4693	177.7228
283.3079	386.1322	456.7240
601.2240	874.9606	939.4915
972.4745	1427.6719	1765.6178
2138.1058	3102.6921	3194.8297

TS3_5

0 3

C,0,-6.4870565042,1.4142807764,-0.2867267996
 C,0,-5.2088309529,0.9260416521,0.3680503812
 H,0,-6.4268154881,2.1638839758,-1.0626621264
 H,0,-5.2030302915,0.1075999662,1.075263167
 H,0,-7.4147687997,0.8991256014,-0.0856713537
 N,0,-4.0554003931,1.4753862691,0.0432108847
 C,0,-3.0384775706,2.0105517589,-0.2807941533

Frequencies

-442.7572	149.6047	193.4406
357.3381	420.7073	503.1609
871.2670	1089.5233	1212.3266
1404.7117	1462.6830	1925.6334
3183.9454	3223.5460	3312.5885

TS3_p3*0 3*

C,0,-1.0421339217,0.0550052862,0.013689475
 C,0,0.1981504263,0.4374552449,0.0085601128
 H,0,-5.6032181583,-2.2046261825,-0.1606146238
 H,0,-1.6816584944,0.1917959864,-0.8568630123
 H,0,-1.4868758016,-0.4161915228,0.8887517812
 N,0,1.4127292609,0.8119902242,0.0033973462
 C,0,2.5601856888,1.1657499635,-0.0014120791

Frequencies

-293.6589	4.7189	16.5964
27.2911	217.7150	331.0665
488.4548	885.4859	929.4039
956.6245	1434.8390	1815.8373
1988.0035	3092.3803	3168.7719

TS3_p5*0 3*

C,0,-2.2436509667,0.9283655743,0.3058380692
 C,0,0.3850468059,-1.4381816358,-0.5070848964
 H,0,-2.5846486369,-0.0811615152,0.4891549947
 H,0,-2.2836077499,1.3375291492,-0.6941464678
 H,0,-1.8771457839,1.5352288896,1.1221534251
 N,0,0.8892228908,-0.3687155354,-0.1249491105
 C,0,1.3858304406,0.7018410733,0.2638219858

Frequencies

-30.5965	63.9205	76.3359
98.6467	130.2534	248.5524
404.9324	507.1844	1321.9105
1403.9346	1404.8753	1469.2617
3112.4597	3298.1908	3298.7694

TS4_7*0 3*

C,0,-8.8349247232,0.4851132647,0.2116950796
 C,0,-7.557761776,1.032876327,0.000507844
 H,0,-8.1352089391,3.0731330568,-0.0744112054
 H,0,-9.6751420827,1.1151637848,0.4776678854
 H,0,-8.9802971591,-0.5864690393,0.1497077163
 C,0,-7.3166020496,2.459938062,0.3409123574
 N,0,-6.5809832704,0.3122645441,-0.4622696773

Frequencies

-381.4647	321.7593	417.0897
481.0359	522.5601	791.1182
868.4914	929.5450	1023.5056
1119.1582	1315.6265	1477.3984
3012.8282	3158.2550	3272.5673

TS5_p3*0 3*

C,0,1.5979917525,-0.319769602,-0.066748974
 C,0,0.4034033758,0.1764838522,-0.3700944966
 H,0,2.411716778,-0.263957297,-0.779716549
 H,0,1.814920774,-0.6806909299,0.936901941
 N,0,-0.8447448625,0.049933616,0.0478103778
 H,0,0.6389290332,1.9987309587,0.1743935926
 C,0,-2.0045968511,-0.0194405979,0.2788341081

Frequencies

-1119.6108	213.8829	251.2996
428.3456	461.1173	482.9977
636.1876	871.9262	919.1170
1018.8225	1419.1687	1660.8417
2088.2946	3120.2543	3234.8323

TS5_p4*0 3*

C,0,1.3662289231,-0.2924994788,0.0657043365
C,0,0.3246639722,0.5196533014,0.0811553256
H,0,2.4382900656,-0.1869769768,0.1157951725
H,0,1.5301977466,-0.9378991184,2.010790481
N,0,-0.9515200862,0.1217027148,-0.2515080199
H,0,0.4059312098,1.5524365684,0.4186543337
C,0,-2.051534362,-0.1773424467,-0.5270718046

Frequencies

-807.1817	193.7213	226.4369
332.9270	385.7702	516.1105
759.7618	774.8537	851.3459
1052.8550	1285.7774	1627.2531
2224.0058	3130.9199	3285.9670

TS5_p4'*0 3*

C,0,1.6569782204,-0.0181629013,0.2732561784
C,0,0.5403270479,0.6497346939,0.0485388971
H,0,2.150936562,-0.7961791964,-1.5715797529
H,0,1.9652682651,-0.9838653133,0.643273594
N,0,-0.6959585835,0.033424542,-0.0202407794
H,0,0.5318045459,1.7171612602,-0.148156715
C,0,-1.7477268188,-0.4820376526,-0.0860699607

Frequencies

-791.9551	187.2759	229.5391
326.5280	387.0768	485.8104
767.7570	828.4154	885.6295
1019.3965	1295.2032	1614.4490
2216.0507	3183.5922	3278.0760

TS6_8*0 3*

C,0,-1.6079550731,-0.3348977741,0.0230150037
 C,0,-0.2791876826,-0.1624938198,0.0344835236
 C,0,1.0370557203,-0.0338170265,0.0411659839
 N,0,2.2582247274,-0.0766326918,0.0325587207
 H,0,-2.1576315307,-0.4665324182,0.9488486899
 H,0,-2.1639132403,-0.2945499322,-0.9075408129
 H,0,0.3529523905,1.0996980319,0.1488246732

Frequencies

-1812.3911	126.6976	292.4709
407.2595	627.8294	647.4865
710.2618	872.6122	962.4801
1411.1426	1547.9889	1641.0254
1963.8752	3137.6166	3231.3479

TS6_p1*0 3*

C,0,-1.7195098449,-0.3317813005,-0.031527454
 C,0,-0.4942327427,0.1123776746,-0.2125817155
 C,0,0.8373635662,0.1568156282,0.024363563
 N,0,1.997194104,0.181979806,0.1508659525
 H,0,-2.105760152,-0.533737333,0.9668533633
 H,0,-2.4106406208,-0.4349601168,-0.8639934081
 H,0,-0.6432655457,2.0451439627,-0.0264090432

Frequencies

-1029.6935	126.8386	266.6005
437.3929	445.3224	466.1371
599.2725	877.1432	910.0283
964.2555	1427.8795	1747.8275
2170.5362	3103.4013	3194.0701

TS7_8*0 3*

C,0,1.450247,0.070656,0.012917
 C,0,0.046684,0.137042,0.054618
 H,0,1.964601,-0.77527,0.451452
 H,0,2.013721,0.793478,-0.563516
 C,0,-1.157658,0.553252,0.299445
 N,0,-1.134398,-0.585523,-0.532626
 H,0,-1.856808,1.246419,0.736515

Frequencies

-373.1144	310.4591	332.8340
445.5331	555.4458	743.7449
892.8482	1002.9281	1036.0879
1137.6168	1431.5709	1849.9000
3159.2385	3265.7128	3283.8619

TS7_9*0 3*

C,0,1.9587926335,0.0154744178,0.013886881
 C,0,0.6051649524,-0.0955511347,0.340386143
 N,0,-0.5015651751,-0.7277270738,-0.1394808573
 C,0,-0.476145707,0.1620602907,1.0789525062
 H,0,2.627204547,0.6206771874,0.6118504735
 H,0,2.3392995258,-0.5134893372,-0.8505910291
 H,0,-1.1221707765,0.5470056498,1.8389058827

Frequencies

-506.1679	354.1663	363.1783
427.8678	745.6855	767.4125
822.4059	972.4572	1062.4049
1184.6844	1459.5505	1712.9443
3169.4505	3284.8697	3377.2320

TS7_p6

0 3

C,0,1.4827142089,0.1349953862,0.0740559655
 C,0,0.1957659192,0.0606932535,-0.1526222604
 H,0,1.9853750786,-0.6354905833,0.648837119
 H,0,2.0595205326,0.9690476437,-0.3071047396
 C,0,-1.2044971796,0.4739776178,-0.4330004248
 N,0,-0.9789389783,-0.7365634939,-0.1668724242
 H,0,-1.6364966914,1.768569222,1.258216234

Frequencies

-593.9535	151.4569	253.6787
314.6706	329.1597	465.8604
611.1704	812.5312	831.5720
970.2338	1377.2770	1512.9964
1840.1503	3151.1655	3247.4942

TS8_p1

0 3

C,0,-1.7060961967,-0.023166081,-0.1192110734
 C,0,-0.4523652446,-0.2980441003,-0.3538751254
 H,0,-1.9778319924,0.8487479287,0.4779622392
 H,0,-2.5114358745,-0.6412552162,-0.5029638669
 C,0,0.851473004,0.0747662288,-0.1544238143
 N,0,2.0306460304,0.0458590522,-0.2188841107
 H,0,0.5922402737,1.5907721879,0.8729857515

Frequencies

-823.2710	154.0360	213.6291
338.0381	543.8645	586.2133
627.4399	890.1680	946.6403
994.8418	1417.2392	1785.2720
2068.8768	3096.9492	3206.8711

TS9_p3*0 3*

C,0,1.8978053818,0.0453316102,-0.0552584824
C,0,0.6700321167,0.4975708137,-0.0219941572
N,0,-0.569910325,0.0670721726,-0.1032263308
C,0,-1.7322983024,-0.1618477128,-0.1715437749
H,0,2.7396096181,0.7186727987,0.0502491659
H,0,2.1013149444,-1.0158335718,-0.1897708841
H,0,-2.6091134335,-0.2118061106,-2.1338155365

Frequencies

<i>-508.5432</i>	<i>134.9371</i>	<i>168.9610</i>
<i>227.3080</i>	<i>299.4018</i>	<i>452.7730</i>
<i>600.8514</i>	<i>898.0075</i>	<i>926.3545</i>
<i>1024.8312</i>	<i>1420.4168</i>	<i>1773.8034</i>
<i>2063.3841</i>	<i>3117.8603</i>	<i>3232.6012</i>