Supporting Information for

**Directed Gas-Phase Formation of the 1-Cyanovinyl Radical (H2CCCN, X2A′) in the Interstellar Medium**

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A graph of a flight

AI-generated content may be incorrect.

**Fig. S1.** Normalized time-of-flight (TOF) mass spectra for the reaction of ground-state atomic carbon with acetonitrile-*d3* (CD3CN) at *m*/*z* = 52 and 54.

A diagram of a molecule

AI-generated content may be incorrect.

**Fig. S2.** Potential energy surface (PES) for the reaction of ground-state atomic carbon (C) with acetonitrile (CH3CN) at the CCSD(T)-F12/cc-pVQZ-f12//ωB97XD/6-311G\*\* + ZPE(ωB97XD/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** | A grey spheres on a black background  AI-generated content may be incorrect.  +H | 38.2% | 38.3% | 39.1% |
| **P2′ / P2** | /  + H | 17.7% | 15.7% | 14.8% |
| **P3** | A blue and grey molecule  AI-generated content may be incorrect.  +H | 44.1% | 45.9% | 46.1% |
| **P4** | A blue and grey molecule  AI-generated content may be incorrect.  + H | 0 | 0 | 0 |
| **P4′** | + H | 0 | 0 | 0 |
| **P5** | A blue ball with white pips  AI-generated content may be incorrect.  + CH3 | 0 | 0 | 0 |
| **P6** | A molecule model of a molecule  AI-generated content may be incorrect.  + 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** | A grey spheres on a black background  AI-generated content may be incorrect.  +H | 2.70% | 0.3% | 0.01% |
| **P2′ / P2** | /  + H | 1.25% | 0.1% | 0 |
| **P3** | A blue and grey molecule  AI-generated content may be incorrect.  +H | 96.0% | 99.6% | 99.9% |
| **P4** | A blue and grey molecule  AI-generated content may be incorrect.  + H | 0 | 0 | 0 |
| **P4′** | + H | 0 | 0 | 0 |
| **P5** | A blue ball with white pips  AI-generated content may be incorrect.  + CH3 | 0 | 0 | 0 |
| **P6** | A molecule model of a molecule  AI-generated content may be incorrect.  + 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** | A grey spheres on a black background  AI-generated content may be incorrect.  +H | 38.2% | 38.2% | 38.7% |
| **P2′ / P2** | /  + H | 17.7% | 15.8% | 14.8% |
| **P3** | A blue and grey molecule  AI-generated content may be incorrect.  +H | 44.1% | 46.0% | 46.5% |
| **P4** | A blue and grey molecule  AI-generated content may be incorrect.  + H | 0 | 0 | 0 |
| **P4′** | + H | 0 | 0 | 0 |
| **P5** | A blue ball with white pips  AI-generated content may be incorrect.  + CH3 | 0 | 0 | 0 |
| **P6** | A molecule model of a molecule  AI-generated content may be incorrect.  + 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:**

***i1***

*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***

*-712.7454 36.2184 342.9137*

*375.7776 795.1277 862.0247*

*1037.8382 1053.7091 1399.1494*

*1476.8528 1483.6321 1690.7151*

*3066.8788 3149.1965 3167.6720*

***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***

*-731.1690 314.8156 361.7248*

*410.0894 628.7840 690.7090*

*958.0149 1005.6431 1013.4990*

*1193.4629 1417.7359 1914.5494*

*3100.6830 3162.8190 3260.2668*

***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,-0.53373733,0.9668533633

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***

*-508.5432 134.9371 168.9610*

*227.3080 299.4018 452.7730*

*600.8514 898.0075 926.3545*

*1024.8312 1420.4168 1773.8034*

*2063.3841 3117.8603 3232.6012*