

Supporting Information: Reaction Mechanisms of Cylco[18]carbon and Triplet Oxygen

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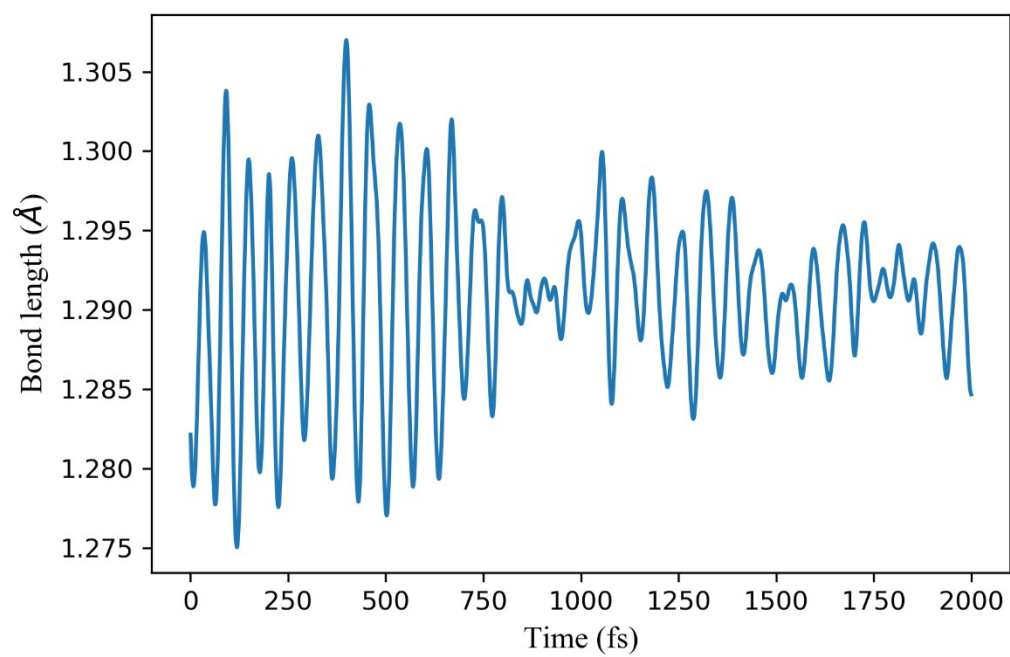


Figure S1 Mean bond length of triplet C₁₆ evolves with time at 300 K.

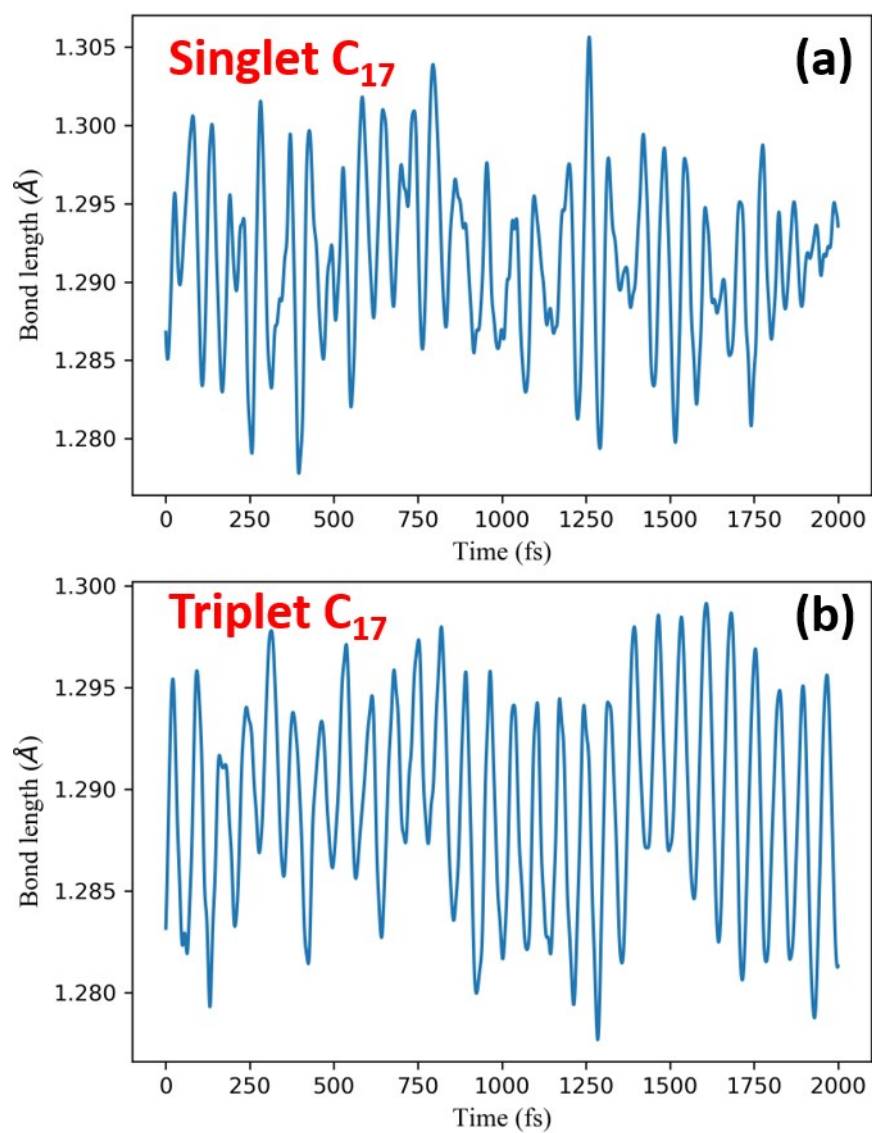


Figure S2 Mean bond length of singlet (a) and triplet (b) C_{17} evolves with time at 300 K.

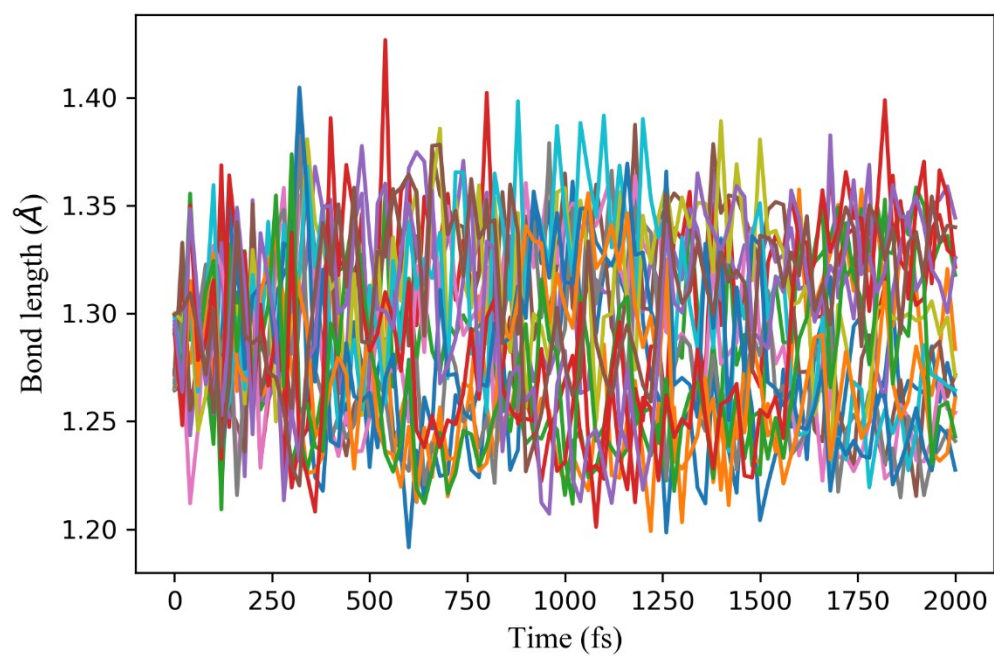


Figure S3 Evolutions of all C-C bonds of triplet C_{16} at 300 K. Different colors denote different bonds.

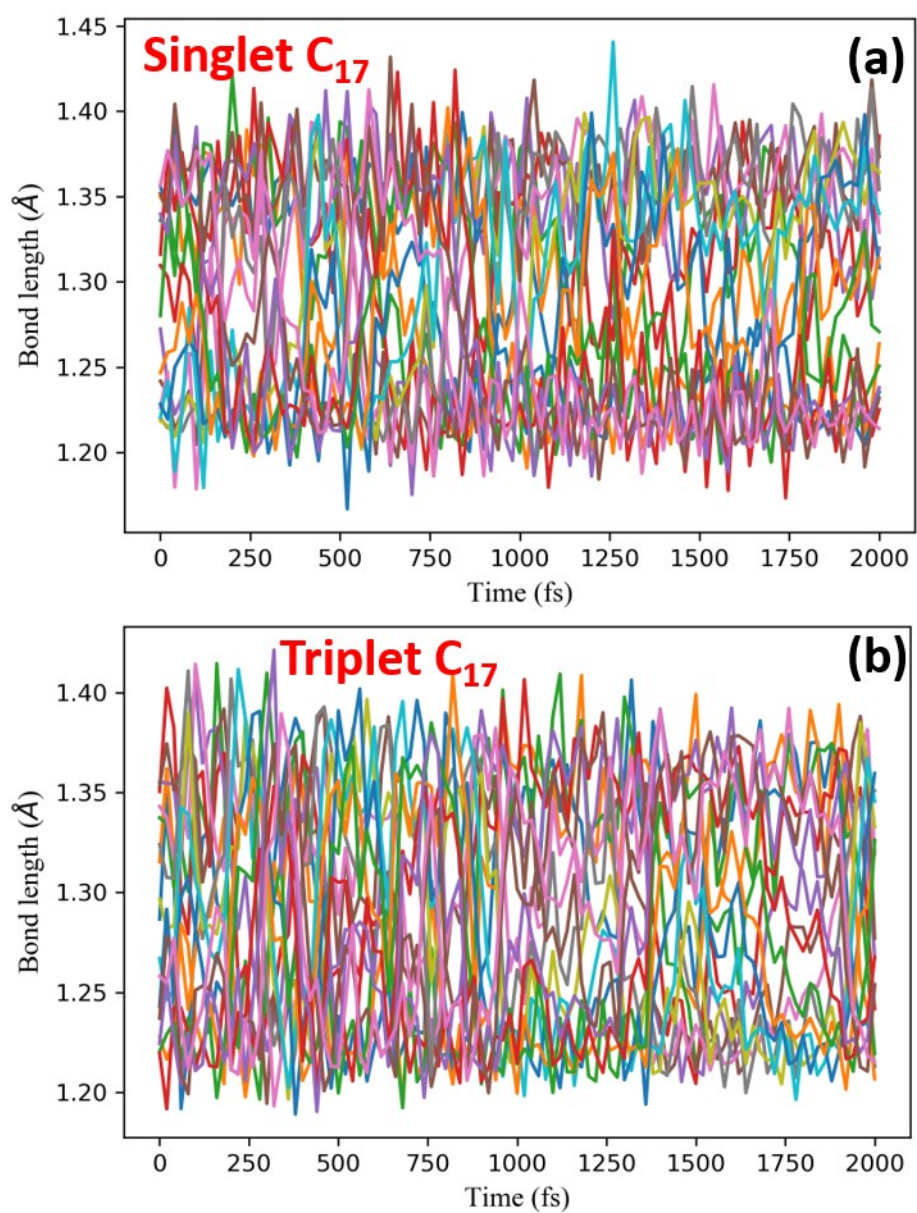


Figure S4 Evolutions of all C-C bonds of singlet (a) and triplet (b) C₁₇ at 300 K. Different colors denote different bonds.

Table S1. Energies and free energies of all optimized structures at ω B97XD/6-311G (d, p) level.

Structure	Energy/eV	Free energy/eV
Int0	-0.033	0.162
Int1	0.041	0.386
Int2	0.249	0.725
Int3	-2.512	-2.029
Int4	-4.208	-3.720
Int5	-4.163	-3.601
Int6	-4.265	-4.071
Int7	-4.169	-4.282
Int8	-2.332	-2.910
P1	-2.156	-3.073
Int9	-4.962	-4.489
Int10	-4.404	-3.916
Int11	-3.023	-2.554
Int12	-4.392	-4.231
P2	-4.315	-4.512
Int13	-2.805	-2.707
Int14	-2.730	-2.862
P3	-5.150	-4.729
TS0	0.889	1.180
TS1	0.915	1.281
TS2	-2.416	-2.051
TS3	-4.009	-3.605
TS4	-3.567	-3.248
TS5	-1.942	-2.346
TS6	-2.385	-1.997
TS7	-4.316	-3.854
TS8	-2.751	-2.298
TS9	-2.730	-2.317
TS10	-3.552	-3.203
TS11	-2.386	-2.070
TS12	-2.524	-2.256
TS13	-2.059	-2.290
TS14	-2.321	-1.879

Optimized structures of singlets at ωB97XD/def2-TZVP level:

Cyclo[16]carbon:

C	2.73544700	1.84828300	0.00009100
C	1.88283500	2.71102700	0.00006900
C	0.62726500	3.24089600	0.00003300
C	-0.58567900	3.24853300	-0.00000400
C	-1.84831000	2.73545300	-0.00004500
C	-2.71103500	1.88282600	-0.00007400
C	-3.24093100	0.62726800	-0.00009600
C	-3.24855900	-0.58567600	-0.00010100
C	-2.73546900	-1.84830300	-0.00009100
C	-1.88283400	-2.71102000	-0.00006900
C	-0.62726900	-3.24089600	-0.00003300
C	0.58567600	-3.24853900	0.00000400
C	1.84829600	-2.73543700	0.00004500
C	2.71105200	-1.88283800	0.00007400
C	3.24089900	-0.62726100	0.00009600
C	3.24861500	0.58568400	0.00010100

Frequencies (cm⁻¹):

73.78 74.01 94.20 94.46 195.92 195.92 213.93 213.93 233.24 320.61 322.48 342.11 367.95 441.65
441.66 441.69 452.03 452.03 486.07 486.08 490.14 500.15 500.64 510.79 510.79 510.82 511.02 665.86
665.86 1009.83 1010.08 1326.88 1326.89 1474.25 2153.45 2221.44 2221.44 2265.95 2265.95 2295.94
2299.80 2300.07

Cyclo[17]carbon:

C	2.62947000	2.29126200	0.00000400
C	1.56576000	3.12420900	0.00018800
C	0.37916800	3.41913800	0.00046500
C	-0.95987200	3.36342200	0.00062700
C	-2.03634900	2.75566400	0.00034500
C	-3.01808300	1.87601000	-0.00008700
C	-3.37393400	0.66318000	-0.00077300
C	-3.52641900	-0.61129400	-0.00106200
C	-2.93979400	-1.77297300	-0.00081500
C	-2.18214200	-2.76549700	-0.00061300
C	-0.95975900	-3.29049200	0.00000500
C	0.25380100	-3.47985000	0.00024300
C	1.54491100	-3.09751000	0.00046500
C	2.54960300	-2.40627400	0.00054300
C	3.27293600	-1.26231800	0.00035800
C	3.51790900	-0.07041100	0.00013600
C	3.28279400	1.26373400	-0.00003100

Frequencies (cm⁻¹):

24.64 61.67 83.52 84.23 118.80 168.48 175.70 193.67 194.11 219.13 223.03 262.97 311.69 318.18
323.97 376.38 403.44 413.71 425.09 429.29 447.12 463.68 467.15 470.15 474.75 492.15 492.57 519.62
519.96 604.59 659.18 781.39 993.21 1000.68 1326.95 1327.90 1516.71 1735.98 1923.05 2055.18
2108.12 2149.55 2184.86 2242.67 2251.34

P3:

O	-3.81592100	-0.45760300	-11.37920500
O	3.81597900	0.45922300	11.37913000
C	3.04243000	0.36558200	9.07290300
C	2.63462400	0.31639700	7.85667800
C	2.23471200	0.26816600	6.66406600
C	1.82194000	0.21845900	5.43308200
C	1.42535900	0.17073000	4.25042500
C	1.00931800	0.12070900	3.00974300
C	0.61465400	0.07328900	1.83284400

C	0.19705700	0.02315000	0.58756100
C	-0.19701300	-0.02413800	-0.58753800
C	-0.61461600	-0.07422300	-1.83282100
C	-1.00929300	-0.12153500	-3.00972200
C	-1.42535200	-0.17139000	-4.25040400
C	-1.82195200	-0.21889700	-5.43306300
C	-2.23475100	-0.26832900	-6.66404900
C	-2.63467900	-0.31621300	-7.85666800
C	-3.04251800	-0.36503800	-9.07289500
C	-3.44740200	-0.41349600	-10.28027100
C	3.44740500	0.41461600	10.28023000

Frequencies (cm⁻¹):

10.25 25.03 25.46 44.92 45.08 72.02 72.21 108.49 108.54 152.69 152.81 194.47 203.81 204.03 262.18
262.48 348.68 348.92 401.89 411.98 412.25 444.87 445.09 467.34 467.62 486.98 487.46 503.72 504.36
518.89 519.54 527.18 527.22 537.29 537.49 586.97 587.07 604.33 804.43 963.56 1000.28 1189.14
1368.68 1531.47 1757.80 1763.61 1793.75 2043.89 2066.04 2108.15 2168.63 2170.06 2292.26 2311.30

Optimized structures of triplets at ωB97XD/def2-TZVP level:

Cyclo[16]carbon:

C	-3.34593500	-0.00629700	0.00000000
C	-2.91648600	-0.00558700	1.20791000
C	-2.36531100	-0.00420500	2.36532400
C	-1.20791200	-0.00215600	2.91654900
C	-0.00000200	0.00022100	3.34597300
C	1.20791700	0.00235400	2.91654100
C	2.36532300	0.00422500	2.36534700
C	2.91648500	0.00516700	1.20791700
C	3.34590800	0.00625900	0.00000000
C	2.91648500	0.00516700	-1.20791700
C	2.36532300	0.00422500	-2.36534700
C	1.20791700	0.00235400	-2.91654100
C	-0.00000200	0.00022100	-3.34597300
C	-1.20791200	-0.00215600	-2.91654900
C	-2.36531100	-0.00420500	-2.36532400
C	-2.91648600	-0.00558700	-1.20791000

Frequencies (cm⁻¹):

60.09 60.15 92.38 92.60 156.74 156.74 213.85 215.73 215.74 325.16 361.20 385.09 435.96 435.96
445.58 445.58 461.04 461.80 471.15 471.15 479.61 479.95 496.61 496.61 539.42 539.46 673.33 673.35
700.31 785.57 785.57 1095.70 1096.10 1150.47 1461.48 1461.49 1725.06 1849.92 2024.84 2024.84
2095.75 2096.58

Cyclo[17]carbon:

C	3.49012600	-0.43174000	0.00013500
C	3.36534300	0.84604200	0.00011500
C	2.87747200	2.01392300	0.00008200
C	1.90903200	2.90001100	0.00003600
C	0.77925300	3.41486300	-0.00001200
C	-0.55568500	3.43526100	-0.00006200
C	-1.71927500	3.04859800	-0.00010100
C	-2.73902000	2.16587000	-0.00012800
C	-3.32428400	1.09696600	-0.00013700
C	-3.49093900	-0.24672000	-0.00012700
C	-3.19112400	-1.42673800	-0.00010200
C	-2.41512000	-2.53338400	-0.00006000
C	-1.38774000	-3.19587100	-0.00001300
C	-0.08133300	-3.49966300	0.00003900
C	1.13439200	-3.28389700	0.00008200
C	2.29608000	-2.65276700	0.00011800

C 3.05282300 -1.65075500 0.00013400

Frequencies (cm⁻¹):

36.44 64.55 70.92 83.69 84.09 171.65 172.36 191.45 191.99 277.36 294.66 309.41 326.86 391.73 393.29
396.85 405.63 410.27 437.00 447.62 454.82 458.72 461.86 467.99 471.54 477.99 481.62 482.05 500.75
502.65 649.77 672.04 990.29 991.48 1327.32 1327.40 1519.56 1758.18 1816.24 1982.85 2032.68
2104.11 2152.74 2205.93 2237.04

P3:

O	0.00000000	0.00000000	11.97901400
O	0.00000000	0.00000000	-11.97901400
C	0.00000000	0.00000000	-9.54443600
C	0.00000000	0.00000000	-8.27274200
C	0.00000000	0.00000000	-7.00071100
C	0.00000000	0.00000000	-5.72705500
C	0.00000000	0.00000000	-4.45517200
C	0.00000000	0.00000000	-3.18149900
C	0.00000000	0.00000000	-1.90957300
C	0.00000000	0.00000000	-0.63598300
C	0.00000000	0.00000000	0.63598300
C	0.00000000	0.00000000	1.90957300
C	0.00000000	0.00000000	3.18149900
C	0.00000000	0.00000000	4.45517200
C	0.00000000	0.00000000	5.72705500
C	0.00000000	0.00000000	7.00071100
C	0.00000000	0.00000000	8.27274200
C	0.00000000	0.00000000	9.54443600
C	0.00000000	0.00000000	10.82135500
C	0.00000000	0.00000000	-10.82135500

Frequencies (cm⁻¹):

10.99 10.99 27.55 27.55 50.65 50.65 79.37 79.37 114.53 114.53 157.39 157.39 206.01 208.15 208.15
266.88 266.88 351.86 351.86 411.02 429.65 429.65 465.33 465.33 491.12 491.12 509.54 509.54 522.27
522.27 530.50 530.50 535.15 535.15 557.95 557.95 557.97 557.97 616.27 819.23 1019.39 1214.09
1402.29 1581.28 1749.87 1891.59 1955.53 2019.50 2093.77 2127.00 2208.77 2246.66 2256.70 2312.96
2343.71

Optimized structures of singlets at ω B97XD/6-311G level:**

Cyclo[18]carbon

C	-3.63813500	-0.68129600	0.00000300
C	-3.21506000	-1.82832800	0.00000800
C	-2.34782000	-2.85764900	0.00000900
C	-1.28620800	-3.46397200	0.00000700
C	0.03960400	-3.69575700	0.00000600
C	1.24290300	-3.47966800	0.00000500
C	2.40844200	-2.80666100	0.00000200
C	3.19204500	-1.86824200	0.00000200
C	3.65206300	-0.60331800	0.00000100
C	3.64740800	0.61923500	0.00000000
C	3.18488300	1.88323400	-0.00000200
C	2.39474800	2.81616400	-0.00000500
C	1.22783000	3.48688200	-0.00000800
C	0.02301500	3.69452000	-0.00000500
C	-1.30224900	3.45976600	-0.00000700
C	-2.35936100	2.84565200	-0.00000900
C	-3.22468700	1.81475700	-0.00000400
C	-3.63942400	0.66467900	-0.00000100

Frequencies (cm⁻¹):

59.24 59.25 75.29 76.64 137.81 160.63 160.67 176.67 177.08 280.19 280.24 291.86 292.24 391.46
391.64 405.81 406.00 419.16 419.84 432.77 459.09 459.13 468.02 473.97 474.06 482.20 482.55 525.52
525.97 526.12 527.06 614.55 615.41 944.38 944.54 1274.51 1274.57 1517.28 1517.44 1928.43 2142.02
2142.43 2249.67 2249.81 2251.96 2252.14 2313.53 2313.68

Cyclo[17]carbon

C	-2.61753800	-2.30850100	0.00043300
C	-1.54957400	-3.13919700	0.00034200
C	-0.35677800	-3.41678700	0.00022200
C	0.98426600	-3.36112300	0.00004700
C	2.05412500	-2.73752600	-0.00008300
C	3.04218000	-1.86126800	-0.00026900
C	3.37931000	-0.64032500	-0.00032200
C	3.53932800	0.63578400	-0.00046000
C	2.92891100	1.78862700	-0.00041500
C	2.17076200	2.78332500	-0.00041500
C	0.93835400	3.29071100	-0.00027700
C	-0.27686600	3.48213900	-0.00016300
C	-1.56579200	3.08550400	0.00002100
C	-2.57306200	2.39471400	0.00016700
C	-3.28758900	1.24276200	0.00031500
C	-3.52689400	0.04791000	0.00040700
C	-3.28314100	-1.28674900	0.00045000

Frequencies (cm⁻¹):

10.18 60.95 82.16 83.78 119.17 166.28 173.66 192.68 192.83 245.68 257.80 258.75 310.60 315.72
323.31 361.77 399.18 413.57 426.31 430.50 448.11 457.64 460.92 475.83 476.06 497.28 498.13 525.28
529.65 617.92 659.77 808.99 991.89 1000.16 1326.29 1327.02 1518.47 1728.11 1935.97 2056.54
2113.12 2152.40 2191.75 2248.00 2259.76

Cyclo[16]carbon

C	-1.37899100	3.00621200	0.00009100
C	-2.36938600	2.30215900	0.00006900
C	-3.10063700	1.15062000	0.00003300
C	-3.30328900	-0.04751700	-0.00000400
C	-3.00623400	-1.37894900	-0.00004500
C	-2.30222500	-2.36938500	-0.00007400

C	-1.15060300	-3.10050500	-0.00009600
C	0.04752500	-3.30320600	-0.00010100
C	1.37896100	-3.00615700	-0.00009100
C	2.36941700	-2.30218000	-0.00006900
C	3.10061300	-1.15060000	-0.00003300
C	3.30327100	0.04753200	0.00000400
C	3.00629800	1.37899200	0.00004500
C	2.30217700	2.36933700	0.00007400
C	1.15062600	3.10057400	0.00009600
C	-0.04752100	3.30307300	0.00010100

Frequencies (cm⁻¹):

72.70 73.90 93.23 94.47 99.94 194.31 194.31 212.45 212.45 315.37 318.31 340.65 366.06 430.72 432.77
 432.77 446.84 446.84 447.57 447.57 479.03 480.89 490.29 504.90 504.90 505.65 506.62 666.10 666.12
 1010.59 1011.12 1330.17 1330.17 1479.92 2151.12 2222.17 2222.19 2273.69 2273.71 2303.36 2304.55
 2306.73

P3

O	12.01922400	-0.11295000	0.06392500
O	-12.01921100	-0.11336800	-0.06360600
C	-9.58848100	0.01265500	0.04282400
C	-8.30346100	0.01350500	0.03330300
C	-7.04282100	0.02378700	0.03363100
C	-5.74205600	0.02758100	0.02747100
C	-4.49199600	0.03091200	0.02180400
C	-3.18092300	0.03347000	0.01548800
C	-1.93698100	0.03507200	0.00949200
C	-0.62101200	0.03589400	0.00296300
C	0.62100900	0.03585300	-0.00309300
C	1.93697800	0.03495100	-0.00961500
C	3.18092000	0.03328600	-0.01559700
C	4.49199300	0.03067800	-0.02189200
C	5.74205300	0.02732900	-0.02754200
C	7.04281800	0.02353100	-0.03368000
C	8.30345800	0.01330200	-0.03332400
C	9.58847800	0.01247500	-0.04284200
C	10.86009000	-0.06117800	0.02112000
C	-10.86008300	-0.06134600	-0.02093800

Frequencies (cm⁻¹):

8.94 21.97 25.64 42.72 46.36 69.18 72.95 105.16 108.58 150.78 153.15 194.43 204.63 206.14 265.87
 266.63 354.60 355.07 401.40 421.91 421.92 454.53 454.67 484.92 486.14 486.85 487.29 501.94 502.01
 515.56 515.63 534.15 534.42 543.26 544.19 570.38 584.88 604.59 804.25 964.09 999.87 1188.43
 1367.86 1531.03 1758.09 1771.01 1795.04 2045.37 2073.71 2111.23 2173.03 2176.17 2305.62 2324.53

Optimized structures of triplets at ωB97XD/6-311G level:****Cyclo[17]carbon**

C	3.48238200	-0.55117300	0.00013500
C	3.39494300	0.73245400	0.00011400
C	2.95054300	1.91900500	0.00008400
C	2.00708600	2.83545500	0.00003800
C	0.89625400	3.39322900	-0.00001100
C	-0.43966900	3.45550900	-0.00006200
C	-1.61829700	3.11125900	-0.00010200
C	-2.66669600	2.25995700	-0.00013000
C	-3.28975600	1.21037700	-0.00013800
C	-3.50163600	-0.12832200	-0.00012700
C	-3.24176300	-1.31994000	-0.00010100
C	-2.50498600	-2.45482600	-0.00005900
C	-1.49717700	-3.15035400	-0.00001200
C	-0.20095600	-3.50210700	0.00004100
C	1.02300100	-3.32224500	0.00008300
C	2.20941800	-2.73459300	0.00011700
C	2.99730900	-1.75368300	0.00013200

Frequencies (cm⁻¹):

11.44 63.88 69.45 81.70 83.43 170.35 171.04 189.82 190.12 275.24 291.57 306.92 325.23 355.61 386.86
389.72 403.70 409.20 434.89 442.94 454.65 458.20 468.21 468.32 469.25 470.58 484.15 502.42 505.25
515.75 648.52 667.69 988.57 989.78 1326.44 1326.95 1520.95 1755.26 1823.06 1988.38 2032.90
2105.44 2155.57 2211.33 2245.56

Cyclo[16]carbon

C	-2.24896500	-2.44895100	0.00009400
C	-1.12550700	-3.02925300	0.00006600
C	0.14168200	-3.32036300	0.00003600
C	1.34820600	-2.93936100	-0.00000500
C	2.44685600	-2.24782900	-0.00004500
C	3.03280000	-1.12316300	-0.00007500
C	3.31958000	0.13904600	-0.00009700
C	2.93728200	1.35192500	-0.00010000
C	2.25053400	2.44532600	-0.00009100
C	1.11946700	3.03088000	-0.00006700
C	-0.13777200	3.32117900	-0.00003100
C	-1.35012400	2.93401000	0.00000400
C	-2.44752300	2.25111900	0.00004500
C	-3.02761900	1.12193500	0.00007100
C	-3.32246900	-0.14032800	0.00009700
C	-2.93642900	-1.34617200	0.00009700

Frequencies (cm⁻¹):

68.13 68.82 90.78 91.64 185.41 185.58 202.44 202.86 247.39 258.95 275.86 279.57 331.49 358.20
393.83 394.65 396.00 396.16 401.76 418.49 419.72 467.11 467.45 471.68 524.74 525.82 582.57 623.45
645.69 672.18 744.91 762.01 1081.35 1081.96 1456.99 1457.20 1727.36 1856.60 2028.73 2029.08
2075.23 2076.15

P3

O	11.99245100	0.02626300	0.00096800
O	-11.99249700	0.01114100	-0.00615600
C	-9.55625500	0.01331500	-0.00040300
C	-8.28333500	0.00828600	0.00130900
C	-7.00951000	0.00464900	0.00298300
C	-5.73439100	0.00048000	0.00406700
C	-4.46078200	-0.00302900	0.00461700

C	-3.18556400	-0.00674100	0.00433700
C	-1.91197000	-0.01007100	0.00344000
C	-0.63678100	-0.01327700	0.00201900
C	0.63680900	-0.01604400	0.00038900
C	1.91200000	-0.01806700	-0.00111800
C	3.18559200	-0.01850300	-0.00238300
C	4.46081200	-0.01763400	-0.00314400
C	5.73440400	-0.01315000	-0.00310400
C	7.00951700	-0.00717100	-0.00222000
C	8.28332400	0.00259000	-0.00120700
C	9.55621900	0.01320900	0.00029200
C	10.83351400	0.01966100	0.00053700
C	-10.83354400	0.01162500	-0.00349300

Frequencies (cm⁻¹):

6.39 21.38 23.45 43.70 43.85 68.82 68.97 103.00 103.56 148.88 148.95 204.19 204.26 205.54 267.29
267.32 355.25 355.27 410.24 430.20 430.24 459.58 459.66 489.05 489.15 497.23 497.32 510.93 510.96
519.67 519.69 524.76 524.77 554.97 554.99 555.00 555.02 615.35 818.35 1018.59 1213.30 1401.54
1580.63 1749.80 1892.83 1962.61 2021.88 2104.80 2130.39 2213.20 2253.95 2262.10 2326.80 2358.03

Int0

O	-6.02768700	0.58669700	0.10392800
O	-6.22914800	-0.57308700	0.31298000
C	-1.92506600	-2.37485200	-0.12440300
C	-0.99777800	-3.17103900	-0.09590900
C	0.26135300	-3.64502600	-0.05595300
C	1.48324800	-3.65707400	-0.01715300
C	2.75151000	-3.20821500	0.02414600
C	3.69438300	-2.43059400	0.05504100
C	4.37719800	-1.27093700	0.07834700
C	4.60025900	-0.06892900	0.08718200
C	4.37995600	1.25884600	0.08207500
C	3.78020300	2.32404100	0.06463300
C	2.75940500	3.20069100	0.03326700
C	1.61574000	3.63128400	-0.00296700
C	0.27054200	3.64504800	-0.04677200
C	-0.88144400	3.23738600	-0.08460000
C	-1.91921400	2.38102200	-0.11898200
C	-2.53941200	1.32773000	-0.13999800
C	-2.78370900	0.00431100	-0.14955900
C	-2.58472900	-1.20184000	-0.14427300

Frequencies (cm⁻¹):

6.20 8.77 20.94 44.49 58.37 61.78 72.02 75.11 76.53 126.32 160.58 162.73 176.47 176.81 279.96 281.00
291.66 291.99 391.22 391.79 405.85 406.07 416.16 418.31 433.20 458.34 459.00 468.89 472.23 474.07
482.63 482.87 525.55 526.28 527.28 530.16 614.79 615.44 944.35 944.54 1274.45 1274.50 1517.18
1517.37 1719.36 1928.71 2141.80 2142.20 2249.07 2250.00 2251.85 2251.94 2313.35 2313.44

Int1

O	5.71842200	-0.66787500	-0.00008000
O	5.03973200	0.44449900	0.00006700
C	2.90753900	1.42854900	0.00026800
C	1.95989900	2.21358000	0.00013500
C	0.81915500	2.89529900	-0.00007700
C	-0.37787500	3.21937000	-0.00015800
C	-1.69498200	3.27344700	0.00003100
C	-2.88420000	2.88257500	-0.00041400
C	-3.95726700	2.14008200	0.00038700
C	-4.58204000	1.03691300	-0.00051400
C	-4.81631400	-0.22948400	0.00052800

C	-4.42575000	-1.45534400	-0.00017700
C	-3.66697800	-2.47258200	0.00032100
C	-2.51169900	-3.07683300	0.00008000
C	-1.28228800	-3.31752300	-0.00005700
C	0.01821600	-3.10851300	-0.00019900
C	1.16806400	-2.64229900	-0.00025100
C	2.22202300	-1.83422100	-0.00009800
C	3.07367300	-0.94541400	0.00005900
C	3.68662000	0.29023200	0.00015300

Frequencies (cm⁻¹):

37.99 53.18 57.02 72.46 95.00 124.09 148.37 152.81 181.40 189.38 211.70 251.86 290.32 291.93 303.66
354.85 360.37 380.70 391.34 391.99 407.36 430.71 435.45 451.00 460.69 465.48 474.75 484.08 505.62
509.40 524.09 540.14 574.83 576.43 593.14 610.29 635.31 704.09 887.06 975.63 1104.95 1243.34
1280.83 1312.84 1498.91 1551.75 1659.02 1773.57 1885.83 1995.21 2083.56 2090.71 2119.15 2166.74

Int2

O	-4.96638300	-0.73277200	-0.00005500
O	-4.96638000	0.73272800	-0.00002000
C	-2.70157700	1.71847500	0.00003100
C	-1.65181900	2.39960500	0.00003600
C	-0.46041100	2.97054300	0.00001400
C	0.74984300	3.21882000	-0.00001100
C	2.08844300	3.15023000	-0.00004600
C	3.22643300	2.69968400	0.00005100
C	4.22660500	1.78882900	-0.00009800
C	4.72940100	0.67854600	-0.00000800
C	4.72935200	-0.67850900	-0.00003500
C	4.22666000	-1.78883800	-0.00014100
C	3.22643700	-2.69964000	0.00008500
C	2.08848300	-3.15026800	-0.00015500
C	0.74987600	-3.21880800	0.00000400
C	-0.46037900	-2.97054300	0.00006700
C	-1.65175400	-2.39953600	0.00009300
C	-2.70157000	-1.71849500	0.00009500
C	-3.58516900	-0.73545000	0.00005200
C	-3.58517100	0.73541300	0.00006500

Frequencies (cm⁻¹):

42.20 53.53 56.40 60.09 108.52 134.86 140.17 157.71 195.81 200.76 244.67 268.46 287.12 307.89
329.28 363.54 367.76 374.23 386.31 392.08 400.06 428.63 434.33 446.31 459.01 469.97 471.47 476.34
481.63 519.48 528.90 531.67 549.80 610.76 612.89 706.03 899.36 928.75 1001.52 1049.85 1211.03
1226.93 1289.89 1382.72 1457.30 1631.76 1696.79 1900.75 2070.73 2111.32 2146.97 2198.40 2226.60
2254.44

Int3

O	-4.87571400	-1.50417300	-0.00021100
O	-5.10508200	1.26774000	-0.00009300
C	-2.76534800	1.48448200	0.00015800
C	-1.71293100	2.08108000	0.00024100
C	-0.46420800	2.61625300	0.00023300
C	0.70866500	2.93242100	0.00027600
C	2.06254300	2.94735900	0.00004600
C	3.23725700	2.62620800	-0.00014400
C	4.30033100	1.78912600	-0.00023600
C	4.88642300	0.71890300	-0.00025500
C	4.88748600	-0.63340600	-0.00018700
C	4.37509800	-1.74246500	-0.00007200
C	3.31254900	-2.57386200	0.00003300
C	2.14869000	-2.94984600	0.00014000

C	0.80538900	-2.91765000	0.00019700
C	-0.38276700	-2.61605200	0.00024500
C	-1.60187600	-2.06554700	0.00003500
C	-2.63903500	-1.40388100	-0.00021000
C	-3.84021400	-0.72548500	-0.00011000
C	-4.01032300	0.74760700	0.00001400

Frequencies (cm⁻¹):

40.34 46.13 51.43 56.36 82.46 115.55 122.09 154.36 159.40 200.28 212.10 241.10 248.19 283.67 308.84
 309.24 349.55 365.88 380.29 385.61 411.70 414.86 444.19 458.69 460.49 468.93 482.26 483.64 522.88
 536.21 555.37 566.64 608.32 633.06 658.72 677.29 706.66 869.04 940.58 1101.87 1180.58 1283.27
 1321.01 1433.50 1512.29 1688.44 1754.43 2110.48 2149.21 2187.24 2228.85 2253.34 2297.98 2343.75

Int4

O	4.89090500	1.65267200	-0.00036600
O	4.89089300	-1.65268300	0.00012100
C	2.56478300	-0.73038700	0.00008800
C	1.54111400	-1.59539200	0.00021600
C	0.48960500	-2.25988700	0.00031800
C	-0.75538700	-2.70211800	0.00036200
C	-1.98361900	-2.84677300	0.00035900
C	-3.27511400	-2.51596800	0.00030900
C	-4.27838300	-1.80427300	0.00020900
C	-4.89800500	-0.61382100	0.00007000
C	-4.89802900	0.61382400	-0.00005700
C	-4.27837300	1.80425900	-0.00017900
C	-3.27512500	2.51598300	-0.00023800
C	-1.98361900	2.84675700	-0.00026200
C	-0.75538600	2.70213200	-0.00023000
C	0.48960200	2.25987600	-0.00018900
C	1.54112700	1.59541300	-0.00015100
C	2.56479000	0.73039400	-0.00010900
C	4.07381300	0.79321300	-0.00020800
C	4.07380900	-0.79321700	0.00001800

Frequencies (cm⁻¹):

33.83 48.78 64.79 65.68 107.54 109.79 139.53 185.15 207.17 217.86 218.28 249.09 262.10 304.84
 314.10 323.86 349.31 380.63 407.69 411.80 418.29 432.62 433.38 441.47 451.38 462.68 469.64 470.70
 475.71 520.53 531.67 587.82 644.38 708.42 759.17 796.27 860.85 930.07 990.31 1033.35 1078.96
 1254.65 1302.68 1441.12 1543.40 1613.73 1878.37 1910.22 1921.46 2084.27 2114.65 2137.57 2195.06
 2195.87

Int5

O	-4.89067900	1.79379400	-0.00033800
O	-4.89195300	-1.79234400	0.00051700
C	-2.63939400	-0.71812000	-0.00940600
C	-1.56010700	-1.59385300	0.00364100
C	-0.50820100	-2.20612200	-0.00379600
C	0.76025700	-2.68087700	0.00084700
C	1.97187300	-2.80454100	0.00060200
C	3.29499400	-2.51087800	0.00132400
C	4.28706600	-1.80327800	0.00074000
C	4.93354400	-0.60978500	0.00007000
C	4.93363300	0.60924900	-0.00119800
C	4.28784600	1.80315300	-0.00161900
C	3.29573500	2.51069600	-0.00180800
C	1.97259400	2.80460200	-0.00067700
C	0.76105800	2.68033200	-0.00056200
C	-0.50748000	2.20571200	0.00427500

C	-1.55916900	1.59310600	-0.00295900
C	-2.63894700	0.71792000	0.00997800
C	-4.02054900	1.02059100	0.00235500
C	-4.02124300	-1.01983900	-0.00204800

Frequencies (cm⁻¹):

39.90 53.89 63.27 66.65 109.28 119.15 125.78 143.35 189.73 208.48 225.16 243.91 306.01 311.05
316.39 337.77 342.84 376.98 405.86 418.30 426.17 427.10 436.46 462.16 468.10 474.39 482.64 486.25
502.59 528.44 545.29 561.14 577.71 582.57 610.46 676.84 693.35 940.36 946.54 1090.62 1173.00
1314.03 1324.66 1485.88 1530.25 1956.69 2018.81 2151.05 2168.78 2180.92 2223.09 2246.67 2277.19
2281.68

Int6

O	-4.88185900	2.42901500	1.42608200
O	-4.94197600	-1.66254600	-0.60074500
C	-2.54922000	-1.02586100	-0.40140600
C	-1.55614800	-2.01760600	-0.17268400
C	-0.48152300	-2.55579200	0.01072900
C	0.80266600	-2.93354400	0.19800100
C	2.02355800	-2.87462300	0.32517700
C	3.29623100	-2.48367500	0.41692100
C	4.20648100	-1.62987100	0.41082300
C	4.86145900	-0.49588200	0.34212100
C	4.77060400	0.76854800	0.17524900
C	4.29343500	1.93815700	-0.02141000
C	3.20889600	2.64580200	-0.22882700
C	2.02063500	2.98551600	-0.40146300
C	0.71315900	2.74318900	-0.51536500
C	-0.40105400	2.22830000	-0.57314800
C	-1.37910200	1.29542200	-0.56303800
C	-2.10041500	0.31762900	-0.51948500
C	-4.78672800	1.42855400	0.92264100
C	-3.84448800	-1.35622300	-0.50528600

Frequencies (cm⁻¹):

10.01 22.21 41.84 63.76 64.25 73.96 82.85 92.48 106.60 113.74 123.26 178.04 192.66 205.57 210.61
286.36 316.26 335.92 346.43 401.28 403.32 415.94 417.22 419.65 438.24 455.57 464.14 469.69 481.81
487.59 497.66 500.48 520.29 542.44 552.37 563.46 663.38 720.86 954.50 985.36 1046.24 1256.39
1292.28 1417.52 1485.16 1721.66 1829.22 1983.58 2107.09 2117.80 2227.63 2233.22 2264.49 2287.43

Int7

O	6.52971500	0.30952000	0.00023200
C	2.29248000	-0.49201700	-0.00045400
C	1.94889800	-1.71853400	-0.00039200
C	1.01105200	-2.60054600	-0.00024800
C	-0.10461200	-3.22202200	-0.00007700
C	-1.39118200	-3.18942900	0.00011600
C	-2.61778800	-2.83888600	0.00029000
C	-3.51175800	-1.90751500	0.00041600
C	-4.12682100	-0.79552100	0.00050000
C	-4.09955200	0.50123400	0.00048600
C	-3.74915700	1.71706000	0.00042900
C	-2.80702000	2.61535700	0.00028100
C	-1.70342300	3.22806400	0.00011300
C	-0.40151700	3.19155600	-0.00008700
C	0.81464100	2.84910000	-0.00026000
C	1.70524500	1.90383800	-0.00038800
C	2.32988600	0.80028800	-0.00046500
C	5.70433800	-0.45472100	-0.00056800

Frequencies (cm⁻¹):

41.37 65.00 65.63 90.99 105.79 107.41 178.83 192.60 204.34 210.50 285.78 315.17 336.30 347.64
403.19 403.31 416.42 416.60 420.24 439.96 456.22 463.66 471.20 483.84 487.68 498.43 501.77 521.92
543.57 551.95 567.41 663.41 720.22 954.89 985.03 1046.91 1257.05 1291.84 1416.75 1485.20 1722.16
1830.07 1984.53 2107.47 2118.11 2230.09 2237.06 2286.21

Int8

O	-6.46457400	0.31518800	-0.00002100
C	-2.22998500	-0.51430800	0.00043200
C	-1.95018600	-1.76583500	0.00038600
C	-0.94689400	-2.56681500	0.00023800
C	0.13571700	-3.25737000	0.00007800
C	1.41080500	-3.11503600	-0.00010800
C	2.66583800	-2.83913700	-0.00029000
C	3.46615600	-1.83702900	-0.00040300
C	4.15867100	-0.75414500	-0.00049900
C	4.01394200	0.52025400	-0.00047200
C	3.73727100	1.77513200	-0.00042800
C	2.73292700	2.57399600	-0.00027900
C	1.65074600	3.26522700	-0.00012000
C	0.37464500	3.12056600	0.00006700
C	-0.87871300	2.84555000	0.00024900
C	-1.68094500	1.84175300	0.00036200
C	-2.37550500	0.76318400	0.00045700
C	-5.66505800	-0.47623600	0.00035800

Frequencies (cm⁻¹):

5.16 18.06 25.22 40.34 59.29 59.81 90.56 92.45 98.58 154.07 156.01 210.85 214.29 214.48 323.35
358.48 383.53 432.33 432.53 451.99 454.14 458.95 463.80 468.00 468.75 475.81 476.79 492.85 493.09
534.76 535.94 686.85 688.38 699.33 787.65 789.07 1091.53 1091.93 1110.75 1457.68 1458.39 1723.06
1849.21 2025.99 2026.78 2100.42 2100.71 2257.77

Int9

O	-4.39531200	1.73931800	0.00001200
O	-5.59707200	-1.44746900	-0.00003600
C	-3.35356100	-0.38278700	-0.00005500
C	-2.20711100	-1.20310500	-0.00001900
C	-1.17588000	-1.84506200	0.00000700
C	0.04037700	-2.43163400	0.00005000
C	1.22835900	-2.73842800	0.00007100
C	2.56228800	-2.78195800	0.00007900
C	3.71915100	-2.32130900	0.00007600
C	4.72970900	-1.48143200	0.00005100
C	5.02758400	-0.23851700	0.00000800
C	4.88319900	1.03203600	-0.00002200
C	3.98257600	1.98834300	-0.00007100
C	2.89635100	2.59692300	-0.00010400
C	1.56902000	2.73803400	-0.00008800
C	0.35070200	2.60000500	-0.00004100
C	-0.94172000	2.20389700	0.00005700
C	-2.05617500	1.72519700	0.00011600
C	-3.36307700	1.10734900	0.00000900
C	-4.56861300	-0.95668400	-0.00009000

Frequencies (cm⁻¹):

34.88 49.42 56.08 60.68 92.59 114.45 120.57 151.49 169.11 185.53 214.75 233.56 274.54 300.67 337.50
341.06 375.60 380.31 395.90 404.35 424.44 426.56 441.06 459.25 470.22 482.65 485.60 493.79 500.50
554.51 558.49 581.90 595.89 617.38 677.89 714.18 801.35 914.90 965.47 1081.62 1155.24 1219.47
1320.20 1399.07 1489.52 1713.90 1754.73 1849.60 1990.61 2133.11 2139.65 2252.14 2265.21 2294.39

Int10

O	4.42878600	-1.08813900	0.00013600
O	5.58707300	0.95950500	-0.00027600
C	3.09715100	0.51544900	0.00007400
C	2.12202800	1.49835200	0.00003400
C	1.12308600	2.19962100	-0.00002700
C	-0.08600700	2.78216300	0.00001700
C	-1.30010800	3.00719500	-0.00013900
C	-2.62044800	2.91573000	-0.00004200
C	-3.72919300	2.32540000	-0.00010200
C	-4.63385900	1.39305600	-0.00018600
C	-4.88336400	0.12955700	-0.00022200
C	-4.71504200	-1.12659800	0.00005700
C	-3.85835900	-2.12882500	0.00031600
C	-2.81235800	-2.79640300	-0.00000100
C	-1.48823500	-2.98417400	-0.00027000
C	-0.26746300	-2.87781600	-0.00021700
C	0.99113300	-2.39119100	0.00025900
C	2.05460400	-1.80140900	0.00049100
C	3.07134200	-0.85393200	0.00025100
C	4.58061300	0.36533700	-0.00010900

Frequencies (cm⁻¹):

36.83 58.85 61.37 70.30 97.48 139.53 146.59 166.45 189.56 224.25 230.96 284.26 292.56 321.64 338.70
 377.60 388.03 390.64 400.35 422.35 430.98 443.27 460.54 464.46 474.78 481.20 494.19 500.12 505.14
 528.19 568.45 572.93 579.01 640.55 702.00 730.94 778.01 848.86 910.40 998.52 1087.57 1231.33
 1328.63 1379.03 1529.67 1627.86 1745.68 1829.05 2002.01 2025.57 2074.21 2154.02 2196.83 2269.04

Int11

O	-5.29306300	-1.03916500	-0.00006400
O	-5.29200400	1.04127200	0.00001800
C	-3.12882900	0.00020700	-0.00006400
C	-2.40019400	1.18115500	0.00001200
C	-1.53170600	2.04315500	0.00006800
C	-0.39300700	2.76550200	0.00008600
C	0.77583200	3.11685500	0.00009700
C	2.12886000	3.10894600	0.00010200
C	3.27339400	2.69106000	0.00009800
C	4.28432000	1.78655800	0.00008200
C	4.78922000	0.67844100	0.00005800
C	4.78892800	-0.67930700	0.00002500
C	4.28230500	-1.78661900	-0.00000600
C	3.27190400	-2.69171500	-0.00003800
C	2.12709400	-3.10876400	-0.00006200
C	0.77402500	-3.11885800	-0.00007900
C	-0.39439500	-2.76611100	-0.00008700
C	-1.53295400	-2.04339800	-0.00008700
C	-2.40072000	-1.18073900	-0.00008300
C	-4.60065400	0.00082200	-0.00006200

Frequencies (cm⁻¹):

32.57 59.37 59.42 68.13 93.24 98.24 98.85 164.14 188.83 194.68 201.44 286.81 295.86 304.62 308.89
 323.67 350.75 371.33 386.57 408.87 417.46 418.31 419.71 449.42 463.48 467.17 470.35 479.57 483.83
 493.39 522.68 526.84 530.85 614.71 652.68 690.02 695.60 890.40 964.06 1009.87 1130.21 1244.40
 1334.98 1433.49 1492.40 1587.57 1845.68 2142.68 2146.45 2179.09 2212.08 2246.79 2273.06 2276.77

Int12

O	5.53163700	1.15505000	-0.00059100
O	5.53109000	-1.15765600	0.00001100
C	2.25221800	-0.61070300	-0.00013600
C	1.77126200	-1.87721200	-0.00012400

C	0.93277400	-2.76668200	-0.00002800
C	-0.26414900	-3.38306900	0.00011500
C	-1.49436700	-3.46566700	0.00027600
C	-2.78196000	-3.13467800	0.00037400
C	-3.75419600	-2.34610600	0.00042400
C	-4.48085200	-1.26316300	0.00028400
C	-4.66427900	0.00232300	0.00002600
C	-4.47930300	1.26349200	-0.00005900
C	-3.75102000	2.35000600	-0.00019500
C	-2.77933300	3.13429500	0.00005100
C	-1.48954500	3.46810600	0.00011900
C	-0.26142300	3.38247000	0.00011700
C	0.93792100	2.76723600	0.00003500
C	1.77250100	1.87526300	-0.00004500
C	2.25526700	0.60886600	-0.00014300
C	5.52818200	-0.00130200	-0.00031700

Frequencies (cm⁻¹):

12.19 19.07 26.15 48.09 62.79 73.26 78.19 83.38 84.18 131.71 171.97 173.53 190.97 191.69 275.64
294.04 308.33 325.94 369.62 388.14 389.75 406.49 410.21 435.86 446.34 452.13 457.73 470.44 470.49
471.49 476.45 495.10 505.79 520.25 523.08 648.94 669.41 672.45 677.58 988.61 990.54 1326.77
1326.98 1402.77 1520.88 1754.69 1823.74 1979.66 2053.41 2091.26 2169.35 2212.08 2249.49 2474.22

Int13

O	-4.25543300	1.32905000	-0.11039600
O	-6.81524500	-0.96125800	0.11003000
C	-2.49753700	-0.26131300	-0.08225900
C	-1.80247100	-1.26673100	-0.07929900
C	-0.82277700	-2.17184300	-0.07030100
C	0.22238000	-2.83815600	-0.05878600
C	1.50676700	-3.10466300	-0.03833700
C	2.76418000	-3.06651000	-0.01710300
C	3.87681300	-2.40738400	0.00873500
C	4.73045600	-1.46384100	0.03251000
C	4.95096800	-0.19747500	0.04811100
C	4.73853500	1.05779800	0.05767700
C	3.94451600	2.08000500	0.05343100
C	2.88938300	2.76568000	0.04307400
C	1.60633800	3.05191100	0.02332800
C	0.37015600	2.97987700	0.00140200
C	-0.90827600	2.58523500	-0.02548900
C	-1.98431600	2.00870000	-0.05034800
C	-3.07395600	1.05919200	-0.08359000
C	-5.75025600	-1.30087100	0.23773100

Frequencies (cm⁻¹):

5.77 9.13 21.65 43.05 53.58 63.01 68.17 79.32 106.78 124.64 167.09 168.55 176.55 196.59 254.98
264.20 270.09 288.70 310.51 356.69 359.79 380.52 397.83 410.77 425.69 432.96 446.80 457.35 463.39
486.99 510.24 530.34 544.90 574.53 623.04 664.80 679.22 768.78 958.95 966.09 1130.59 1239.77
1302.47 1466.57 1665.41 1709.72 1755.77 1945.48 2009.22 2084.63 2132.19 2190.23 2209.82 2256.76

Int14

O	5.19874200	-0.04867900	0.00041400
C	3.11352100	-1.17271000	0.00035400
C	2.20439500	-1.98864200	0.00028900
C	1.03814700	-2.64014900	0.00003600
C	-0.13445500	-3.03783900	-0.00019400
C	-1.44757800	-2.99512700	-0.00038400
C	-2.65787600	-2.65633000	-0.00041300
C	-3.58549700	-1.75275400	-0.00017000

C	-4.18505800	-0.63147500	0.00011000
C	-4.10256500	0.65191100	0.00040100
C	-3.59526000	1.81917500	0.00058300
C	-2.58664000	2.62998900	0.00043100
C	-1.39864300	3.04541000	0.00008800
C	-0.08438300	3.02628500	-0.00052100
C	1.09882900	2.65965500	-0.00074300
C	2.24913600	1.97630300	-0.00047800
C	3.15384800	1.15619600	-0.00015300
C	3.98842400	-0.02499200	0.00021000

Frequencies (cm⁻¹):

41.35 58.87 64.21 80.87 104.13 159.60 167.66 178.04 192.16 230.70 261.47 266.11 288.30 309.35
344.28 354.30 374.75 396.24 411.31 423.37 431.96 446.75 463.78 464.74 493.29 507.74 535.88 543.39
599.25 626.48 666.17 677.45 788.58 958.43 965.15 1137.30 1246.14 1301.19 1464.70 1664.86 1717.03
1792.55 1948.09 2014.61 2085.50 2134.87 2193.44 2215.54

TS0

O	-5.68792500	-0.68798600	-0.00176600
O	-5.17441900	0.42641500	-0.00016900
C	-2.74687100	1.51947600	0.00055300
C	-1.85803500	2.45812400	0.00052000
C	-0.81040300	3.15688200	0.00039400
C	0.46276000	3.46506200	0.00022700
C	1.70931400	3.43966600	0.00001900
C	2.93257100	2.93879000	-0.00018500
C	3.87996300	2.14053400	-0.00034700
C	4.49389700	0.96077900	-0.00042100
C	4.65192000	-0.26279300	-0.00041200
C	4.29402000	-1.54910000	-0.00029800
C	3.56438000	-2.53976100	-0.00014400
C	2.42773100	-3.24581600	0.00005800
C	1.22750000	-3.50584200	0.00023400
C	-0.10156500	-3.33826400	0.00039400
C	-1.21660200	-2.82745400	0.00047900
C	-2.21913300	-1.93674200	0.00052400
C	-2.87261600	-0.90086600	0.00051500
C	-3.33570500	0.37608600	0.00046900

Frequencies (cm⁻¹):

-708.28 24.07 51.41 56.02 60.09 77.06 92.61 94.76 146.13 171.25 177.03 186.06 258.69 279.67 292.06
298.70 323.08 349.72 369.67 398.77 402.12 408.41 412.47 431.10 436.27 447.44 455.29 481.71 482.49
484.02 504.49 519.64 527.95 546.69 575.10 608.97 628.22 662.85 915.32 943.24 983.63 1267.98
1289.07 1412.84 1530.88 1558.30 1828.07 1898.14 1998.46 2073.42 2138.07 2159.62 2217.06 2228.82

TS1

O	-5.25408300	0.73971000	0.00054700
O	-4.95916200	-0.62854900	0.00055100
C	-2.79416000	-1.65192700	-0.00038800
C	-1.78149800	-2.33047400	-0.00021300
C	-0.58999200	-2.95136800	-0.00012400
C	0.61500300	-3.19185800	-0.00003200
C	1.94695000	-3.20548500	0.00005400
C	3.09475300	-2.72979600	0.00013000
C	4.15233700	-1.94723800	0.00035900
C	4.65054700	-0.78489800	-0.00066900
C	4.80037300	0.49630900	0.00048300
C	4.26787300	1.67392200	-0.00054400
C	3.40313300	2.59244400	0.00057800
C	2.21271500	3.14712300	0.00001900

C	0.97063000	3.23429500	-0.00003400
C	-0.34236000	3.06754700	-0.00009100
C	-1.43154800	2.47163500	-0.00024800
C	-2.52684100	1.73678200	-0.00024300
C	-3.35478800	0.79858100	-0.00044700
C	-3.67546800	-0.57380900	-0.00005500

Frequencies (cm⁻¹):

-512.26 42.13 52.53 56.80 68.29 100.16 133.12 150.43 152.12 186.99 224.87 237.37 276.33 282.77
290.11 323.94 328.32 362.45 380.29 385.23 405.82 413.15 421.22 432.58 454.23 464.97 465.12 484.97
497.72 504.20 529.51 542.25 571.63 578.09 589.88 633.02 711.80 888.63 934.63 954.97 1014.78
1241.88 1279.28 1409.04 1505.45 1536.10 1761.46 1777.81 1891.43 2008.63 2077.62 2092.98 2145.23
2227.57

TS2

O	4.97502600	1.55934900	0.22918900
O	5.00783400	-1.48849300	-0.38555100
C	2.66317000	-1.06071000	-0.07477800
C	1.64083900	-1.75529600	-0.02960300
C	0.42692500	-2.30034800	0.04079800
C	-0.75669200	-2.63127600	0.09655900
C	-2.08049600	-2.75977300	0.13126500
C	-3.27519300	-2.43728100	0.12399000
C	-4.41226900	-1.76238600	0.07059600
C	-4.92548900	-0.61963600	0.00560500
C	-5.04753200	0.67575400	-0.10393500
C	-4.32059500	1.72372800	-0.12599700
C	-3.30833400	2.51132200	-0.14613200
C	-2.04240600	2.71285100	-0.10698600
C	-0.77181500	2.63623600	-0.02799400
C	0.43843700	2.23497500	0.04941200
C	1.60536600	1.70903900	0.14302800
C	2.65477100	0.99498500	0.22916200
C	4.08652200	0.76633400	0.10277600
C	4.11431300	-0.73299100	-0.16928300

Frequencies (cm⁻¹):

-682.73 36.77 41.32 58.06 61.21 100.37 104.72 141.67 171.88 195.48 202.21 237.75 281.00 291.64
292.35 309.17 328.89 351.47 389.15 394.40 410.65 414.82 432.27 437.03 447.41 459.81 464.36 482.15
485.52 511.08 533.73 566.70 646.43 659.45 673.34 682.85 787.56 889.68 904.80 945.44 1095.22
1135.76 1317.46 1380.71 1466.76 1625.43 1775.60 1815.41 1863.99 1910.56 2029.84 2061.31 2131.40
2155.57

TS3

O	-4.87494400	1.65202900	0.12213900
O	-4.87494400	-1.65202900	0.12213900
C	-2.57169400	-0.72924800	-0.12805400
C	-1.54801000	-1.62406700	-0.08465800
C	-0.50451600	-2.27532500	-0.06330700
C	0.75051700	-2.74240600	-0.02514800
C	1.97059800	-2.85651400	-0.00973600
C	3.27770600	-2.53466300	0.02440600
C	4.26085200	-1.80781900	0.03615100
C	4.88803800	-0.61099000	0.05135500
C	4.88803800	0.61099000	0.05135500
C	4.26085200	1.80781900	0.03615100
C	3.27770600	2.53466300	0.02440600
C	1.97059800	2.85651400	-0.00973600
C	0.75051700	2.74240600	-0.02514800
C	-0.50451600	2.27532500	-0.06330700

C	-1.54801000	1.62406700	-0.08465800
C	-2.57169400	0.72924800	-0.12805400
C	-4.02356500	0.84334900	0.03614000
C	-4.02356500	-0.84334900	0.03614000

Frequencies (cm⁻¹):

-2298.61 39.11 44.60 59.25 67.52 105.14 107.63 112.56 163.63 189.82 206.43 219.77 240.63 256.55
 273.27 315.07 331.54 335.99 348.78 407.13 410.85 416.16 425.05 432.09 436.26 456.82 468.08 471.31
 472.96 483.73 497.67 507.87 534.36 637.48 676.91 703.74 733.85 859.41 876.02 1034.09 1048.55
 1251.19 1307.65 1431.31 1503.74 1808.66 1855.33 1879.90 1973.33 2114.15 2164.44 2166.48 2238.83
 2239.46

TS4

O	4.98214500	1.91437700	-0.00011200
O	4.42496600	-2.52388400	-0.00269300
C	2.52348300	-0.56034700	0.00092700
C	1.50012700	-1.33676000	0.00178000
C	0.48181900	-2.11727900	0.00215500
C	-0.70778100	-2.61182000	0.00133400
C	-1.95679100	-2.82568100	0.00063300
C	-3.22851600	-2.52145500	0.00001500
C	-4.28543100	-1.85014800	-0.00050200
C	-4.86051900	-0.65256500	-0.00072000
C	-4.91789400	0.58354200	-0.00113100
C	-4.23960500	1.74381400	-0.00075900
C	-3.27613200	2.50192700	-0.00052800
C	-1.95923800	2.80526400	0.00019800
C	-0.74194000	2.74391600	-0.00003100
C	0.54364900	2.30660200	0.00044400
C	1.61725000	1.74399900	0.00063400
C	2.72739900	0.86142400	0.00073400
C	3.96402700	1.39189400	0.00023500
C	4.27327700	-1.39365100	-0.00167900

Frequencies (cm⁻¹):

-609.44 25.74 41.47 57.43 67.57 97.58 109.88 110.38 127.61 142.91 186.35 199.52 212.57 219.99
 270.48 323.08 340.87 343.21 347.08 373.43 411.40 415.55 422.57 427.82 436.97 451.15 454.19 467.18
 470.64 480.62 505.97 513.18 515.46 530.98 542.12 543.26 674.56 718.40 935.89 987.39 1065.01
 1252.80 1294.51 1404.86 1490.36 1687.83 1821.83 1971.64 2033.91 2098.39 2126.60 2224.20 2243.57
 2311.87

TS5

O	-5.94027000	0.00001400	-0.13152100
C	-2.99039700	-0.00000100	-0.23782100
C	-2.35720000	-1.17343900	-0.04341400
C	-1.55509500	-2.11840500	-0.06581900
C	-0.40943300	-2.79233800	0.01466100
C	0.80406300	-3.04405600	-0.00527400
C	2.12210300	-2.90988400	0.02908500
C	3.18580400	-2.24778200	0.00937200
C	4.04851400	-1.26575600	0.01593800
C	4.23259900	-0.00000200	0.00716700
C	4.04852000	1.26576700	0.01593400
C	3.18580900	2.24777500	0.00937100
C	2.12210400	2.90989100	0.02908000
C	0.80407100	3.04404500	-0.00527200
C	-0.40943200	2.79233200	0.01466100
C	-1.55508700	2.11839600	-0.06581300
C	-2.35719900	1.17343200	-0.04341100

C -4.99938400 0.00000400 0.49691600

Frequencies (cm⁻¹):

-389.37 22.90 27.49 62.46 71.14 88.67 93.58 152.16 156.35 188.69 190.50 211.87 240.06 300.71 313.52
320.01 321.17 326.69 384.88 395.09 400.72 405.06 423.86 430.59 447.76 455.47 463.33 473.55 486.22
497.33 512.41 552.49 625.37 719.62 808.18 1011.09 1042.12 1344.78 1374.70 1525.21 1727.44 1761.67
1818.79 2012.08 2064.42 2066.28 2068.87 2168.04

TS6

O -4.23605800 0.13536000 -1.91872300
O -4.64059300 0.04422600 1.90746000
C -2.96699400 -0.50948400 0.21295400
C -1.89298500 -1.42992300 0.10370800
C -0.87683900 -2.07689200 -0.02341700
C 0.37850400 -2.58859400 -0.09833800
C 1.57462400 -2.81252600 -0.14913400
C 2.91046700 -2.60514200 -0.13165700
C 3.97926900 -2.01216300 -0.08521000
C 4.72735300 -0.89562700 0.01724100
C 4.86466600 0.32251900 0.11312300
C 4.35320800 1.55762100 0.19024200
C 3.40967700 2.35901300 0.20861900
C 2.15555500 2.77979700 0.16695400
C 0.91134700 2.72643000 0.06553500
C -0.34468200 2.39779500 -0.07235200
C -1.44824600 1.81983000 -0.27905100
C -2.50467200 1.07924900 -0.42211400
C -3.44485700 0.27277500 -1.04621700
C -3.94986000 -0.62412700 1.24413000

Frequencies (cm⁻¹):

-772.82 37.80 50.66 61.80 72.36 91.41 105.48 123.95 160.82 175.72 188.39 213.10 256.57 274.62
301.28 309.50 327.14 350.00 369.51 398.07 405.18 412.26 428.65 433.63 446.86 450.61 457.44 465.31
485.93 489.31 499.19 509.91 533.22 583.70 644.57 657.12 680.42 791.07 884.87 949.71 1107.27
1245.32 1336.01 1372.97 1477.96 1661.28 1931.41 1939.69 2015.12 2049.08 2104.96 2162.99 2240.43
2313.06

TS7

O -4.41549600 -1.21862300 -0.00001600
O -5.58627300 1.05597500 -0.00001700
C -3.13867000 0.48961700 -0.00001100
C -2.13473100 1.44981200 -0.00000800
C -1.12766500 2.13707200 -0.00000300
C 0.08431700 2.71930300 0.00000200
C 1.29268500 2.96007000 0.00000700
C 2.61833700 2.88959600 0.00001200
C 3.73553200 2.32516100 0.00001500
C 4.65752300 1.40191800 0.00001700
C 4.91413500 0.14537000 0.00001800
C 4.74577400 -1.11637100 0.00001600
C 3.87762400 -2.10285000 0.00001300
C 2.82133900 -2.76050200 0.00000800
C 1.49833100 -2.93412700 0.00000300
C 0.27627500 -2.82459100 -0.00000200
C -0.99015900 -2.36070600 -0.00000600
C -2.07097400 -1.80488700 -0.00000900
C -3.15681600 -0.91486300 -0.00001200
C -4.56716500 0.51784200 -0.00001500

Frequencies (cm⁻¹):

-366.98 37.04 58.70 59.93 66.48 97.76 137.65 138.77 167.25 187.51 219.95 228.28 273.09 296.73

323.63 334.85 379.47 387.02 396.02 399.48 427.29 430.62 442.04 459.67 461.94 477.04 479.32 495.39
 495.43 498.60 528.44 549.54 610.59 619.59 654.91 726.69 747.81 906.47 984.72 1037.98 1101.33
 1281.27 1304.01 1440.08 1539.97 1559.73 1738.96 1824.28 1997.39 2093.07 2118.95 2142.61 2218.17
 2271.39

TS8

O	-4.73067100	-1.20843000	-0.00010600
O	-5.48378700	0.88244700	-0.00005100
C	-3.10407300	0.30001200	-0.00001200
C	-2.30415500	1.42639900	0.00003400
C	-1.39806000	2.24602000	0.00006900
C	-0.21203200	2.89195100	0.00009800
C	0.97136000	3.18502200	0.00011400
C	2.31980800	3.06514300	0.00011600
C	3.43902800	2.58389000	0.00010600
C	4.35949600	1.58946000	0.00007800
C	4.80258500	0.45335400	0.00004600
C	4.67484300	-0.89384500	0.00000700
C	4.11047200	-1.97819700	-0.00002300
C	3.03680300	-2.79153700	-0.00005200
C	1.86457100	-3.15780200	-0.00006900
C	0.53137300	-3.07576700	-0.00007400
C	-0.63353400	-2.65765200	-0.00007200
C	-1.70006600	-1.87910300	-0.00005700
C	-2.56237100	-0.97236000	-0.00004400
C	-4.57677100	0.09965500	-0.00005500

Frequencies (cm⁻¹):

-368.00 32.21 59.50 62.38 68.29 96.88 107.05 134.56 165.84 197.64 199.10 224.95 275.31 286.16
 301.90 328.39 335.34 359.59 382.11 408.71 413.20 417.13 426.05 452.11 465.30 480.24 480.81 486.18
 490.19 496.84 501.33 525.41 566.60 602.20 640.07 662.28 734.35 887.69 973.52 1107.14 1161.39
 1261.21 1326.34 1395.39 1499.53 1557.28 1806.00 1999.78 2107.59 2120.43 2163.55 2196.84 2249.13
 2266.13

TS9

O	-5.18473400	1.03683300	0.50321600
O	-5.11802600	-1.04055700	-0.43766300
C	-3.10625100	-0.05829500	-0.04074600
C	-2.38366800	-1.23071600	-0.02518200
C	-1.51858700	-2.09767900	0.00188000
C	-0.37233600	-2.80578400	0.02400900
C	0.79977500	-3.14767100	0.03772600
C	2.15206500	-3.10894400	0.04900700
C	3.29078500	-2.67495700	0.04964600
C	4.27863500	-1.74552300	0.04290600
C	4.77146800	-0.63194500	0.02844800
C	4.74446400	0.72507200	0.00663000
C	4.23217900	1.83005000	-0.01395100
C	3.21056200	2.72082100	-0.03548000
C	2.06382900	3.13576000	-0.04882800
C	0.71278800	3.12782700	-0.05823400
C	-0.45512500	2.76559700	-0.05894700
C	-1.57705100	2.02441700	-0.05299600
C	-2.41598100	1.12835900	-0.04229100
C	-4.69053600	0.04857400	0.04899900

Frequencies (cm⁻¹):

-678.72 33.52 38.14 59.51 61.88 84.10 98.30 111.91 164.56 191.93 195.38 200.78 285.09 296.56 300.47
 318.62 324.18 333.13 352.71 404.14 417.10 419.88 426.76 449.50 463.74 467.90 470.49 475.79 486.17
 494.86 510.36 523.35 524.45 529.16 612.72 631.70 725.72 762.41 956.79 968.44 1113.04 1241.26

1314.70 1428.75 1492.32 1783.68 1809.55 2104.57 2138.62 2167.86 2200.36 2234.09 2267.84 2271.67

TS10

O	-4.90818400	-1.52642500	0.00000300
O	-5.05294900	1.75824200	0.00000200
C	-2.17958600	0.70771700	0.00000100
C	-1.29908500	1.58263100	0.00000000
C	-0.27345400	2.43018800	-0.00000100
C	0.90201400	2.82042700	-0.00000100
C	2.21925400	2.96523700	-0.00000200
C	3.38425700	2.50830800	-0.00000200
C	4.42769900	1.71851800	-0.00000300
C	4.83579100	0.50878700	-0.00000200
C	4.84622500	-0.77166700	-0.00000200
C	4.12383100	-1.86097200	-0.00000100
C	3.13906500	-2.63273400	0.00000000
C	1.83899200	-2.91381300	0.00000000
C	0.61002900	-2.83264300	0.00000100
C	-0.64353000	-2.33948800	0.00000100
C	-1.66656600	-1.67743600	0.00000100
C	-2.61443000	-0.64094800	0.00000100
C	-4.01201000	-0.74735900	0.00000200
C	-4.35698600	0.86615600	0.00000200

Frequencies (cm⁻¹):

-192.81 34.69 48.80 57.83 64.86 96.90 107.20 126.81 177.56 202.28 205.77 211.54 228.00 288.99
300.86 306.14 329.67 345.49 366.93 382.04 409.50 413.89 421.60 432.41 438.65 453.37 458.84 464.11
477.24 478.50 494.65 494.82 514.34 536.18 640.22 651.02 692.16 719.82 953.53 974.28 1043.32
1229.61 1323.27 1398.81 1512.92 1728.28 1768.17 1896.53 1958.20 2048.81 2077.95 2100.36 2180.62
2219.99

TS11

O	-4.68165400	-1.13350100	-0.00039600
O	-5.50364200	1.00574500	-0.00020700
C	-2.95004600	0.50024500	-0.00014500
C	-2.06116800	1.55851600	0.00001300
C	-1.17268600	2.39368300	0.00015300
C	0.04144200	2.97853500	0.00029300
C	1.24596900	3.22086600	0.00039800
C	2.56512500	3.02651300	0.00046800
C	3.64996100	2.41582100	0.00047800
C	4.49943700	1.41641900	0.00043200
C	4.76791900	0.17434500	0.00032300
C	4.62637400	-1.10056800	0.00018300
C	3.84841800	-2.14144600	0.00002700
C	2.85505000	-2.91040100	-0.00011500
C	1.55664800	-3.15062200	-0.00022600
C	0.31758400	-3.11744900	-0.00030300
C	-0.89175000	-2.56173000	-0.00032700
C	-1.91324400	-1.87097500	-0.00032100
C	-2.63470100	-0.75134300	-0.00025400
C	-4.76993800	0.08993300	-0.00027100

Frequencies (cm⁻¹):

-767.32 34.51 39.76 59.59 66.01 67.61 86.70 111.36 157.70 158.98 189.86 202.80 247.97 280.12 291.11
316.67 327.39 335.77 393.15 398.86 399.07 410.56 419.18 438.78 450.25 459.76 463.31 483.79 487.15
496.52 509.06 520.58 545.11 564.42 602.93 657.33 708.27 745.85 858.73 978.37 997.89 1233.93
1313.36 1341.55 1520.79 1735.75 1781.15 1863.03 1994.43 2055.39 2078.23 2124.15 2134.49 2226.64

TS12

O	-4.38401600	1.51455900	0.00121400
O	-6.04306000	-1.34338200	0.00079200
C	-2.85418100	-0.30642700	-0.00099900
C	-1.99586600	-1.24718400	-0.00103900
C	-0.99080100	-2.03107600	-0.00100900
C	0.11703300	-2.69376300	-0.00059800
C	1.35387800	-2.94661100	-0.00020100
C	2.65280600	-2.94952700	0.00031100
C	3.77511400	-2.36145500	0.00058200
C	4.69787600	-1.45869400	0.00073100
C	4.95619200	-0.19684900	0.00055000
C	4.77335600	1.05766900	0.00024100
C	3.92738800	2.06359900	-0.00008900
C	2.86499700	2.70905000	-0.00034600
C	1.54838300	2.92529100	-0.00040900
C	0.32668000	2.81913900	-0.00034900
C	-0.95978700	2.40793400	-0.00020300
C	-2.04913400	1.87228600	-0.00002500
C	-3.25233400	1.06442700	0.00016400
C	-4.98882900	-0.95604500	0.00001300

Frequencies (cm⁻¹):

-279.85 19.34 46.19 48.73 60.35 73.27 79.17 108.63 133.35 151.69 170.77 196.97 201.62 248.21 281.55
 285.80 308.44 314.09 359.04 390.19 392.40 401.11 417.07 420.65 425.87 436.07 453.49 453.72 474.95
 484.65 498.54 510.35 553.03 592.73 604.80 676.63 683.87 753.67 961.10 971.68 1167.49 1187.32
 1297.78 1420.59 1490.08 1663.43 1714.44 1820.24 1952.52 2027.57 2069.44 2149.60 2262.78 2267.85

TS13

O	-5.50571700	0.06557900	0.00052600
C	-3.23961100	-0.89657300	0.00021300
C	-2.19825300	-1.68684500	-0.00011300
C	-1.08206400	-2.25441400	-0.00034100
C	0.14347300	-2.70644600	-0.00042600
C	1.40040500	-2.76701200	-0.00025800
C	2.67927500	-2.54583200	-0.00019000
C	3.66952500	-1.73899700	0.00041800
C	4.38272600	-0.67624300	0.00001500
C	4.26613700	0.62479200	0.00069500
C	3.77924600	1.78088800	0.00014600
C	2.64676700	2.47158700	0.00033400
C	1.46420000	2.83411200	-0.00007600
C	0.14139200	2.66798900	-0.00092400
C	-1.03841400	2.31804100	-0.00044300
C	-2.19089100	1.65152500	-0.00021100
C	-3.17166500	0.89829000	0.00014000
C	-4.31129100	-0.06230000	0.00032000

Frequencies (cm⁻¹):

-279.85 19.34 46.19 48.73 60.35 73.27 79.17 108.63 133.35 151.69 170.77 196.97 201.62 248.21 281.55
 285.80 308.44 314.09 359.04 390.19 392.40 401.11 417.07 420.65 425.87 436.07 453.49 453.72 474.95
 484.65 498.54 510.35 553.03 592.73 604.80 676.63 683.87 753.67 961.10 971.68 1167.49 1187.32
 1297.78 1420.59 1490.08 1663.43 1714.44 1820.24 1952.52 2027.57 2069.44 2149.60 2262.78 2267.85

TS14

O	-5.00867600	-0.87292600	-0.99899900
O	-4.83922800	0.99374700	1.08387300
C	-2.68975500	1.42201800	0.21019900
C	-1.63089700	1.99560800	0.05986000
C	-0.40107200	2.53635900	-0.08860000

C	0.77950700	2.82332400	-0.16346900
C	2.12741600	2.89657700	-0.22015800
C	3.28603300	2.51561900	-0.20748300
C	4.39411600	1.74321900	-0.14911700
C	4.87328700	0.62140200	-0.05751100
C	4.92800400	-0.71990700	0.07634500
C	4.27997400	-1.75957600	0.14657300
C	3.23418700	-2.59667100	0.22555300
C	2.03281100	-2.86089500	0.19751700
C	0.70002800	-2.84140200	0.16241200
C	-0.48239300	-2.50158900	0.05233600
C	-1.69983600	-1.99770800	-0.08059400
C	-2.78822000	-1.43217900	-0.26464400
C	-3.92468400	-0.72665600	-0.44840400
C	-3.88796700	0.72136600	0.43601900

Frequencies (cm⁻¹):

-161.09 41.10 48.39 56.85 67.42 101.02 124.62 146.47 148.58 187.54 192.77 241.09 259.05 262.32
 288.31 306.82 333.35 348.79 382.32 396.35 405.55 426.25 429.96 441.01 450.81 456.64 465.15 468.86
 476.36 486.95 506.10 514.46 527.08 553.44 590.35 639.42 646.59 701.86 886.49 971.16 1167.74
 1269.62 1428.67 1494.29 1640.15 1660.67 1876.42 2062.58 2107.19 2164.15 2198.20 2218.36 2284.32
 2305.23