Supporting Information for

Thermal decomposition of graphene oxyradicals under the influence of an embedded

five-membered ring

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In this supporting information, we present:

·   **Table S1**. Total energies, relative energies, zero-point energies, expectation values of S2 operator (projected values are in parentheses), vibrational frequencies, rotational constants for all optimized structures at B3LYP/6-311G(d,p) level in this work for oxyradicals a-g.

·   **Table S2**. Cartesian coordinates of optimized structures at B3LYP/6-311G(d,p) level for oxyradcials a-g.

·   **Table S3**. Rate coefficients (units: s-1) of product formation from oxyradical a.

·   **Table S4**. Rate coefficients (units: s-1) of product formation from oxyradical b.

·   **Table S5**. Rate coefficients (units: s-1) of product formation from oxyradical c.

·   **Table S6**. Rate coefficients (units: s-1) of product formation from oxyradical d.

·   **Table S7**. Rate coefficients (units: s-1) of product formation from oxyradical e.

·   **Table S8**. Rate coefficients (units: s-1) of product formation from oxyradical f.

·   **Table S9**. Rate coefficients (units: s-1) of product formation from oxyradical g.

·   **Figure S1**. Potential energy surface of oxyradical c calculated at B3LYP/6-311G(d,p) level at 0 K (units: kcal/mol).

·   **Figure S2**. Potential energy surface of oxyradical d calculated at B3LYP/6-311G(d,p) level at 0 K (units: kcal/mol).

·   **Figure S3**. Potential energy surface of oxyradical e calculated at B3LYP/6-311G(d,p) level at 0 K (units: kcal/mol).

·   **Figure S4**. ln(concentration fraction)s and concentrations as functions of time for oxyradical g at 0.1 atm, (a) 1500 K, (b) 2000 K, (c) 2500 K.

·   **Figure S5**. Comparison of concentration profiles of the reactant (oxyradical g) from the master equation modelling with those from the fitting formula e^{-kt}, where *k* is the effective rate constant derived from three different methods.

·   **Figure S6**. Densities of states as functions of energy, (a) f, (b) f5.

·   **Figure S7.** Microcanonical rate constants for isomerization from species f to f5, f5 to f, f5 to f3, and f3 to f4.

·   **Figure S8**. Concentration profiles from the kinetic modelling at 1500 K, (a) xO_2=0.001, (b) xO_2=0.01, (c) xO_2=0.1.

·   **Figure S9**. Concentration profiles from the kinetic modelling at 2000 K, (a) xO_2=0.001, (b) xO_2=0.01, (c) xO_2=0.1.

Table S1. Total energies, relative energies, zero-point energies, expectation values of S2 operator (projected values are in parentheses), vibrational frequencies, rotational constants for all optimized structures at B3LYP/6-311G(d,p) level in this work for oxyradicals a-g.

Oxyradical a					
Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	<S^2>	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
a	-766.51403	0.0	0.20972	0.79(0.75)	62.2 95.3 138.2 208.3 212.8 280.7 291.4 323.4 392.1 410.7 425.0 428.6 465.2 473.3 533.7 540.5 557.2 577.4 589.7 605.1 636.5 649.9 658.0 690.1 728.7 767.6 769.5 774.5 817.9 827.8 837.1 846.8 858.7 897.9 939.3 961.7 963.2 973.2 991.8 994.5 1030.1 1035.0 1074.7 1140.6 1146.2 1156.9 1178.4 1199.6 1215.4 1225.7 1246.0 1274.0 1323.8 1342.1 1385.1 1395.1 1415.4 1425.6 1436.6 1467.3 1475.7 1478.9 1506.4 1528.4 1575.9 1606.8 1637.4 1670.6 1694.2 3159.5 3160.4 3162.3 3165.1 3177.2 3178.6 3181.0 3188.8 3199.0	0.59918 0.44183 0.25431
a3	-766.40214	70.2	0.20694	0.76(0.75)	41.1* 59.6 111.9 145.7 173.1 211.9 278.6 291.9 315.9 340.8 395.8 453.9 457.8 465.9 490.4 525.5 551.8 589.9 590.8 600.0 618.0 641.7 664.1 674.1 686.1 737.5 746.3 760.9 790.4 808.2 817.6 829.7 842.8 872.5 913.1 919.2 950.1 963.2 963.8 979.8 983.7 1038.5 1066.8 1094.7 1104.4 1119.0 1159.2 1160.8 1192.6 1204.8 1215.9 1236.1 1261.3 1280.2 1366.2 1384.4 1399.2 1424.6 1442.7 1452.4 1494.7 1504.0 1512.5 1582.5 1595.5 1622.3 1650.5 1706.8 1903.8 2994.8 3157.3 3158.4 3162.1 3174.4 3177.2 3180.1 3188.5 3213.2	0.55981 0.46423 0.26918
a5	-766.40373	69.2	0.20626	0.80(0.75)	44.6 66.2 91.6 106.4 187.1 189.2 216.7 269.3 279.7 299.3 357.7 420.0 441.8 449.1 495.8 513.1 529.1 532.5 554.1 564.7 590.4 601.1 640.3 651.6 676.3 676.9 701.4 726.3 762.6 784.1 796.5 824.9 829.7 837.0 879.5 915.4 958.4 958.8 969.7 977.5 1014.8 1045.4 1050.5 1077.0 1140.4 1157.7 1182.4 1192.2 1215.4 1225.8 1231.3 1240.1 1276.2 1333.3 1359.3 1387.1 1394.1 1432.0 1455.6 1464.0 1472.7 1501.9 1518.9 1560.8 1596.8 1625.3 1643.0 1690.7 2203.7 3133.2 3155.7 3156.3 3161.2 3165.4 3173.1 3174.5 3177.9 3185.1	0.74140 0.25363 0.18898
a6	-766.43472	49.8	0.20515	0.76(0.75)	51.6 90.3 101.0 127.8 150.7 165.7 210.9 287.6 299.8 308.1 353.9 412.9 430.2 461.6 466.4 497.2 510.9 519.6 530.6 559.1 565.9 576.5 611.9 627.1 656.7 667.9 694.9 739.7 748.5 771.1 792.0 811.9 835.2 843.4 853.7 864.8 888.4 901.9 952.3 969.4 971.8 980.2 1054.7 1061.9 1135.3 1145.1 1169.3 1191.6 1200.3 1237.6 1247.2 1251.4 1282.7 1322.4 1368.6 1397.2 1413.0 1422.2 1438.9 1479.0 1490.6 1514.6 1530.9 1599.9 1622.5 1643.8 1651.5 1670.8 2172.3 3024.3 3156.4 3157.1 3161.7 3172.7 3174.0 3177.6 3184.6 3266.4	0.57950 0.41894 0.24316
a7	-766.42516	55.8	0.20729	0.75(0.75)	58.8 92.3 115.9 132.5 188.3 214.9 283.6 289.8 307.4 322.3 396.1 435.7 463.9 480.6 485.8 506.9 550.1 559.2 576.3 603.3 606.7 640.3 678.3 695.8 707.6 723.1 755.5 771.8 792.4 807.2 827.8 838.0 853.6 878.2 902.0 919.8 949.0 962.0 962.3 973.4 982.1 1043.5 1054.3 1069.8 1095.5 1136.2 1154.4 1176.4 1194.1 1219.3 1223.4 1243.3 1250.4 1309.7 1346.1 1367.7 1384.7 1428.6 1435.9 1465.7 1470.8 1504.8 1513.9 1543.6 1618.8 1633.0 1650.5 1665.8 1894.2 3157.1 3159.8 3162.4 3174.6 3176.9 3177.5 3189.5 3191.1 3216.9	0.54230 0.50770 0.28903
a10	-766.46210	32.6	0.20659	0.78(0.75)	41.4 49.0 91.1 136.1 188.9 195.7 211.5 265.5 275.0 298.8 350.9 411.5 445.8 459.1 500.7 517.7 531.3 547.9 567.1 570.5 582.1 582.3 630.1 653.6 684.0 693.2 719.5	0.68984 0.26855 0.19330

					760.0 775.5 792.6 815.1 817.6 835.0 846.4 917.1 920.3 942.3 964.2 973.6 982.1 1004.2 1028.6 1034.1 1053.4 1104.2 1162.5 1175.9 1178.5 1200.9 1227.2 1233.2 1257.4 1295.9 1297.8 1356.3 1387.8 1396.4 1422.7 1440.1 1470.8 1481.5 1489.5 1514.8 1554.0 1613.0 1650.1 1675.9 1715.3 2207.0 3061.5 3160.9 3161.2 3164.2 3175.6 3177.9 3179.6 3187.1 3243.9	
a11	-766.44735	41.8	0.20801	0.78(0.75)	57.1 85.9 123.3 145.4 209.2 280.0 283.5 287.1 339.3 388.0 434.9 458.4 465.6 477.1 494.0 504.0 543.4 550.3 590.9 595.9 616.3 653.4 673.7 679.7 695.2 707.3 751.8 765.9 787.7 796.1 805.2 826.2 845.7 853.6 915.6 947.8 957.7 967.2 978.9 990.8 1036.4 1049.0 1095.7 1127.1 1155.2 1160.6 1170.9 1182.1 1207.5 1220.6 1236.1 1243.0 1248.8 1290.2 1330.7 1364.5 1375.9 1390.6 1430.9 1443.2 1457.3 1465.4 1502.1 1509.5 1595.1 1620.6 1637.7 1645.4 2181.7 3010.3 3155.4 3157.8 3159.2 3169.3 3173.6 3177.6 3182.6 3215.9	0.58226 0.41992 0.25424
CO	-113.34134	N/A	0.00506		2219.8	58.03862
a4	-653.10710	N/A	0.19845	0.78(0.75)	84.2 135.1 198.8 262.2 297.4 308.6 343.6 427.6 464.6 467.6 484.8 493.6 546.4 557.6 587.5 599.3 617.9 641.6 654.5 682.4 705.3 724.8 760.4 772.9 793.8 803.5 820.3 836.7 855.2 881.2 905.4 913.1 952.1 964.3 971.1 978.7 992.5 1042.2 1071.8 1091.9 1140.9 1146.8 1170.9 1203.6 1216.2 1220.3 1250.0 1276.1 1310.0 1342.7 1351.4 1366.8 1409.1 1425.5 1436.6 1460.5 1471.9 1507.5 1510.7 1600.9 1633.2 1657.8 1715.8 3155.2 3157.4 3161.0 3172.6 3173.9 3174.4 3185.8 3194.7 3215.9	0.84583 0.55821 0.34196
C₂H₂	-77.32860	N/A	0.02699		643.0 643.0 773.6 773.6 2070.6 3419.9 3523.0	35.64470
a8	-689.04077	N/A	0.17386	0.76(0.75)	68.1 101.5 102.6 191.0 227.9 288.8 322.7 334.5 430.4 441.2 485.4 488.6 494.1 512.2 526.8 538.9 562.4 603.5 604.4 628.1 674.6 720.1 723.7 764.6 776.2 787.6 833.8 838.5 888.4 893.3 900.1 941.1 971.9 980.4 1011.2 1055.2 1066.3 1119.6 1143.1 1167.8 1197.9 1228.9 1245.4 1255.7 1312.2 1335.5 1384.9 1409.0 1416.2 1434.7 1460.4 1488.3 1499.0 1521.7 1583.6 1618.8 1639.1 1665.6 2213.8 3158.6 3160.7 3162.7 3174.2 3175.9 3177.3 3185.7	0.62187 0.60189 0.30586
H	-0.50216	N/A		0.75(0.75)		
a9	- 765.87671	N/A	0.19553	0.75(0.75)	52.9 86.3 100.6 114.4 124.3 200.2 241.1 294.0 310.9 333.1 390.8 415.6 421.9 470.6 471.8 495.8 524.5 529.1 547.3 560.0 595.4 599.3 614.8 625.7 647.9 670.1 698.0 701.2 747.7 748.4 771.8 812.6 839.7 843.2 850.0 890.4 902.0 946.1 961.1 973.4 981.9 1051.8 1063.0 1123.0 1144.7 1167.9 1193.7 1216.3 1239.1 1249.0 1264.0 1318.4 1368.9 1391.8 1418.1 1420.0 1437.9 1478.1 1489.1 1511.3 1528.4 1606.5 1624.5 1647.7 1669.9 2195.7 2212.2 3158.5 3162.4 3170.3 3173.4 3176.0 3185.3 3190.3 3475.5	0.60082 0.39439 0.23810
a12	-653.04884	N/A	0.19891	0.76(0.75)	107.5 137.0 204.3 269.1 286.3 301.4 356.3 430.2 458.7 467.8 479.4 503.6 544.3 550.9 588.1 596.1 607.3 643.2 680.1 699.4 717.8 764.9 789.4 791.0 795.2 808.9 838.1 847.3 859.8 892.1 919.7 945.8 959.4 972.3 981.6 996.7 1042.4 1050.9 1095.6 1136.5 1153.8 1170.2 1175.3 1186.0 1210.1 1222.3 1232.4 1239.1 1261.2 1323.2 1364.7 1381.5 1420.1 1435.7 1461.2 1469.5 1496.8 1513.8 1530.7 1616.8 1626.5 1650.7 1655.0 3017.2 3156.3 3158.6 3160.0 3172.6 3174.0 3176.3 3184.7 3200.6	0.85073 0.56422 0.35276
aTS1-3	-766.38630	80.1	0.20541	0.77(0.75)	-268.7 57.3 85.4 134.3 175.5 210.3 279.6 281.2 286.1 332.2 416.2 430.3 462.9 465.6 479.3 499.9 533.8 559.4 576.6 596.7 607.8 610.6 621.7 644.6 686.4 691.3 744.5 759.7 787.6 794.5 819.0 833.2 861.7 873.1 892.1 897.4 937.9 944.3 955.7 961.7 969.5 1043.6 1066.0 1072.1 1103.6 1147.8 1158.8 1171.4 1182.2 1209.3 1214.0 1231.6 1256.1 1263.2 1353.6 1359.7 1377.3 1411.8 1419.4 1436.5 1452.6 1461.8 1504.6 1508.4 1597.0 1613.5 1651.3 1675.3 2091.1 2988.1 3152.9 3156.1 3157.5 3167.7 3170.5 3177.4 3180.2 3223.8	0.61021 0.42050 0.26629
aTS1-5	-766.39998	71.6	0.20524	0.78(0.75)	-321.0 45.1 68.5 98.5 141.0 196.7 229.1 238.4 292.1 298.6 389.3 398.0 423.7 442.9 459.2 497.0 511.7 533.1 546.1 569.2 588.4 602.0 622.4 649.3 666.4 678.5 716.0 725.8 762.9 778.6 787.9 828.8 834.3 838.9 893.2 907.8 918.8 960.1 969.0 978.3 980.6 1000.5 1044.9 1053.3 1142.9 1159.1 1169.9 1185.6 1210.6 1221.4 1229.8	0.61042 0.37055 0.23075

					1242.1 1282.0 1344.8 1371.7 1384.7 1428.0 1435.1 1455.6 1460.4 1468.4 1513.7 1517.3 1558.0 1587.8 1623.0 1642.9 1689.5 2115.5 3127.5 3156.8 3157.3 3161.8 3169.5 3174.0 3175.7 3177.7 3186.4	
aTS1-6	-766.43400	50.2	0.20472	0.76(0.75)	-206.8 48.0 86.4 115.1 179.9 196.0 224.2 277.1 307.9 341.6 361.6 402.2 414.2 452.3 460.1 492.2 504.1 515.7 528.6 564.5 574.1 576.8 602.8 616.4 649.2 657.0 694.2 747.1 747.8 770.7 778.2 829.0 834.9 847.3 848.1 868.5 890.8 905.8 949.3 972.1 972.8 980.3 1052.0 1065.2 1136.0 1143.9 1167.2 1182.9 1201.4 1231.3 1246.0 1251.4 1280.5 1315.3 1368.7 1396.8 1413.4 1423.2 1438.8 1477.5 1488.6 1513.6 1527.8 1594.4 1621.0 1641.0 1654.7 1674.7 2055.7 3050.4 3156.1 3158.1 3160.8 3173.3 3174.1 3177.8 3184.4 3277.5	0.58318 0.42943 0.24732
aTS1-7	-766.39901	72.2	0.20601	0.78(0.75)	-603.3 76.6 100.8 127.5 206.1 210.7 277.8 284.9 288.3 354.8 404.5 438.5 454.6 467.9 474.7 490.5 532.0 548.6 563.4 593.3 598.0 632.1 654.5 697.9 705.6 720.1 744.7 768.4 790.1 806.7 815.7 833.3 843.9 849.7 888.7 909.8 925.7 956.9 961.6 971.3 981.1 1041.8 1058.0 1062.8 1107.5 1120.5 1159.4 1177.8 1195.0 1216.2 1224.1 1235.4 1248.0 1301.4 1324.4 1349.1 1373.7 1391.1 1433.9 1444.4 1464.8 1467.5 1509.4 1513.5 1612.8 1625.2 1648.2 1654.3 1904.7 3157.4 3160.4 3162.1 3174.6 3175.5 3179.2 3187.0 3199.5 3216.1	0.56545 0.47806 0.28290
aTS5-3	-766.36406	94.1	0.20458	0.79(0.75)	-591.3 31.8 59.5 105.0 130.5 197.7 250.5 276.7 281.0 290.2 358.5 383.6 417.6 450.0 452.6 508.1 518.8 534.0 565.4 580.8 597.5 609.9 617.1 642.2 667.2 680.2 721.9 734.9 753.1 770.2 804.5 817.4 829.8 840.0 844.6 924.3 955.9 957.7 968.4 978.9 982.4 985.5 1032.8 1056.7 1076.6 1130.7 1156.3 1169.4 1197.7 1206.9 1217.6 1238.8 1259.2 1287.1 1363.2 1381.0 1404.4 1415.0 1444.3 1455.6 1488.0 1503.6 1530.5 1576.0 1596.2 1625.9 1657.0 1716.8 2087.9 3067.5 3156.9 3157.9 3159.8 3171.8 3174.0 3177.4 3183.0 3201.6	0.61152 0.35267 0.22874
aTS3-4	-766.39979	71.7	0.20469	0.83(0.75)	-509.6 40.6 63.3 102.1 125.5 159.5 209.3 286.1 293.7 316.3 339.0 392.6 442.3 458.3 465.0 486.8 507.1 551.1 569.2 591.6 600.0 613.5 637.2 648.1 686.6 698.0 748.0 749.8 776.3 802.0 811.3 817.8 840.9 868.7 898.4 912.0 927.6 958.9 963.6 974.0 979.0 984.3 1037.8 1073.3 1119.5 1137.7 1157.7 1179.7 1183.8 1210.4 1219.8 1240.9 1271.0 1296.0 1357.0 1375.7 1384.1 1412.3 1438.5 1443.1 1447.9 1479.6 1502.7 1542.8 1599.3 1620.1 1650.6 1699.9 1957.0 3109.1 3156.7 3159.3 3160.8 3173.7 3176.1 3178.8 3186.6 3212.7	0.55023 0.47220 0.27577
aTS6-7	-766.37919	84.6	0.20424	0.78(0.75)	-656.0 72.1 88.2 103.8 130.6 199.8 245.4 276.3 295.7 304.6 359.6 403.0 426.9 434.9 463.4 478.6 502.4 517.0 541.3 563.5 577.5 605.3 612.6 633.5 664.5 680.9 694.0 743.4 760.7 770.4 805.2 825.9 840.4 849.9 862.0 893.2 912.7 915.4 959.6 973.9 976.7 981.2 1029.2 1051.0 1115.4 1128.9 1155.9 1173.6 1185.4 1226.0 1228.1 1236.4 1250.7 1270.1 1331.0 1367.0 1381.9 1431.7 1437.0 1474.7 1480.2 1511.4 1520.7 1560.4 1616.7 1638.4 1656.9 1662.5 2075.9 3108.5 3157.7 3160.7 3163.0 3174.9 3176.5 3177.1 3188.2 3200.1	0.55179 0.46366 0.27580
aTS6-8	-766.36415	94.0	0.20098	0.77(0.75)	-291.3 27.4 29.8 68.8 73.3 104.7 109.2 175.3 209.0 245.4 292.0 324.7 337.2 430.4 444.5 461.0 494.5 494.9 505.2 529.5 537.3 558.2 567.2 606.5 607.3 631.3 653.6 673.8 709.7 728.4 752.3 768.1 769.1 782.6 797.6 837.1 839.2 884.5 893.2 898.7 942.3 970.8 979.1 1006.3 1054.7 1064.4 1120.5 1142.9 1167.6 1198.3 1230.5 1244.9 1256.1 1312.4 1341.9 1384.6 1407.3 1415.8 1435.2 1460.6 1488.9 1500.6 1519.6 1585.0 1617.6 1638.8 1666.0 1951.2 2208.2 3153.1 3156.3 3161.2 3171.4 3172.6 3174.3 3184.4 3397.9 3485.8	0.59019 0.36480 0.22814
aTS6-9	-766.37177	89.3	0.19673	0.76(0.75)	-690.8 45.3 58.4 89.5 116.2 118.2 152.3 202.1 250.1 294.4 315.9 335.0 411.9 418.3 427.2 473.9 476.5 494.6 521.9 524.1 529.2 548.6 561.5 584.9 600.4 614.9 624.8 645.8 671.0 681.2 702.7 745.9 748.7 771.8 812.1 839.7 844.3 850.5 889.6 902.5 945.5 961.5 973.8 982.6 1051.6 1062.6 1121.4 1145.0 1167.8 1191.1 1216.8 1238.5 1248.9 1264.1 1318.8 1368.3 1390.2 1418.4 1418.9 1438.2 1476.5 1489.9 1511.9 1527.3 1602.6 1624.0 1647.8 1670.2 2099.6 2206.4 3159.0 3163.0 3171.2 3173.8 3176.4 3185.8 3188.7 3460.8	0.59308 0.39710 0.23806
aTS7-4	-766.42298	57.1	0.20553	0.76(0.75)	-418.3 67.4 83.6 108.0 129.6 184.7 211.8 270.5 287.6 303.2 317.5 380.1 436.3 468.0 477.7 485.9 502.7 553.7	0.53290 0.49839

Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
					561.1 598.5 604.7 623.9 647.9 663.0 698.3 711.0 739.1 769.1 771.2 792.7 815.1 828.1 839.0 881.2 902.0 915.2 933.7 958.4 962.1 972.8 980.8 1045.7 1066.3 1090.3 1104.4 1133.5 1153.0 1177.3 1204.7 1215.3 1222.8 1247.6 1256.9 1316.2 1346.1 1366.1 1382.2 1423.0 1434.7 1460.8 1470.3 1481.7 1511.0 1519.1 1614.1 1632.1 1651.4 1675.6 1978.6 3156.2 3158.6 3162.2 3173.6 3175.6 3175.9 3187.6 3192.8 3216.9	0.28593
aTS5-10	-766.39706	73.4	0.20156	0.77(0.75)	-887.1 46.8 89.1 90.5 140.1 191.9 241.6 256.0 285.6 291.3 301.1 391.1 418.5 443.6 461.3 506.3 521.0 536.4 560.1 569.7 578.1 596.3 639.3 647.2 660.2 682.3 722.8 744.9 770.2 789.8 796.3 829.9 835.0 849.8 903.7 928.3 957.4 965.2 973.4 979.8 986.0 1019.8 1038.9 1047.1 1083.5 1151.6 1159.5 1180.7 1199.6 1219.9 1223.2 1243.8 1259.0 1295.1 1352.2 1379.9 1398.0 1423.8 1436.4 1456.8 1472.8 1483.8 1513.0 1548.8 1575.9 1616.8 1646.4 1672.7 1682.4 2181.8 3149.4 3157.1 3157.4 3160.7 3173.2 3174.3 3176.2 3184.3	0.68351 0.28299 0.20016
aTS10-11	-766.42207	57.7	0.20651	0.76(0.75)	-401.0 53.8 88.1 108.3 144.6 204.7 267.9 279.2 311.4 322.6 399.1 426.4 456.9 470.9 484.5 506.3 535.2 545.8 574.8 579.8 592.7 607.2 621.9 646.7 675.0 692.1 750.2 769.8 777.3 783.9 806.4 824.3 839.5 855.7 895.2 923.2 961.4 965.3 971.7 982.4 1005.8 1010.0 1046.6 1058.2 1118.1 1160.8 1171.0 1182.7 1194.1 1218.6 1228.6 1249.0 1267.9 1329.2 1354.6 1375.7 1409.2 1430.0 1439.9 1465.7 1472.0 1499.1 1509.6 1527.2 1593.9 1622.7 1645.2 1671.2 2161.7 3157.7 3160.7 3161.7 3162.3 3172.9 3174.9 3175.0 3177.9 3184.9	0.58148 0.38063 0.23861
aTS11-12	-766.38946	78.2	0.20458	0.76(0.75)	-104.7 17.2 21.2 67.8 106.2 142.0 185.5 206.0 271.8 286.7 304.5 357.6 429.4 458.6 468.5 479.9 504.5 544.7 551.0 587.9 596.0 607.5 642.5 680.6 699.6 716.3 766.4 789.6 791.1 795.5 807.7 836.1 847.1 867.1 892.4 923.1 944.9 959.6 972.9 983.3 996.4 1041.9 1050.8 1095.9 1137.3 1154.4 1170.3 1176.8 1186.2 1211.5 1222.3 1233.8 1239.7 1262.5 1324.1 1364.9 1382.0 1420.8 1435.8 1461.5 1469.2 1497.4 1513.8 1532.6 1616.5 1626.2 1650.6 1654.3 2150.3 3017.0 3156.4 3158.9 3160.8 3173.4 3174.3 3177.3 3185.4 3204.3	0.56928 0.37784 0.23489
Oxyradical b						
Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
b	-766.51286	0.0	0.20957	0.79(0.75)	65.8 100.2 179.9 185.1 231.1 239.5 295.1 322.9 383.0 407.3 429.7 430.9 457.2 483.4 525.9 539.2 548.4 591.1 598.7 621.0 623.5 650.5 666.8 692.3 718.7 762.8 778.8 783.7 800.7 827.9 835.8 844.8 868.9 900.8 912.8 928.8 950.9 970.3 975.2 978.2 986.9 1043.2 1064.8 1137.4 1154.9 1159.2 1188.6 1200.9 1220.0 1238.5 1246.3 1252.7 1290.0 1353.8 1367.7 1398.4 1414.5 1436.6 1448.4 1469.5 1480.3 1496.0 1514.3 1525.0 1597.3 1629.3 1634.4 1658.1 1685.0 3160.5 3164.0 3164.1 3176.3 3177.4 3180.9 3187.3 3188.2 3191.3	0.67724 0.37253 0.24033
b2	-766.41749	59.9	0.20764	0.77(0.75)	56.1 92.4 135.6 150.9 215.5 282.9 291.2 319.4 381.4 426.0 456.6 461.4 472.6 497.7 530.9 536.2 554.6 593.9 595.2 603.1 618.0 643.1 682.0 692.5 696.2 754.0 769.2 781.0 799.7 821.2 838.5 847.1 876.7 890.5 899.7 925.8 944.8 948.2 969.6 977.0 998.3 1015.7 1044.3 1058.3 1116.6 1123.2 1140.7 1161.4 1188.1 1205.1 1209.0 1219.7 1244.1 1286.4 1295.6 1343.2 1369.5 1372.9 1414.6 1434.9 1458.1 1468.0 1493.1 1506.7 1580.3 1624.9 1661.8 1691.5 1916.6 3132.9 3145.3 3156.4 3161.0 3163.0 3173.8 3174.5 3180.2 3184.8	0.64266 0.41257 0.27898
b3	-766.40214	69.5	0.20694	0.76(0.75)	41.1 59.6 111.9 145.7 173.1 211.9 278.6 291.9 315.9 340.8 395.8 453.9 457.8 465.9 490.4 525.5 551.8 589.9 590.8 600.0 618.0 641.7 664.1 674.1 686.1 737.5 746.3 760.9 790.4 808.2 817.6 829.7 842.8 872.5 913.1 919.2 950.1 963.2 963.8 979.8 983.7 1038.5 1066.8 1094.7 1104.4 1119.0 1159.2 1160.8 1192.6 1204.8 1215.9 1236.1 1261.3 1280.2 1366.2 1384.4 1399.2 1424.6 1442.7 1452.4 1494.7 1504.0 1512.5 1582.5 1595.5 1622.3 1650.5 1706.8 1903.8 2994.8 3157.3 3158.4 3162.1 3174.4 3177.2 3180.1 3188.5 3213.2	0.55981 0.46423 0.26918
b5	-766.40537	67.5	0.20443	0.85(0.75)	45.4 85.3 88.2 103.9 136.9 211.5 211.9 277.1 287.6 304.9 374.5 388.6 437.9 445.2 445.4 485.2 505.0 521.9 532.3 546.0 573.2 603.0 609.6 615.4 640.5 668.4 680.0 716.3 754.5 757.9 769.9 796.7 830.0 837.9 841.1 853.3	0.51346 0.42396 0.23222

					892.1 923.8 957.8 965.0 974.9 980.7 1045.8 1061.5 1099.0 1119.7 1149.2 1165.6 1212.6 1215.3 1232.7 1243.1 1291.7 1328.1 1359.1 1397.6 1410.8 1417.3 1451.8 1468.5 1481.9 1508.5 1514.9 1557.5 1574.2 1632.3 1656.0 1693.3 2195.1 3141.5 3157.9 3159.1 3161.1 3171.7 3176.2 3182.1 3184.3 3240.6	
b6	-766.43192	50.8	0.20514	0.77(0.75)	37.0 87.7 89.5 127.6 131.0 210.6 215.6 273.1 285.2 309.4 361.2 414.3 433.0 443.5 454.6 505.5 531.4 532.6 549.8 565.2 571.9 603.4 609.5 642.8 655.4 668.0 671.0 713.9 761.2 766.5 777.3 789.6 815.1 834.6 843.4 883.9 912.0 914.2 953.5 955.3 971.7 980.0 1038.5 1048.7 1105.8 1123.4 1157.3 1174.0 1195.0 1225.7 1236.5 1242.8 1267.6 1328.7 1357.3 1386.3 1411.9 1435.1 1439.4 1485.2 1489.9 1515.4 1533.3 1613.5 1625.4 1641.2 1657.8 1676.4 2205.0 3147.4 3152.3 3157.0 3160.9 3173.1 3173.4 3175.0 3184.6 3254.0	0.80282 0.28527 0.21048
b7	-766.42883	52.7	0.20781	0.75(0.75)	39.3 70.4 101.7 147.7 177.7 213.9 266.7 290.0 304.9 390.4 417.4 431.7 459.5 466.4 498.0 538.4 548.0 576.3 587.4 616.9 629.2 653.1 659.4 687.6 702.0 733.9 764.6 776.5 798.0 824.6 833.6 843.7 860.8 892.1 915.3 922.6 948.9 954.5 971.0 974.7 983.0 1041.7 1069.0 1106.6 1132.7 1142.3 1153.3 1161.0 1171.6 1212.2 1223.1 1237.5 1254.9 1285.4 1348.3 1369.9 1375.4 1425.8 1436.1 1468.9 1471.7 1509.2 1530.5 1592.3 1620.4 1653.1 1679.7 1747.6 1916.0 2996.5 3156.6 3161.5 3165.1 3174.1 3174.9 3185.4 3186.6 3208.2	0.74016 0.34290 0.24787
b8	-766.45943	33.5	0.20630	0.80(0.75)	46.5 51.1 89.0 118.1 181.1 213.0 233.0 281.7 292.2 309.5 358.2 422.3 432.5 444.4 456.8 475.8 519.6 537.3 548.7 563.3 572.0 602.3 614.9 650.3 657.2 675.3 692.1 757.8 763.6 784.9 806.4 832.3 838.1 847.8 857.5 871.6 925.1 934.3 967.6 980.7 989.3 995.9 1032.1 1053.0 1099.6 1156.3 1161.5 1180.1 1197.1 1228.4 1242.4 1255.1 1301.7 1350.6 1357.2 1410.8 1428.2 1438.3 1452.4 1470.7 1478.1 1509.3 1523.0 1564.6 1629.7 1652.6 1663.8 1714.5 2203.8 3146.8 3160.8 3161.5 3165.1 3176.9 3177.8 3178.9 3188.2 3251.5	0.51326 0.40187 0.22539
b9	-766.46500	30.0	0.20703	0.78(0.75)	44.7 51.6 100.2 120.7 160.2 210.3 244.5 276.3 285.5 321.4 340.4 408.6 429.8 446.1 462.7 527.3 531.6 544.8 566.2 566.9 575.4 589.6 621.8 629.1 661.3 674.5 726.0 729.8 763.2 784.0 797.0 820.5 840.6 854.6 867.9 921.1 948.9 965.7 972.8 980.1 985.9 1011.0 1046.9 1074.6 1107.3 1152.2 1157.7 1172.9 1205.3 1232.1 1249.0 1267.8 1325.0 1358.8 1394.5 1429.9 1433.2 1436.7 1452.8 1468.4 1486.3 1516.1 1562.2 1595.8 1625.1 1646.7 1657.0 1679.7 2174.0 3143.5 3161.3 3163.6 3167.8 3174.1 3178.1 3186.2 3191.0 3239.4	0.76949 0.28548 0.20823
b10	-766.45738	34.8	0.20847	0.77(0.75)	52.2 80.6 103.8 146.8 205.1 265.8 275.1 309.6 312.2 382.3 406.6 458.7 460.8 473.6 482.6 493.8 513.3 548.9 574.3 594.3 619.3 644.5 648.6 675.9 691.7 732.6 745.3 764.1 779.4 820.0 829.1 835.1 879.3 894.2 907.5 930.0 949.3 966.8 974.4 980.9 1045.9 1055.3 1112.0 1133.6 1156.1 1158.3 1177.7 1202.3 1217.5 1223.8 1238.4 1267.2 1299.4 1347.7 1353.3 1371.3 1402.8 1416.9 1434.6 1461.0 1468.1 1474.2 1505.7 1510.3 1585.0 1631.8 1664.4 1715.5 2187.0 3035.5 3070.1 3153.9 3158.7 3159.6 3171.6 3172.3 3175.3 3183.2	0.58899 0.40190 0.24211
b11	-766.45218	38.1	0.20819	0.77(0.75)	45.5 95.4 103.2 136.3 200.2 246.5 280.3 285.0 337.6 372.6 394.5 437.4 463.0 469.6 518.2 533.2 540.0 555.7 582.7 603.2 608.9 627.4 645.4 667.9 700.4 715.2 739.1 759.7 784.5 818.9 831.8 846.2 876.4 896.0 908.8 922.3 939.2 966.0 973.2 977.0 1041.9 1046.7 1109.0 1124.8 1144.5 1151.3 1172.0 1201.7 1213.7 1227.2 1246.1 1275.8 1292.9 1345.8 1371.5 1376.7 1403.5 1419.1 1434.4 1455.0 1462.1 1472.0 1492.5 1505.5 1578.4 1622.8 1660.4 1692.3 2196.8 3018.1 3044.6 3155.1 3159.1 3161.0 3171.2 3172.8 3178.0 3182.7	0.77137 0.31857 0.22954
CO	-113.34134	N/A	0.00506		2219.8	58.03862
b4	-653.10710	N/A	0.19845	0.78(0.75)	84.2 135.1 198.8 262.2 297.4 308.6 343.6 427.6 464.6 467.6 484.8 493.6 546.4 557.6 587.5 599.3 617.9 641.6 654.5 682.4 705.3 724.8 760.4 772.9 793.8 803.5 820.3 836.7 855.2 881.2 905.4 913.1 952.1 964.3 971.1 978.7 992.5 1042.2 1071.8 1091.9 1140.9 1146.8 1170.9 1203.6 1216.2 1220.3 1250.0 1276.1 1310.0 1342.7 1351.4 1366.8 1409.1 1425.5 1436.6 1460.5 1471.9 1507.5 1510.7 1600.9 1633.2 1657.8 1715.8 3155.2 3157.4 3161.0 3172.6 3173.9 3174.4 3185.8 3194.7	0.84583 0.55821 0.34196

					3215.9	
b12	-653.05300	N/A	0.19886	0.77(0.75)	53.3 134.3 195.6 249.4 278.3 299.2 317.9 415.8 430.0 459.8 461.6 497.2 512.9 555.8 573.3 588.1 618.8 636.2 645.0 681.3 693.2 745.2 774.6 785.5 786.0 828.3 840.5 864.9 890.8 895.2 913.9 920.8 951.2 970.2 973.0 981.5 1041.3 1060.9 1108.3 1131.4 1136.5 1171.4 1172.1 1201.7 1215.0 1223.9 1248.7 1262.6 1325.4 1363.3 1371.1 1423.3 1434.7 1436.7 1469.4 1471.9 1510.5 1522.1 1583.5 1621.2 1650.6 1678.4 1741.3 3039.6 3071.5 3154.7 3157.8 3160.8 3172.2 3174.5 3175.3 3188.0	0.86125 0.54063 0.33475
b13	-653.02503	N/A	0.19789	0.81(0.75)	74.5 129.2 191.7 240.1 255.7 290.7 314.6 366.5 436.9 454.6 465.0 491.5 515.3 561.5 590.0 598.0 600.7 608.6 638.9 677.9 693.2 726.6 761.9 784.5 797.6 817.6 837.2 850.4 872.4 879.4 914.1 919.7 961.4 962.7 976.6 979.0 1037.1 1062.8 1099.4 1105.8 1129.0 1159.6 1177.8 1196.5 1211.7 1233.3 1252.3 1263.1 1347.9 1379.7 1386.8 1409.3 1421.4 1440.3 1450.7 1468.6 1495.1 1500.5 1560.7 1588.3 1617.8 1645.4 1704.4 3033.7 3062.7 3157.5 3158.7 3160.5 3170.3 3174.7 3182.3 3183.0	0.84361 0.55398 0.33993
bTS1-2	-766.41533	61.2	0.20637	0.77(0.75)	-331.0 63.8 106.6 150.4 169.5 212.9 267.2 284.1 310.3 392.8 427.1 451.8 455.8 467.2 490.9 529.1 542.9 557.1 593.1 605.6 627.4 637.1 662.4 672.9 695.4 747.6 764.1 774.5 798.4 813.0 822.1 836.8 870.3 901.2 904.6 927.2 947.1 953.2 969.5 976.9 987.2 1024.5 1045.0 1055.4 1121.4 1129.0 1143.4 1161.4 1195.3 1209.5 1211.4 1235.3 1246.7 1295.7 1318.8 1349.2 1368.7 1375.2 1417.3 1435.3 1462.0 1472.2 1499.7 1507.7 1586.4 1629.6 1660.3 1695.7 1878.4 3145.1 3148.0 3157.1 3162.2 3162.6 3174.1 3174.9 3180.0 3185.8	0.68775 0.37341 0.24962
bTS1-5	-766.40364	68.5	0.20352	0.81(0.75)	-378.5 57.7 84.1 117.3 138.9 171.1 217.6 270.5 289.9 300.8 350.9 397.9 404.9 446.0 450.7 455.7 494.1 518.2 530.6 537.7 578.4 583.5 606.0 615.3 640.9 656.8 671.9 703.3 756.2 763.0 770.8 781.1 800.1 829.3 837.9 839.8 916.4 920.5 952.1 958.2 976.9 979.6 1036.9 1062.0 1068.0 1115.1 1152.6 1169.3 1198.3 1216.2 1236.0 1248.5 1265.0 1331.4 1371.6 1402.1 1415.1 1442.7 1465.8 1467.3 1480.0 1510.4 1512.7 1563.9 1567.7 1633.1 1658.0 1694.9 2107.1 3133.1 3157.4 3158.9 3159.5 3168.7 3176.4 3183.4 3183.7 3248.6	0.62309 0.37215 0.23324
bTS1-6	-766.42663	54.1	0.20443	0.77(0.75)	-436.0 57.5 82.9 134.9 154.3 187.8 221.4 281.7 303.0 315.0 363.5 414.3 415.3 446.7 461.4 494.2 519.4 537.7 543.7 559.5 580.0 589.9 601.0 624.6 643.7 650.9 657.5 697.8 758.5 765.2 775.3 781.5 813.6 832.9 844.4 888.7 908.1 919.1 958.6 963.6 971.2 981.5 1044.6 1052.0 1077.4 1135.3 1156.4 1170.2 1190.8 1207.6 1231.8 1241.9 1252.9 1324.2 1365.7 1399.1 1419.8 1435.4 1449.0 1483.8 1488.4 1514.1 1527.9 1614.0 1625.6 1644.9 1666.6 1681.2 2026.7 3138.8 3156.9 3158.5 3161.9 3174.1 3175.0 3175.9 3186.4 3275.7	0.68091 0.35070 0.23169
bTS2-3	-766.38695	79.0	0.20597	0.79(0.75)	-548.5 51.7 92.3 110.7 163.7 212.7 273.1 290.6 316.7 336.9 373.5 426.6 447.1 461.3 466.9 492.0 532.3 560.5 598.8 603.2 613.6 630.1 646.4 688.1 695.5 744.9 749.0 772.6 789.8 805.3 821.3 821.9 842.9 882.7 890.3 912.9 951.8 959.1 964.2 971.3 979.0 1041.3 1072.5 1103.3 1124.0 1145.3 1160.1 1173.0 1184.9 1208.9 1214.9 1237.0 1272.1 1276.2 1342.9 1375.6 1382.1 1422.6 1437.0 1444.5 1453.6 1467.9 1504.4 1538.1 1594.9 1619.7 1655.5 1695.2 1914.7 2993.9 3157.1 3161.0 3161.2 3173.4 3174.4 3181.1 3184.3 3217.0	0.59962 0.42880 0.27488
bTS2-7	-766.39852	71.8	0.20608	0.78(0.75)	-665.5 44.9 85.6 101.4 154.8 218.8 283.2 291.8 311.2 351.6 423.2 459.1 461.0 463.9 489.1 512.7 542.3 569.2 586.3 599.0 613.2 637.1 653.4 686.7 691.2 747.9 757.8 772.4 778.4 800.7 826.3 839.7 840.3 879.3 891.8 905.7 928.9 943.2 952.3 971.1 978.4 1042.5 1059.5 1072.8 1110.7 1129.1 1140.5 1151.9 1170.4 1209.5 1221.1 1222.9 1251.0 1283.2 1345.0 1358.1 1371.5 1405.0 1420.9 1434.3 1462.7 1472.4 1506.7 1513.1 1596.7 1637.7 1669.8 1721.3 1924.9 3102.2 3154.6 3160.1 3163.5 3172.6 3173.6 3180.8 3184.4 3217.9	0.66197 0.39639 0.27705
bTS5-3	-766.36622	92.0	0.20390	0.80(0.75)	-630.8 35.7 59.8 99.7 136.9 190.6 237.9 274.0 285.9 302.7 381.3 384.6 424.3 449.5 451.7 471.6 488.0 520.8 551.3 581.7 588.8 609.4 632.7 640.7 646.1 688.1 703.1 743.7 747.3 770.2 788.2 809.8 825.0 841.7 868.8 896.4 916.7 919.4 954.4 961.7 977.5 980.9 1028.6 1036.8	0.55943 0.41207 0.24881

					1062.0 1127.2 1147.8 1160.4 1196.5 1214.5 1230.5 1240.1 1258.4 1303.9 1363.1 1384.3 1394.3 1418.1 1442.3 1454.3 1494.4 1503.4 1522.9 1566.9 1592.9 1624.0 1656.9 1711.3 2079.7 3073.8 3157.2 3158.0 3159.9 3171.9 3174.5 3180.2 3183.1 3187.7	
bTS6-7	-766.39591	73.4	0.20474	0.78(0.75)	-620.5 36.2 77.4 90.3 143.5 184.2 233.0 277.5 293.5 307.8 391.4 417.9 418.4 441.1 460.6 480.4 505.9 532.0 557.6 579.3 596.5 618.8 636.4 655.2 659.8 682.7 721.7 749.9 760.9 782.9 794.1 829.4 834.2 839.6 846.8 909.0 920.8 934.3 952.6 963.4 974.6 982.0 1031.5 1045.9 1067.6 1127.7 1148.0 1170.8 1183.1 1216.0 1224.9 1248.8 1251.4 1288.3 1333.7 1367.7 1376.7 1429.2 1436.2 1474.0 1480.4 1514.6 1527.6 1604.6 1618.3 1654.5 1683.0 1715.9 2091.8 3096.5 3155.4 3160.0 3162.8 3173.0 3173.7 3179.1 3184.5 3199.1	0.73427 0.31997 0.23115
bTS5-8	-766.39409	74.5	0.20073	0.80(0.75)	-807.9 55.5 76.2 90.1 135.0 182.9 229.6 257.2 291.1 296.6 307.6 387.7 419.2 446.9 449.9 457.2 482.0 521.7 538.5 553.9 579.3 591.0 629.8 642.9 649.5 680.5 702.5 747.1 757.6 774.9 807.3 820.6 831.6 848.5 858.1 904.5 927.0 952.9 970.5 973.6 984.3 987.1 1011.6 1044.5 1063.6 1112.6 1145.3 1164.3 1203.5 1210.0 1222.3 1239.5 1263.5 1313.1 1360.5 1376.5 1410.8 1430.9 1442.9 1467.9 1477.4 1483.8 1512.3 1564.4 1571.3 1629.4 1653.9 1682.8 1837.2 2176.9 3040.8 3157.5 3160.4 3164.3 3173.8 3175.6 3177.5 3186.9	0.52322 0.41392 0.23115
bTS6-9	-766.41576	60.9	0.20055	0.76(0.75)	-1448.4 42.5 90.8 100.7 128.8 176.9 230.3 282.2 284.0 325.0 358.3 425.7 428.3 460.9 463.1 498.4 504.7 527.9 544.4 544.9 554.0 585.5 593.5 637.5 646.7 658.6 670.1 711.9 757.7 773.0 777.8 803.4 826.0 831.2 841.7 843.9 880.6 920.7 939.9 954.0 972.1 982.3 982.9 1041.3 1060.1 1116.3 1156.3 1170.5 1173.0 1207.2 1228.7 1239.2 1256.1 1327.6 1364.0 1388.3 1424.7 1439.1 1448.4 1483.3 1491.7 1504.7 1522.1 1544.2 1612.6 1630.3 1649.1 1679.7 1684.2 2187.4 3157.9 3161.9 3162.5 3174.5 3175.5 3180.2 3186.7 3237.4	0.78297 0.29351 0.21348
bTS8-10	-766.41927	58.7	0.20599	0.76(0.75)	-514.0 56.6 74.5 102.6 149.9 196.3 240.7 281.6 303.0 310.4 374.9 427.2 454.4 457.3 460.2 477.2 509.0 526.8 546.7 584.8 591.0 612.1 640.3 643.5 651.6 693.4 698.4 750.9 756.8 773.4 792.2 824.3 839.4 843.8 882.8 907.4 920.9 938.6 963.2 972.0 982.2 1011.3 1046.9 1068.2 1089.4 1146.5 1162.3 1194.0 1214.3 1223.4 1247.1 1254.6 1283.0 1352.5 1365.4 1393.4 1427.5 1432.6 1464.2 1471.2 1477.6 1495.2 1511.7 1593.7 1603.4 1627.1 1657.0 1675.4 2176.9 3126.2 3157.9 3160.7 3162.8 3174.9 3175.6 3178.5 3186.9 3218.2	0.57082 0.39369 0.23632
bTS9-11	-766.41639	60.5	0.20603	0.76(0.75)	-536.2 48.7 83.4 108.9 149.0 189.8 239.9 281.0 292.3 325.0 377.6 403.1 430.9 462.3 469.1 528.4 532.9 548.9 551.8 586.9 600.9 607.1 624.6 633.1 647.6 678.7 721.4 739.2 756.3 770.6 798.6 826.7 833.9 839.3 873.3 915.2 936.4 948.2 962.5 970.6 980.0 1020.6 1041.3 1057.7 1126.4 1154.2 1160.2 1167.4 1211.0 1216.7 1243.3 1255.2 1329.1 1355.2 1392.0 1408.1 1423.3 1429.6 1452.0 1466.5 1481.2 1499.5 1503.8 1554.5 1584.5 1616.1 1650.7 1673.4 2172.3 3116.9 3158.5 3162.4 3162.5 3173.7 3175.7 3185.6 3185.8 3194.7	0.74415 0.31304 0.22619
bTS3-4	-766.39979	71.0	0.20469	0.83(0.75)	-509.6 40.6 63.3 102.1 125.5 159.5 209.3 286.1 293.7 316.3 339.0 392.6 442.3 458.3 465.0 486.8 507.1 551.1 569.2 591.6 600.0 613.5 637.2 648.1 686.6 698.0 748.0 749.8 776.3 802.0 811.3 817.8 840.9 868.7 898.4 912.0 927.6 958.9 963.6 974.0 979.0 984.3 1037.8 1073.3 1119.5 1137.7 1157.7 1179.7 1183.8 1210.4 1219.8 1240.9 1271.0 1296.0 1357.0 1375.7 1384.1 1412.3 1438.5 1443.1 1447.9 1479.6 1502.7 1542.8 1599.3 1620.1 1650.6 1699.9 1957.0 3109.1 3156.7 3159.3 3160.8 3173.7 3176.1 3178.8 3186.6 3212.7	0.55023 0.47220 0.27577
bTS7-4	-766.42265	56.6	0.20577	0.77(0.75)	-442.4 49.7 62.6 96.1 121.6 160.3 205.4 262.9 306.7 312.3 325.7 414.9 433.3 464.3 470.9 490.5 517.8 556.2 561.1 592.0 616.1 619.7 642.9 658.7 691.9 700.0 759.8 773.7 794.1 807.7 824.4 836.6 847.3 886.7 909.6 918.1 924.2 952.0 962.4 972.9 980.9 1016.9 1042.9 1073.0 1108.8 1141.9 1156.0 1170.7 1202.7 1214.9 1223.4 1245.9 1270.2 1302.5 1348.5 1367.4 1373.7 1424.4 1436.6 1465.2 1470.1 1507.2 1520.1 1524.5 1612.5 1644.9 1670.1 1733.0 2000.6 3155.5 3160.3 3160.9 3172.9 3174.1 3174.8 3176.9 3185.5 3208.2	0.69925 0.35966 0.25584
bTS10-12	-766.39288	75.3	0.20450	0.77(0.75)	-124.8 17.0 26.8 58.2 70.6 136.1 183.4 197.2 249.8	0.57877

Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	⟨S²⟩	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
					278.1 299.0 321.4 417.7 428.7 460.5 462.3 497.8 513.8 555.9 573.8 588.7 617.3 637.1 647.6 680.8 691.8 746.8 775.8 782.2 786.5 828.2 841.0 864.4 884.0 894.2 910.5 923.5 952.8 971.4 973.6 982.6 1041.3 1061.1 1110.0 1131.8 1137.4 1171.2 1173.3 1201.9 1214.5 1223.8 1249.4 1263.6 1326.7 1363.5 1371.2 1423.6 1434.6 1436.3 1469.4 1471.8 1510.2 1522.3 1585.5 1622.5 1651.1 1678.9 1740.8 2148.6 3039.3 3071.3 3155.0 3157.9 3160.9 3172.6 3174.7 3176.0 3190.0	0.34983 0.22058
bTS11-13	-766.36535	92.6	0.20354	0.81(0.75)	-112.6 17.5 28.1 64.4 82.8 129.7 180.2 192.3 239.5 256.6 291.8 315.7 367.1 437.5 454.7 465.5 490.1 516.5 562.3 590.6 598.6 601.6 609.3 639.5 676.1 693.2 727.7 763.0 786.0 793.8 818.0 838.5 849.2 872.6 876.5 915.3 917.1 962.5 963.2 978.0 981.7 1037.0 1062.5 1100.4 1106.4 1129.3 1159.5 1177.4 1196.6 1211.9 1233.0 1252.6 1262.7 1349.5 1380.3 1387.1 1409.0 1422.0 1440.6 1450.7 1471.2 1495.6 1500.9 1563.0 1590.6 1618.4 1646.0 1704.8 2152.8 3033.1 3062.1 3157.4 3159.2 3161.5 3170.9 3174.5 3182.6 3187.5	0.75138 0.28248 0.21071
Oxyradical c						
Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees	⟨S²⟩	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
c	-766.51951	0.0	0.20981	0.78(0.75)	58.4 118.2 125.0 206.6 234.3 266.3 290.6 333.3 338.6 416.4 431.9 444.9 455.4 500.7 513.5 554.2 558.7 574.7 586.7 620.9 635.6 646.6 659.6 689.0 724.9 749.3 763.3 781.5 808.9 837.9 842.8 855.7 863.8 920.5 921.1 943.3 973.3 974.2 983.2 987.8 1038.2 1049.4 1055.0 1138.5 1143.6 1154.5 1161.8 1202.4 1215.5 1240.3 1249.6 1276.3 1293.6 1356.4 1369.4 1390.8 1421.8 1427.7 1438.9 1471.5 1479.1 1482.9 1513.6 1527.0 1595.0 1611.4 1647.3 1679.0 1693.5 3160.1 3164.0 3165.5 3168.1 3175.1 3177.4 3187.3 3190.9 3192.0	0.73750 0.36498 0.24415
c3	-766.42866	57.0	0.20779	0.75(0.75)	33.3 54.8 98.9 126.7 197.2 211.3 255.0 307.8 317.0 325.5 414.4 443.2 465.1 479.5 497.2 521.6 559.3 576.9 612.6 619.3 622.5 641.3 662.4 691.7 699.4 738.9 767.7 777.8 801.9 825.8 831.3 840.4 861.3 888.8 910.8 922.9 931.4 955.1 968.7 975.1 983.4 1040.9 1070.4 1104.4 1136.2 1152.9 1156.4 1163.1 1171.7 1212.9 1223.3 1240.0 1256.7 1285.4 1349.5 1369.8 1374.7 1426.3 1436.3 1469.2 1472.9 1509.5 1535.5 1583.9 1617.4 1656.5 1685.8 1760.1 1913.3 3011.3 3155.6 3161.8 3162.5 3173.4 3175.1 3179.4 3186.9 3211.3	0.72451 0.33713 0.23539
c5	-766.43647	52.1	0.20664	0.76(0.75)	44.9 64.3 95.2 122.2 184.2 189.1 222.7 244.3 274.7 307.4 370.3 406.4 444.8 455.2 493.5 493.6 526.3 535.1 542.4 560.9 605.5 630.0 640.6 653.8 682.6 684.1 713.3 745.1 765.9 779.7 802.5 830.2 838.7 865.8 900.3 905.9 941.8 942.4 971.4 979.6 1014.6 1047.4 1063.2 1099.2 1125.4 1152.8 1164.2 1185.4 1197.6 1227.3 1244.1 1256.8 1306.4 1323.4 1339.9 1380.0 1412.3 1430.7 1439.3 1460.0 1486.7 1501.6 1521.1 1582.9 1621.8 1645.0 1650.6 1674.4 2208.4 3147.4 3156.7 3158.7 3159.4 3160.2 3169.4 3174.2 3175.8 3182.4	0.62068 0.29540 0.20014
CO	-113.34134	N/A	0.00506		2219.8	58.03856
c4	-653.10710	N/A	0.19845	0.78(0.75)	84.2 135.1 198.8 262.2 297.4 308.6 343.6 427.6 464.6 467.6 484.8 493.6 546.4 557.6 587.5 599.3 617.9 641.6 654.5 682.4 705.3 724.8 760.4 772.9 793.8 803.5 820.3 836.7 855.2 881.2 905.4 913.1 952.1 964.3 971.1 978.7 992.5 1042.2 1071.8 1091.9 1140.9 1146.8 1170.9 1203.6 1216.2 1220.3 1250.0 1276.1 1310.0 1342.7 1351.4 1366.8 1409.1 1425.5 1436.6 1460.5 1471.9 1507.5 1510.7 1600.9 1633.2 1657.8 1715.8 3155.2 3157.4 3161.0 3172.6 3173.9 3174.4 3185.8 3194.7 3215.9	0.84583 0.55821 0.34196
cTS1-5	-766.42699	58.1	0.20578	0.76(0.75)	-213.8 42.8 74.0 101.0 192.1 234.8 240.6 268.2 275.0 321.6 377.5 414.2 440.7 460.1 477.7 485.8 513.7 540.4 544.9 551.1 585.2 590.0 615.5 632.4 651.7 690.5 735.6 738.2 755.2 774.8 798.0 827.5 838.4 881.6 906.5 918.3 919.5 939.7 967.1 972.2 980.2 1009.9 1053.2 1071.0 1125.9 1137.8 1163.5 1196.1 1203.6 1222.8 1244.7 1265.5 1308.8 1341.9 1362.1 1387.8 1410.8 1427.0 1439.3 1463.8 1480.4 1499.3 1523.6 1602.6 1619.0 1635.9 1649.5 1674.6 2022.0 3138.3 3157.7 3159.7 3166.8 3170.8 3172.1 3175.3 3183.1 3185.3	0.69413 0.35259 0.23382
cTS5-3	-766.39194	80.1	0.20534	0.78(0.75)	-584.8 35.6 72.1 92.2 130.5 197.4 251.1 258.3 283.2 309.6 371.1 406.9 425.6 447.6 458.2 487.3 501.0 549.8	0.69561 0.32275

Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
					561.6 584.9 614.5 625.0 632.1 655.6 659.8 710.2 739.8 755.9 775.5 794.8 810.5 817.3 842.0 847.9 902.2 920.5 937.6 957.0 965.8 972.7 980.7 1008.0 1045.0 1063.3 1087.1 1119.0 1155.2 1161.4 1192.1 1220.8 1233.3 1247.5 1253.4 1283.9 1341.0 1361.8 1374.9 1418.9 1428.8 1462.5 1476.3 1504.6 1525.8 1616.5 1641.1 1656.1 1682.5 1689.1 2091.8 3086.0 3151.6 3156.0 3160.2 3168.3 3172.8 3173.8 3185.0 3195.1	0.22650
cTS1-3	-766.38881	82.0	0.20575	0.78(0.75)	-693.3 65.6 108.0 119.8 198.3 209.3 249.6 286.1 305.5 343.4 405.9 422.5 436.1 459.0 476.4 507.9 518.4 537.6 587.6 589.8 610.2 624.6 656.4 670.4 691.4 741.8 749.7 767.5 784.2 805.5 819.3 838.3 838.8 898.7 910.2 922.0 955.2 958.0 967.0 981.2 988.0 1012.2 1043.6 1052.5 1085.0 1134.2 1152.3 1163.6 1191.2 1211.9 1225.6 1243.2 1253.8 1273.4 1344.6 1377.5 1393.0 1416.1 1431.5 1447.5 1466.2 1491.9 1505.7 1569.6 1620.9 1624.6 1653.2 1675.8 1830.6 3015.2 3157.6 3161.6 3162.3 3174.4 3175.2 3185.4 3186.6 3201.1	0.78843 0.34813 0.24844
cTS3-4	-766.42265	60.8	0.20577	0.77(0.75)	-442.4 49.7 62.6 96.1 121.6 160.3 205.4 262.9 306.7 312.3 325.7 414.9 433.3 464.3 470.9 490.5 517.8 556.2 561.1 592.0 616.1 619.7 642.9 658.7 691.9 700.0 759.8 773.7 794.1 807.7 824.4 836.6 847.3 886.7 909.6 918.1 924.2 952.0 962.4 972.9 980.9 1016.9 1042.9 1073.0 1108.8 1141.9 1156.0 1170.7 1202.7 1214.9 1223.4 1245.9 1270.2 1302.5 1348.5 1367.4 1373.7 1424.4 1436.6 1465.2 1470.1 1507.2 1520.1 1524.5 1612.5 1644.9 1670.1 1733.0 2000.6 3155.5 3160.3 3160.9 3172.9 3174.1 3174.8 3176.9 3185.5 3208.2	0.69925 0.35966 0.25584

Oxyradical d						
Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
d	-766.51935	0.0	0.20983	0.78(0.75)	69.4 96.9 164.9 183.0 247.2 270.3 292.4 304.6 336.3 394.2 426.8 437.7 468.2 486.7 511.7 555.1 568.7 575.1 577.6 618.9 632.3 666.4 667.3 714.8 757.3 761.7 775.9 778.2 799.9 819.6 824.2 834.0 864.4 925.5 931.2 940.8 973.7 982.9 984.3 994.5 1022.2 1041.1 1054.0 1103.0 1145.9 1157.1 1171.5 1182.7 1209.2 1233.5 1252.1 1277.7 1306.2 1330.4 1375.4 1388.0 1410.7 1429.2 1448.4 1466.9 1489.2 1497.5 1522.3 1579.9 1618.2 1621.5 1634.0 1654.9 1663.8 3163.5 3164.7 3166.3 3176.3 3181.1 3181.6 3185.8 3187.3 3197.7	0.68253 0.39091 0.24855
d3	-766.41511	65.4	0.20801	0.75(0.75)	33.4 87.3 96.4 126.6 196.4 206.0 266.0 276.0 300.2 338.5 439.7 444.7 464.2 484.9 502.0 514.2 560.4 563.8 592.5 626.4 632.9 648.8 666.9 716.9 748.0 755.5 771.5 777.7 805.2 810.7 826.3 835.2 864.1 908.0 920.1 939.5 960.1 965.4 971.3 984.7 996.7 1035.6 1036.3 1127.7 1139.2 1147.8 1164.0 1170.5 1177.8 1184.9 1215.8 1240.1 1261.0 1307.2 1335.8 1369.7 1397.6 1418.4 1437.6 1447.0 1484.9 1494.0 1541.1 1588.9 1614.1 1642.6 1650.0 1716.0 1919.4 3035.9 3160.9 3161.5 3162.1 3172.7 3175.1 3178.4 3183.9 3185.7	0.67670 0.38158 0.25416
d5	-766.45083	43.0	0.20677	0.76(0.75)	44.6 83.5 95.6 124.9 128.6 178.5 215.4 281.0 292.0 326.5 352.4 432.1 454.0 462.7 482.5 500.5 515.3 532.5 555.3 574.2 613.7 623.6 626.8 658.6 684.6 688.6 734.8 762.2 767.6 784.8 794.1 818.1 837.7 890.6 905.9 920.6 930.0 961.2 962.5 979.9 982.5 1054.8 1061.3 1104.4 1123.8 1128.6 1169.7 1178.8 1202.4 1231.9 1240.6 1260.7 1277.0 1321.9 1370.5 1397.3 1400.8 1429.4 1451.3 1460.0 1463.8 1498.9 1527.1 1555.6 1623.7 1638.6 1643.2 1654.5 2206.5 3153.3 3156.6 3160.9 3161.8 3171.0 3172.7 3175.9 3183.9 3185.7	0.50058 0.37067 0.21297
CO	-113.34134	N/A	0.00506		2219.8	58.03862
d4	-653.08607	N/A	0.19848	0.78(0.75)	100.7 138.2 201.2 269.6 283.9 303.2 331.7 445.9 460.2 467.4 493.9 506.2 546.2 561.6 594.2 602.0 625.3 634.0 658.0 666.2 736.3 747.7 751.3 765.9 783.6 794.8 807.3 825.1 855.7 893.1 915.5 932.9 960.3 964.9 973.6 982.5 1003.7 1037.0 1040.7 1099.4 1140.1 1152.4 1173.9 1185.5 1203.3 1211.3 1239.4 1269.6 1301.0 1338.0 1363.6 1394.5 1411.2 1433.0 1445.4 1477.6 1484.6 1527.6 1574.2 1597.3 1608.7 1612.4 1659.1 3157.7 3158.8 3159.7 3170.2 3171.2 3175.1 3182.0 3182.9 3202.0	0.89218 0.53394 0.34677
dTS1-5	-766.43797	51.1	0.20545	0.77(0.75)	-612.8 60.4 82.3 128.8 151.1 192.5 236.1 256.2 287.4 318.9 333.0 428.9 433.7 455.3 480.1 506.2 519.7 530.0 548.0 561.2 573.2 609.1 621.8 627.9 661.6 684.5 729.5	0.62520 0.39024 0.24050

Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
					745.6 756.7 773.7 778.9 813.8 838.9 900.2 913.6 923.9 941.9 962.3 963.6 964.7 978.7 1039.1 1047.8 1081.3 1101.5 1139.7 1165.5 1173.5 1180.5 1209.5 1244.0 1258.2 1297.0 1321.3 1368.9 1400.2 1412.2 1416.9 1444.7 1462.3 1469.1 1504.3 1525.6 1557.7 1632.1 1640.0 1653.6 1667.1 1960.7 3140.4 3159.6 3161.6 3163.6 3171.8 3176.7 3179.3 3185.2 3193.0	
dTS5-3	-766.39163	80.1	0.20572	0.77(0.75)	-558.5 44.5 63.9 93.9 136.3 188.0 234.8 277.3 284.1 315.6 374.3 415.4 432.2 450.1 476.5 493.8 507.7 525.8 558.5 580.0 619.9 632.5 644.7 653.7 679.2 714.6 753.7 764.8 783.8 793.6 802.1 833.1 847.1 904.9 909.8 924.0 955.1 962.2 968.3 982.7 985.1 1023.4 1030.7 1045.5 1083.0 1141.2 1158.8 1173.2 1195.1 1213.7 1231.8 1246.2 1262.8 1302.5 1316.2 1374.2 1394.3 1419.1 1438.9 1446.6 1462.6 1499.5 1536.0 1567.2 1621.0 1648.1 1664.1 1723.1 2051.1 3097.9 3153.2 3160.3 3164.2 3170.2 3172.9 3178.6 3181.7 3183.6	0.57923 0.39807 0.24838
dTS1-3	-766.37679	89.5	0.20583	0.77(0.75)	-719.5 79.7 87.3 152.6 170.8 196.5 235.4 268.9 282.2 334.6 362.7 412.0 438.9 461.2 489.8 501.5 519.3 546.0 564.3 583.8 614.5 631.9 646.4 669.2 690.1 747.0 758.1 765.6 779.4 796.8 808.7 832.5 890.2 904.6 920.5 937.9 961.6 967.2 974.1 982.5 986.3 1034.6 1039.6 1060.6 1086.5 1142.7 1159.5 1171.9 1180.1 1214.4 1234.5 1242.9 1267.2 1312.6 1323.8 1373.5 1394.7 1418.1 1437.9 1445.1 1455.4 1496.2 1528.1 1561.7 1609.1 1621.8 1638.8 1701.0 1807.0 3032.2 3161.3 3163.7 3163.8 3172.6 3181.3 3181.4 3184.3 3195.5	0.72013 0.38082 0.25859
dTS3-4	-766.40737	70.3	0.20565	0.77(0.75)	-428.7 55.3 63.1 99.9 129.5 141.2 205.5 254.2 274.1 294.2 330.7 408.2 445.3 460.4 476.9 495.4 516.1 560.9 579.9 597.6 609.5 632.7 643.0 661.0 699.6 745.5 753.7 769.4 782.9 801.3 810.4 828.1 844.6 900.5 917.2 936.2 949.8 960.1 968.5 978.5 985.0 999.1 1037.6 1040.4 1135.4 1143.0 1152.7 1174.1 1178.2 1203.7 1212.5 1239.6 1270.5 1307.1 1338.3 1368.1 1397.4 1414.5 1436.0 1447.8 1483.4 1489.5 1533.5 1584.2 1609.9 1624.1 1626.3 1684.6 2012.7 3159.7 3160.3 3160.8 3170.8 3172.8 3176.9 3183.1 3184.0 3189.0	0.62689 0.40510 0.27271
Oxyradical e						
Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
e	-766.51808	0.0	0.20975	0.78(0.75)	70.1 100.6 138.1 208.6 256.0 270.3 287.7 305.7 314.7 406.9 436.1 436.8 461.2 482.4 519.1 521.2 576.5 584.1 617.2 628.6 631.8 641.8 666.7 702.6 717.8 754.6 773.4 781.9 798.0 820.5 841.6 857.1 877.4 917.0 917.3 927.7 976.6 980.4 982.4 991.9 1019.6 1042.0 1048.0 1091.8 1142.9 1158.3 1179.6 1197.4 1221.3 1236.4 1255.7 1268.3 1298.4 1340.7 1364.9 1389.2 1414.1 1431.7 1448.6 1454.1 1478.9 1502.2 1522.4 1565.6 1599.8 1618.1 1634.6 1656.1 1703.5 3163.6 3166.5 3167.6 3175.0 3178.9 3182.9 3186.4 3189.1 3193.3	0.57620 0.44440 0.25089
e3	-766.41511	64.6	0.20801	0.75(0.75)	33.4 87.3 96.4 126.6 196.4 206.0 266.0 276.0 300.2 338.5 439.7 444.7 464.2 484.9 502.0 514.2 560.4 563.8 592.5 626.4 632.9 648.8 666.9 716.9 748.0 755.5 771.5 777.7 805.2 810.7 826.3 835.2 864.1 908.0 920.1 939.5 960.1 965.4 971.3 984.7 996.7 1035.6 1036.3 1127.7 1139.2 1147.8 1164.0 1170.5 1177.8 1184.9 1215.8 1240.1 1261.0 1307.2 1335.8 1369.7 1397.6 1418.4 1437.6 1447.0 1484.9 1494.0 1541.1 1588.9 1614.1 1642.6 1650.0 1716.0 1919.4 3035.9 3160.9 3161.5 3162.1 3172.7 3175.1 3178.4 3183.9 3185.7	0.67670 0.38158 0.25416
e5	-766.44862	43.6	0.20675	0.76(0.75)	34.6 82.8 90.0 103.8 172.7 183.6 214.6 266.1 280.0 305.1 368.0 432.6 452.3 468.1 498.3 498.4 516.5 530.7 563.0 568.1 598.2 613.7 629.7 632.7 661.5 736.2 751.6 761.9 772.3 782.6 807.6 812.0 833.2 849.9 895.5 920.4 947.8 952.0 971.4 982.8 995.6 1053.4 1073.8 1099.0 1126.2 1141.3 1157.7 1194.5 1205.2 1215.3 1236.6 1274.5 1295.3 1309.1 1351.9 1389.7 1405.8 1429.0 1435.7 1459.1 1478.1 1494.0 1518.8 1598.8 1616.6 1629.5 1636.7 1647.2 2207.1 3155.7 3157.8 3160.7 3162.7 3172.1 3173.2 3177.2 3185.8 3187.9	0.73629 0.28685 0.20643
CO	-113.34134	N/A	0.00506		2219.8	58.03862
e4	-653.08607	N/A	0.19848	0.78(0.75)	100.7 138.2 201.2 269.6 283.9 303.2 331.7 445.9 460.2 467.4 493.9 506.2 546.2 561.6 594.2 602.0 625.3 634.0 658.0 666.2 736.3 747.7 751.3 765.9 783.6 794.8 807.3 825.1 855.7 893.1 915.5 932.9 960.3 964.9 973.6 982.5	0.89218 0.53394 0.34677

Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
					1003.7 1037.0 1040.7 1099.4 1140.1 1152.4 1173.9 1185.5 1203.3 1211.3 1239.4 1269.5 1301.0 1338.0 1363.6 1394.5 1411.2 1433.0 1445.4 1477.6 1484.6 1527.6 1574.2 1597.3 1608.7 1612.4 1659.1 3157.7 3158.8 3159.7 3170.2 3171.2 3175.1 3182.0 3182.9 3202.0	
eTS1-5	-766.43590	51.6	0.20542	0.77(0.75)	-633.4 55.5 81.5 117.4 166.7 185.9 244.7 264.3 276.1 295.6 350.9 421.5 430.3 443.8 467.7 498.7 518.1 535.7 551.9 573.1 584.1 607.6 622.7 628.9 656.9 664.9 747.6 752.0 764.9 778.4 796.2 807.5 831.7 854.0 900.8 922.7 953.1 956.9 963.0 971.8 983.9 1044.1 1062.3 1078.3 1101.6 1136.1 1160.7 1189.2 1203.7 1218.9 1237.3 1270.5 1285.5 1325.6 1362.3 1399.5 1401.5 1428.8 1430.1 1452.0 1484.3 1496.6 1513.9 1614.5 1622.9 1631.8 1639.6 1660.1 1951.5 3136.8 3162.5 3163.0 3166.0 3173.4 3175.4 3185.7 3187.4 3187.8	0.57199 0.41801 0.24176
eTS5-3	-766.39279	78.6	0.20586	0.77(0.75)	-557.5 36.6 59.8 96.9 132.5 199.7 244.7 272.6 282.8 301.0 379.4 406.2 429.5 448.1 486.2 492.5 513.4 527.9 567.5 585.7 615.0 628.1 636.7 652.3 686.2 739.1 757.2 768.3 792.1 800.5 804.5 826.5 837.6 888.5 919.0 924.2 954.3 961.2 972.3 982.9 986.0 1025.7 1034.3 1043.6 1078.9 1143.5 1153.3 1177.4 1178.3 1221.9 1239.0 1251.4 1264.6 1297.4 1334.2 1363.4 1395.9 1415.9 1429.9 1439.1 1487.2 1493.8 1537.8 1597.3 1620.8 1649.0 1668.8 1704.8 2050.6 3099.9 3153.7 3159.8 3164.3 3171.2 3172.3 3177.1 3182.9 3187.9	0.62263 0.37569 0.24530
eTS1-3	-766.37670	88.7	0.20584	0.77(0.75)	-636.0 82.9 107.4 125.6 171.9 218.2 240.5 274.6 281.8 326.6 427.6 436.2 445.7 472.9 489.7 510.4 535.9 558.2 589.5 601.3 619.9 637.5 652.4 668.6 696.7 750.7 760.9 767.5 781.2 802.7 809.8 822.2 887.9 899.7 907.8 916.4 942.4 964.3 965.4 972.6 983.6 1010.9 1036.5 1042.1 1092.1 1128.5 1150.6 1167.9 1171.1 1178.8 1207.2 1240.5 1265.2 1292.8 1333.2 1355.0 1394.2 1406.0 1420.4 1460.7 1477.9 1486.0 1518.1 1566.2 1583.2 1598.5 1619.1 1625.2 1904.4 3139.7 3157.5 3160.3 3161.6 3169.7 3174.0 3180.8 3183.7 3185.5	0.60600 0.43953 0.27910
eTS3-4	-766.40737	69.5	0.20565	0.77(0.75)	-428.7 55.3 63.1 99.9 129.5 141.2 205.5 254.2 274.1 294.2 330.7 408.2 445.3 460.4 476.9 495.4 516.1 560.9 579.9 597.6 609.5 632.7 643.0 661.0 699.6 745.5 753.7 769.4 782.9 801.3 810.4 828.1 844.6 900.5 917.2 936.2 949.8 960.1 968.5 978.5 985.0 999.1 1037.6 1040.4 1135.4 1143.0 1152.7 1174.1 1178.2 1203.7 1212.5 1239.6 1270.5 1307.1 1338.3 1368.1 1397.4 1414.4 1436.0 1447.8 1483.4 1489.5 1533.5 1584.2 1609.9 1624.1 1626.3 1684.6 2012.7 3159.7 3160.3 3160.8 3170.8 3172.8 3176.9 3183.1 3184.0 3189.0	0.62689 0.40510 0.27271
Oxyradical f						
Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
f	-842.71077	0.0	0.22230	0.78(0.75)	92.9 137.5 138.6 187.8 269.7 281.4 294.2 320.1 338.6 392.3 403.0 434.9 448.0 456.1 481.2 534.3 546.7 554.5 574.7 594.0 609.4 629.9 633.7 646.7 666.0 670.4 709.2 718.4 761.4 769.2 785.8 806.7 815.9 828.6 832.2 856.1 861.0 868.6 929.3 967.1 974.9 979.4 988.3 1012.4 1054.3 1087.9 1093.7 1151.1 1159.8 1162.5 1171.9 1191.0 1207.1 1225.3 1240.0 1259.4 1316.5 1331.6 1359.8 1372.3 1402.9 1426.1 1430.5 1450.3 1451.5 1461.9 1470.2 1476.5 1502.4 1575.4 1596.8 1638.1 1649.3 1655.1 1660.7 3158.1 3159.1 3162.0 3165.5 3175.0 3176.0 3179.4 3182.3 3189.7	0.50222 0.39415 0.22847
f3	-842.61309	61.3	0.22079	0.75(0.75)	26.1 90.3 136.1 147.2 181.5 229.3 285.6 302.4 316.2 325.0 420.3 444.8 449.2 466.1 493.5 499.8 531.5 553.8 558.1 596.9 618.2 624.0 639.1 654.6 669.6 679.8 691.7 740.9 760.4 764.5 786.1 805.2 816.0 825.0 828.4 848.9 854.5 899.4 905.9 958.9 961.6 972.5 979.6 998.2 1044.6 1086.9 1128.2 1144.2 1148.7 1157.1 1164.8 1169.1 1193.9 1202.8 1213.2 1234.1 1263.6 1315.2 1328.5 1364.5 1378.7 1399.5 1421.3 1428.3 1447.2 1454.5 1474.0 1477.5 1500.3 1612.0 1615.7 1628.6 1635.2 1647.7 1918.1 3053.0 3155.5 3156.6 3158.5 3159.3 3173.0 3174.0 3175.7 3176.5	0.55252 0.35917 0.23292
f5	-842.66166	30.8	0.21948	0.76(0.75)	37.3 76.2 83.0 106.1 145.7 195.1 225.8 287.2 295.4 329.3 335.1 400.1 436.0 437.1 464.1 471.4 498.0 514.2 534.3 550.0 560.5 579.8 606.1 631.2 636.2 650.5 651.4 684.3 700.0 760.6 764.8 773.1 776.6 811.8 828.0 835.8	0.53030 0.27472 0.18097

Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
					841.7 847.0 893.2 946.8 948.1 955.8 966.7 973.4 1026.7 1069.9 1095.0 1122.7 1142.9 1158.5 1163.3 1202.5 1205.9 1226.4 1228.3 1252.0 1277.1 1331.9 1338.2 1385.3 1402.5 1424.9 1428.6 1444.7 1447.3 1479.2 1481.3 1522.5 1526.9 1580.0 1616.1 1645.5 1671.6 1693.3 2207.7 3152.2 3157.3 3157.8 3159.8 3171.4 3174.1 3174.6 3175.5 3176.3	
CO	-113.34134	N/A	0.00506		2219.8	58.03862
f4	-729.28569	N/A	0.21115	0.78(0.75)	136.8 158.2 203.4 284.5 293.4 321.8 341.7 421.4 444.1 445.5 473.6 495.0 495.7 554.2 561.8 582.8 589.2 613.3 646.0 655.0 658.8 663.5 685.8 709.9 746.6 753.1 774.0 780.0 799.6 813.5 815.4 841.6 842.6 883.5 921.2 955.0 958.6 966.9 973.7 1011.2 1055.1 1084.8 1105.7 1142.8 1159.3 1159.3 1183.7 1187.7 1207.8 1211.8 1238.4 1258.5 1306.7 1319.7 1375.7 1386.3 1402.4 1414.6 1427.3 1431.4 1448.9 1453.9 1467.3 1492.9 1560.8 1586.2 1605.3 1606.9 1622.9 3153.5 3154.5 3156.0 3156.2 3170.9 3172.0 3173.4 3174.0 3197.8	0.62016 0.56158 0.32054
fTS1-5	-842.63550	47.2	0.21805	0.77(0.75)	-808.1 63.7 109.0 128.9 160.1 179.5 244.2 289.0 294.3 320.6 334.4 389.3 426.9 434.1 446.7 481.1 504.9 527.3 533.0 549.9 558.9 577.1 600.8 612.1 621.9 646.9 649.8 663.8 680.6 737.0 754.7 763.9 770.2 800.9 813.7 823.9 832.2 849.1 902.1 927.0 950.0 960.5 969.5 976.4 1003.2 1074.7 1092.2 1101.3 1142.8 1158.6 1159.4 1175.7 1199.7 1217.9 1232.4 1245.5 1292.1 1323.7 1338.4 1387.3 1411.2 1416.5 1425.4 1440.0 1455.7 1459.5 1474.7 1491.3 1511.5 1600.3 1621.0 1641.0 1655.7 1665.0 1959.6 3139.1 3156.6 3157.7 3159.0 3162.1 3173.6 3175.0 3176.1 3180.0	0.48538 0.37322 0.21502
fTS5-3	-842.58808	77.0	0.21848	0.78(0.75)	-591.1 52.0 91.3 137.7 143.6 179.6 248.7 287.6 300.3 317.6 378.1 387.5 434.7 443.8 453.3 485.8 491.2 496.8 542.0 551.6 561.9 612.0 613.8 630.7 653.2 657.6 666.3 686.1 737.8 758.8 762.3 779.1 795.8 812.6 826.4 829.6 850.1 881.9 917.6 951.0 960.2 961.9 972.3 979.0 1017.3 1052.7 1075.3 1100.5 1143.7 1152.4 1161.9 1167.8 1195.4 1215.3 1227.7 1246.4 1259.7 1314.2 1320.0 1348.9 1376.3 1412.9 1419.5 1427.5 1444.0 1452.4 1468.7 1476.9 1499.3 1612.0 1623.7 1630.7 1643.9 1649.8 2069.5 3104.6 3149.6 3154.8 3155.8 3160.3 3166.9 3172.3 3173.4 3178.2	0.53197 0.34212 0.21907
fTS1-3	-842.57720	83.8	0.21855	0.78(0.75)	-649.5 95.1 124.5 142.2 182.4 200.2 262.8 300.8 306.0 317.3 390.8 433.2 446.1 447.4 472.3 492.7 523.1 536.2 550.2 558.9 606.2 614.5 640.7 644.1 647.6 669.4 674.7 689.9 751.6 762.1 770.5 774.7 792.9 803.7 819.6 839.7 864.9 875.7 920.9 953.4 957.7 964.7 970.2 976.0 1014.7 1027.3 1071.0 1101.2 1137.9 1153.1 1161.9 1163.2 1186.0 1194.4 1211.2 1231.8 1252.7 1312.4 1322.7 1350.3 1384.5 1405.0 1417.7 1423.4 1430.4 1441.6 1455.2 1471.1 1497.8 1530.3 1593.2 1608.0 1619.8 1626.8 1899.3 3139.6 3155.1 3155.9 3157.0 3158.6 3172.7 3173.8 3175.5 3180.3	0.54111 0.38203 0.24554
fTS3-4	-842.60689	65.2	0.21843	0.77(0.75)	-432.2 62.0 69.1 135.8 147.2 157.0 194.8 271.3 302.9 311.8 325.2 404.5 432.5 445.7 459.1 478.8 500.0 504.1 556.4 561.2 599.7 611.1 619.3 651.4 655.5 666.0 676.6 702.8 713.2 756.7 774.3 780.0 804.5 816.4 817.1 833.9 843.0 894.8 910.1 956.2 958.4 969.6 969.6 976.7 1005.4 1057.4 1097.7 1128.9 1142.1 1155.6 1160.6 1172.7 1187.8 1210.9 1212.1 1241.1 1262.0 1313.8 1326.2 1373.1 1383.3 1398.4 1417.7 1429.4 1444.6 1450.6 1467.8 1475.7 1499.0 1593.4 1611.3 1613.1 1618.6 1629.3 2014.0 3154.8 3155.8 3157.9 3158.1 3172.2 3173.3 3175.1 3175.6 3187.5	0.53814 0.36671 0.24152
Oxyradical g						
Species	Total Energy (hartrees)	Relative Energy (kcal/mol)	ZPE (unscaled) (hartrees)	$\langle S^2 \rangle$	Frequencies (unscaled) (cm-1)	Rotational constants (GHz)
g	-1531.11380	0.0	0.37862	0.80	60.2 73.6 93.1 133.9 147.3 165.8 197.3 225.4 237.4 246.4 263.8 278.4 290.9 310.8 317.7 329.6 339.4 362.3 369.0 389.8 395.2 405.9 424.3 440.1 444.7 456.0 473.5 483.9 493.7 505.1 513.8 527.9 543.7 556.5 559.9 579.7 587.9 592.9 597.0 602.7 618.7 627.0 638.2 642.2 649.6 659.9 668.9 686.0 687.9 713.9 724.3 730.1 737.0 739.5 746.9 761.6 768.4 771.2 788.1 790.1 796.4 798.2 817.6 826.7 838.1 844.7 846.7 863.2 874.3 876.3 891.0 902.3 907.4 930.5 946.1 968.3 973.8 980.4 983.7 992.4 1003.8 1034.4 1079.2 1096.9 1121.4 1141.0 1158.5 1167.9	0.14642 0.11654 0.06934

					1170.7 1175.0 1184.0 1188.7 1203.1 1213.0 1215.5 1226.7 1229.0 1256.2 1258.9 1266.5 1297.1 1316.9 1326.6 1331.2 1337.2 1354.5 1366.3 1377.1 1387.3 1394.0 1394.8 1402.9 1410.6 1415.6 1426.2 1429.1 1440.6 1448.5 1455.1 1465.9 1479.0 1490.3 1512.7 1514.2 1527.3 1538.0 1547.4 1571.8 1585.6 1593.9 1613.7 1618.8 1621.0 1631.4 1639.5 1655.5 1663.1 3158.1 3158.6 3159.4 3161.0 3161.9 3162.4 3166.5 3176.6 3176.7 3177.9 3178.9 3179.9 3181.4	
g3	-1531.04244	44.8	0.37755	0.75	23.3 64.9 75.9 87.6 129.6 153.5 161.0 196.6 213.5 234.5 237.6 258.3 287.5 298.1 325.6 329.0 342.6 357.9 363.5 367.1 393.6 397.2 404.2 441.9 446.6 452.1 469.7 472.2 489.1 499.8 504.5 519.1 528.0 542.8 571.3 573.0 578.9 585.3 595.8 599.8 612.1 624.6 637.7 640.8 649.9 656.3 667.5 674.8 714.2 724.7 725.2 738.0 740.9 743.4 752.5 764.7 770.6 782.2 789.9 794.5 795.0 798.6 805.5 813.6 835.0 840.3 849.2 863.0 874.8 887.4 889.9 900.1 902.3 905.9 944.7 966.6 967.7 980.4 980.8 984.9 999.2 1017.7 1060.9 1095.2 1104.4 1141.8 1149.2 1168.1 1169.6 1172.8 1179.2 1188.0 1195.1 1206.3 1210.4 1214.3 1220.0 1231.0 1249.2 1264.4 1267.2 1291.5 1320.2 1320.5 1325.8 1347.2 1354.6 1371.9 1376.0 1388.9 1396.3 1401.7 1404.3 1412.4 1420.3 1438.4 1449.3 1453.2 1462.9 1481.7 1490.3 1509.4 1519.5 1525.1 1533.5 1544.9 1553.2 1581.4 1597.7 1611.6 1615.6 1617.5 1626.0 1634.4 1642.4 1650.6 1919.5 3085.6 3156.6 3157.1 3157.7 3158.4 3159.0 3160.2 3163.1 3167.2 3174.5 3174.9 3176.5 3177.0	0.14002 0.12273 0.07181
g5	-1531.02423	56.2	0.37513	0.76	24.6 53.8 70.5 76.6 115.8 137.4 139.5 168.5 201.9 213.9 233.5 236.5 270.5 285.6 295.6 320.1 331.1 339.1 357.4 364.6 380.8 386.2 393.7 421.2 431.4 441.5 455.4 461.9 471.0 485.7 493.0 503.4 512.7 532.6 543.4 547.7 562.4 571.3 579.4 582.3 587.9 594.5 612.8 624.3 633.3 640.2 643.6 662.6 668.6 674.1 684.4 705.3 723.5 730.5 739.5 744.5 758.0 763.9 766.8 780.3 789.2 790.4 795.7 799.0 811.3 823.5 836.0 840.0 857.8 867.4 879.0 884.9 895.6 903.6 923.2 949.6 966.6 966.7 979.0 980.2 990.1 1010.5 1053.2 1088.9 1098.8 1131.3 1137.3 1153.7 1163.8 1168.9 1171.2 1180.7 1195.8 1197.1 1212.4 1218.4 1225.8 1237.5 1252.9 1266.2 1281.4 1290.0 1308.2 1325.9 1335.8 1348.9 1365.7 1375.1 1377.8 1387.6 1389.2 1398.0 1405.8 1410.3 1415.9 1427.2 1428.8 1448.6 1455.1 1461.2 1480.4 1500.9 1517.0 1525.2 1532.7 1544.7 1549.8 1589.8 1602.9 1607.1 1619.9 1623.0 1626.8 1627.9 1658.3 1669.7 2201.9 3152.0 3152.9 3156.0 3157.0 3157.7 3158.8 3159.6 3160.2 3166.3 3174.4 3175.4 3175.9 3177.1	0.13759 0.11005 0.06529
CO	-113.34134		0.00506		2219.8	58.03862
g4	-1417.72231		0.36803	0.79	72.7 76.6 136.7 152.5 174.5 209.1 236.4 243.2 253.5 288.2 297.5 327.5 332.3 345.4 353.2 369.6 380.0 384.0 401.6 409.6 440.5 447.0 447.7 470.6 475.4 488.7 497.9 510.7 522.0 539.2 565.1 579.4 580.9 582.8 589.7 592.8 601.3 617.4 622.7 635.1 649.1 659.1 664.5 672.5 711.5 722.4 729.0 733.8 737.1 738.4 743.2 755.0 760.0 760.4 771.6 786.8 791.5 794.3 796.4 801.2 831.8 835.8 847.4 857.7 872.3 875.5 876.0 893.3 903.1 911.3 961.2 965.2 965.4 978.6 978.8 1002.8 1007.4 1035.1 1080.6 1090.2 1118.8 1129.1 1164.9 1167.2 1170.5 1171.6 1182.6 1199.2 1199.4 1212.4 1216.6 1219.6 1230.7 1247.1 1262.8 1266.4 1289.7 1320.0 1322.8 1325.2 1347.0 1349.5 1368.9 1368.9 1373.3 1395.9 1399.7 1406.0 1411.1 1414.3 1428.4 1437.0 1447.0 1450.9 1469.9 1483.9 1490.2 1496.3 1509.7 1527.6 1529.4 1541.7 1573.4 1573.9 1588.0 1613.1 1614.2 1620.6 1628.3 1640.4 1648.8 3156.2 3156.4 3157.0 3157.7 3158.6 3159.9 3160.7 3161.3 3174.0 3174.1 3176.1 3176.4 3214.3	0.18892 0.12379 0.08274
gTS1-5	-1531.02232	57.4	0.37454	0.76	-122.0 43.1 70.4 74.3 116.6 137.9 146.3 172.3 205.4 215.6 236.2 254.3 272.0 289.2 298.8 301.6 322.1 334.5 352.1 356.1 363.4 385.0 391.4 420.1 432.4 442.9 448.2 458.0 468.5 480.1 490.5 493.8 512.2 520.0 532.0 542.6 566.3 572.0 577.6 580.3 589.1 596.0 617.2 623.5 626.0 635.1 644.8 658.2 665.6 672.0 684.0 709.1 715.8 728.0 736.3 740.9 747.5 758.3 761.4 771.8 779.8 788.2 795.4 796.8 816.8 823.1 835.4 837.2 857.4 866.3 878.1 881.9 894.3 903.0 911.2 942.0 966.6 967.3 978.7 980.8 990.9	0.13884 0.11656 0.06728

					1014.9 1054.0 1088.1 1092.0 1129.1 1138.3 1160.8 1166.3 1170.6 1173.2 1186.8 1197.1 1200.1 1214.9 1216.8 1229.3 1242.3 1256.3 1263.7 1281.5 1296.9 1313.3 1328.3 1335.7 1343.8 1366.9 1371.7 1383.1 1389.5 1395.6 1401.8 1405.7 1415.1 1421.0 1428.0 1440.2 1449.5 1456.2 1460.3 1480.9 1500.0 1519.2 1526.7 1534.3 1542.5 1549.5 1587.6 1600.3 1609.4 1619.4 1621.9 1625.0 1628.7 1656.0 1666.7 2106.6 3125.8 3156.4 3157.1 3157.8 3158.4 3159.6 3160.0 3160.6 3164.0 3174.7 3176.0 3176.3 3177.7	
gTS5-3	-1531.00304	69.5	0.37472	0.77	-515.7 40.4 70.0 75.4 85.7 132.1 143.5 164.8 193.7 211.3 234.3 245.2 281.1 294.5 305.7 322.4 325.7 337.1 345.4 359.6 362.8 389.7 394.9 406.7 425.8 438.1 451.8 459.4 473.9 485.6 489.2 496.8 507.0 525.4 545.5 549.4 572.4 572.9 584.4 592.5 595.0 599.6 624.3 626.3 635.9 644.3 656.9 664.8 673.7 676.2 707.3 726.0 733.0 737.6 739.1 750.1 753.7 764.2 771.2 787.9 792.8 795.2 798.4 809.8 818.3 832.6 837.9 845.8 863.8 876.7 880.6 891.6 894.4 903.2 914.7 954.8 966.7 967.1 979.3 980.6 991.7 1014.9 1040.7 1077.8 1093.3 1106.3 1131.4 1152.9 1168.3 1172.1 1179.2 1185.2 1191.6 1197.9 1210.7 1213.8 1220.6 1245.8 1259.5 1261.4 1272.6 1296.4 1307.4 1317.0 1325.6 1343.5 1353.9 1371.8 1380.0 1385.7 1393.1 1394.7 1401.4 1409.2 1420.9 1428.5 1444.3 1448.4 1454.7 1459.6 1482.8 1494.0 1518.2 1521.3 1527.4 1541.1 1550.8 1580.8 1595.1 1599.4 1616.4 1619.7 1621.5 1624.4 1647.7 1656.2 2119.9 3124.4 3141.5 3155.7 3156.5 3157.2 3158.0 3158.7 3159.8 3167.7 3173.4 3174.7 3175.4 3176.4	0.13463 0.11972 0.06833
gTS1-3	-1531.00582	67.8	0.37521	0.79	-665.8 61.7 75.3 85.3 127.1 145.9 156.7 174.3 209.9 233.9 235.8 256.5 285.5 298.4 311.9 328.8 332.9 349.9 356.4 365.0 391.5 398.0 405.6 414.7 440.9 444.9 460.8 469.9 472.7 487.1 498.9 507.4 515.0 525.0 546.6 571.5 574.6 583.6 583.8 592.9 597.8 616.9 625.4 635.8 646.8 652.2 663.2 675.5 684.1 709.0 711.9 724.3 735.3 739.4 746.5 751.3 763.8 769.6 782.3 789.3 791.5 797.8 798.3 809.9 823.3 836.9 843.1 851.2 865.3 877.1 888.2 892.0 902.2 921.1 955.8 964.5 965.7 977.6 979.5 996.1 1008.3 1016.6 1050.1 1054.2 1086.5 1102.1 1128.0 1149.7 1167.9 1169.5 1173.3 1182.8 1194.5 1202.7 1203.7 1214.0 1217.0 1226.9 1244.9 1260.2 1267.0 1291.3 1315.6 1320.0 1324.5 1347.1 1350.3 1361.9 1367.8 1375.1 1392.4 1395.7 1402.8 1408.2 1417.8 1433.4 1437.0 1446.5 1459.6 1470.4 1480.1 1486.5 1508.4 1517.5 1531.1 1531.7 1547.1 1567.4 1584.6 1600.2 1610.8 1616.7 1626.3 1626.7 1640.4 1649.5 1849.4 3055.4 3156.4 3157.0 3157.7 3158.6 3159.3 3160.1 3167.8 3174.0 3174.7 3175.9 3176.2 3177.2	0.14324 0.12106 0.07171
gTS3-4	-1531.03896	47.0	0.37533	0.77	-462.0 56.7 58.2 75.5 78.8 131.8 140.7 161.1 166.2 213.6 220.0 237.3 247.9 287.3 298.2 322.0 329.3 343.2 358.4 358.5 368.8 390.4 396.7 400.6 442.8 447.0 447.9 468.3 471.1 473.7 489.7 501.5 513.0 524.0 541.7 570.3 575.8 580.2 585.9 594.5 596.5 611.5 624.7 625.3 638.2 650.2 661.1 674.0 695.1 713.1 726.6 727.9 734.9 741.3 743.9 755.4 768.5 769.7 772.7 788.1 794.2 795.7 798.5 803.1 834.1 838.1 846.5 861.1 873.8 885.7 886.3 892.4 902.2 906.3 952.9 966.3 966.4 980.3 980.4 997.0 1002.3 1019.9 1020.7 1074.4 1095.1 1110.6 1146.3 1150.9 1169.4 1171.6 1176.0 1183.9 1198.9 1204.0 1205.4 1213.6 1214.1 1227.5 1248.4 1262.2 1267.8 1292.0 1320.7 1322.1 1325.7 1347.8 1354.1 1371.5 1372.8 1390.7 1396.3 1399.6 1404.4 1411.7 1417.5 1435.0 1447.6 1451.5 1458.0 1479.6 1488.0 1501.3 1513.0 1521.0 1532.1 1538.3 1549.8 1580.2 1594.8 1599.6 1615.2 1616.6 1622.4 1630.9 1641.0 1649.6 1982.6 3156.4 3156.9 3157.3 3158.1 3158.9 3159.7 3163.2 3163.5 3174.6 3174.6 3176.5 3176.8 3186.1	0.14115 0.12248 0.07275

Table S2. Cartesian coordinates of optimized structures at B3LYP/6-311G(d,p) level for oxyradcials a-g.

Species Name	Geometry (Å)
a	C 3.409567 -0.795807 -0.000307 C 3.349971 0.566817 -0.000280 C 2.065872 1.232369 0.000098 C 0.971257 0.372422 0.000637 C 0.943493 -1.040443 0.000468 C 2.230498 -1.710220 -0.000048 H 4.366074 -1.306270 -0.000606 H 4.265665 1.149926 -0.000588 C -0.335527 0.870671 0.000677 C -1.215538 -0.210963 0.000604 C -2.588309 -0.028338 0.000094 C -3.336157 -1.243359 -0.000347 C -2.666803 -2.461078 -0.000331 C -1.246795 -2.589972 0.000020 C -0.484875 -1.433695 0.000479 H -4.420881 -1.228950 -0.000743 H -3.255571 -3.371614 -0.000682 H -0.791501 -3.572852 -0.000192 O 2.375997 -2.941574 -0.000233 C 1.743007 2.627340 -0.000218 H 2.549971 3.352611 -0.000617 C 0.430698 3.099337 -0.000129 H 0.266567 4.171908 -0.000477 C -0.696027 2.199977 0.000172 C -3.015483 1.354142 -0.000218 H -4.078441 1.572470 -0.000532 C -2.124261 2.414132 -0.000218 H -2.517395 3.425364 -0.000629
a3	C 2.639573 -0.613724 -0.414727 C 2.978720 0.870879 -0.120051 C 1.835746 1.622215 -0.213854 C 0.819622 0.706350 -0.603416 C -0.553334 0.936690 -0.450852 C -1.161253 -0.314683 -0.433600 C -2.476825 -0.450487 -0.007785 C -2.912519 -1.800261 0.147658 C -2.001942 -2.828176 -0.038266 C -0.619566 -2.630152 -0.349250 C -0.157999 -1.344741 -0.550607 C 1.141182 -0.614711 -0.672929 C 3.127711 -1.546621 0.718411 H 3.228843 -0.969112 -1.274380 H 3.978962 1.179183 0.152506 H -3.928400 -2.028452 0.451828 H -2.339553 -3.848313 0.109127 H 0.043533 -3.487383 -0.364967 O 2.619927 -2.531411 1.112107 C -1.067316 2.104281 0.047051 C 1.301963 2.941285 0.150690 H 1.977373 3.756191 0.386263 C -0.052032 3.154302 0.267496 H -0.384540 4.134654 0.594512 C -3.122013 0.784756 0.366744 H -4.158312 0.755019 0.688092 C -2.451926 2.003879 0.418722 H -2.984072 2.873002 0.791547
a5	C 3.536822 -0.712201 -0.000048 C 3.063298 0.640590 0.000014 C 1.736508 0.992573 0.000025 C 0.636009 0.046408 -0.000035 C -0.698510 0.633347 -0.000095 C -1.651097 -0.377170 -0.000113 C -3.022515 -0.135860 -0.000056 C -3.836197 -1.301166 0.000036 C -3.237594 -2.554897 0.000086 C -1.829553 -2.756707 0.000063 C -1.003186 -1.646842 -0.000041 C 0.416078 -1.312381 -0.000006 C 4.821021 -1.044538 -0.000018 H 2.838168 -1.545061 -0.000109 H 3.805390 1.432307 0.000057 H -4.917991 -1.221025 0.000077

	H	-3.874657	-3.432597	0.000162
	H	-1.436599	-3.767313	0.000137
	O	5.936653	-1.351060	0.000010
	C	-1.030533	1.968573	-0.000046
	C	1.368090	2.408967	0.000092
	H	2.190397	3.117517	0.000144
	C	0.092595	2.887049	0.000074
	H	-0.081955	3.957460	0.000228
	C	-3.391630	1.251734	-0.000029
	H	-4.442441	1.522854	0.000000
	C	-2.437872	2.254892	-0.000030
	H	-2.763931	3.290100	-0.000010
a6	C	3.898198	-0.712851	0.000007
	C	3.538613	0.551285	0.000033
	C	2.165963	1.056779	0.000039
	C	1.045224	0.223456	0.000019
	C	0.785340	-1.231393	-0.000001
	C	1.619295	-2.267643	-0.000019
	H	4.785645	-1.324284	-0.000003
	H	4.328592	1.311292	0.000050
	C	-0.221156	0.838764	0.000026
	C	-1.239634	-0.122387	-0.000009
	C	-2.596558	0.205961	-0.000018
	C	-3.483558	-0.893742	-0.000064
	C	-2.972991	-2.189504	-0.000099
	C	-1.588614	-2.483547	-0.000089
	C	-0.698750	-1.421753	-0.000041
	H	-4.556988	-0.738456	-0.000074
	H	-3.669044	-3.021179	-0.000133
	H	-1.261492	-3.517362	-0.000113
	O	2.183482	-3.280232	-0.000052
	C	1.926765	2.461048	0.000070
	H	2.794658	3.112881	0.000088
	C	0.664436	3.038445	0.000081
	H	0.568520	4.118727	0.000105
	C	-0.481870	2.210757	0.000056
	C	-2.879045	1.623016	0.000020
	H	-3.914029	1.949521	0.000016
	C	-1.880587	2.568478	0.000055
	H	-2.150150	3.619709	0.000078
a7	C	2.518584	-0.415861	-0.946582
	C	2.787726	0.915462	-0.980301
	C	1.779482	1.665599	-0.195702
	C	1.016711	0.692525	0.402244
	C	-0.345986	0.848950	0.534800
	C	-0.956391	-0.393122	0.246630
	C	-2.335134	-0.494808	0.060019
	C	-2.786985	-1.763606	-0.376351
	C	-1.866998	-2.769498	-0.650641
	C	-0.462617	-2.588293	-0.552882
	C	0.006025	-1.360820	-0.131527
	C	1.408299	-0.715409	0.063291
	C	2.108212	-1.526165	1.229590
	H	3.112432	-1.189905	-1.413929
	H	3.584156	1.361130	-1.563764
	H	-3.844514	-1.947860	-0.533733
	H	-2.234579	-3.728952	-0.997306
	H	0.205154	-3.392749	-0.838408
	O	2.570171	-2.602332	1.132356
	C	-0.997714	2.073928	0.394126
	C	1.203664	2.967028	-0.258461
	H	1.767361	3.801712	-0.660894
	C	-0.136988	3.170190	0.084788
	H	-0.552942	4.166719	-0.023676
	C	-3.068535	0.750174	0.189433
	H	-4.149110	0.728003	0.092505
	C	-2.439534	1.968463	0.317671
	H	-3.040253	2.872129	0.299497
a10	C	-3.656071	-0.306878	0.000027
	C	-3.081831	0.910237	0.000254
	C	-1.666623	1.181316	0.000030
	C	-0.650655	0.192504	-0.000271
	C	0.691799	0.671915	-0.000501
	C	1.571566	-0.412822	-0.000526
	C	2.950801	-0.271578	-0.000149
	C	3.674102	-1.498140	0.000230

	C	2.983702	-2.706159	0.000331
	C	1.567950	-2.798972	0.000131
	C	0.827275	-1.621100	-0.000290
	C	-0.576076	-1.239808	-0.000157
	C	-4.747972	-0.986005	0.000042
	H	-1.422989	-1.908755	0.000154
	H	-3.712879	1.802768	0.000583
	H	4.758822	-1.500004	0.000483
	H	3.555318	-3.627549	0.000636
	H	1.097133	-3.775799	0.000369
	O	-5.641443	-1.746319	-0.000016
	C	1.128577	1.986213	-0.000159
	C	-1.236563	2.551023	0.000193
	H	-2.012315	3.309839	0.000417
	C	0.083656	2.961514	0.000142
	H	0.316740	4.020777	0.000365
	C	3.426016	1.090498	0.000057
	H	4.494903	1.277335	0.000283
	C	2.558983	2.163325	0.000045
	H	2.965011	3.169439	0.000258
a11	C	-2.520688	0.083481	-0.019945
	C	-2.456965	1.514121	-0.281300
	C	-1.194476	2.009768	0.156743
	C	-0.532988	0.947866	0.762289
	C	0.816271	0.766395	0.555890
	C	1.057062	-0.616056	0.385944
	C	2.296321	-1.083985	-0.056104
	C	2.348595	-2.475443	-0.317593
	C	1.198829	-3.245256	-0.193501
	C	-0.066992	-2.704311	0.158938
	C	-0.150631	-1.353905	0.429347
	C	-1.279725	-0.358273	0.819510
	C	-3.528412	-0.728856	-0.307649
	H	-1.626854	-0.602231	1.831392
	H	-3.213462	2.055800	-0.831366
	H	3.270968	-2.939430	-0.651045
	H	1.256547	-4.304561	-0.418853
	H	-0.937384	-3.351441	0.165307
	O	-4.392110	-1.458285	-0.585324
	C	1.672269	1.760304	0.077741
	C	-0.359954	3.127619	-0.209146
	H	-0.805905	4.041352	-0.586259
	C	1.023683	3.010332	-0.205815
	H	1.614503	3.854363	-0.547771
	C	3.287336	-0.060805	-0.314958
	H	4.281355	-0.365150	-0.625822
	C	2.983159	1.286771	-0.283418
	H	3.740941	1.998964	-0.594821
CO	C	0.000000	0.000000	-0.643976
	O	0.000000	0.000000	0.482982
a4	C	1.685666	-2.530321	-0.170025
	C	2.852682	-1.731217	-0.284868
	C	2.535758	-0.325475	0.055551
	C	1.227168	-0.418893	0.452657
	C	0.319821	0.599755	0.448465
	C	-0.954835	0.007122	0.329148
	C	-2.062167	0.792112	0.038436
	C	-3.253870	0.060899	-0.203580
	C	-3.218781	-1.332853	-0.211419
	C	-2.036574	-2.094350	-0.031348
	C	-0.846805	-1.426859	0.231737
	C	0.607910	-1.714710	0.264387
	H	1.651434	-3.579222	-0.430640
	H	3.807423	-2.106115	-0.632514
	H	-4.187021	0.571857	-0.416597
	H	-4.140726	-1.867838	-0.411372
	H	-2.078807	-3.172629	-0.135208
	C	0.659720	1.908126	0.131484
	C	2.966138	1.013198	-0.184549
	H	3.984887	1.228776	-0.489762
	C	2.059374	2.090851	-0.119436
	H	2.436315	3.080878	-0.354655
	C	-0.505809	2.745755	-0.077624
	H	-0.384258	3.807124	-0.269301
	C	-1.781381	2.215436	-0.097504
	H	-2.613344	2.885717	-0.289029

C₂H₂	C	0.000000	0.000000	0.598990
	C	0.000000	0.000000	-0.598990
	H	0.000000	0.000000	1.661939
	H	0.000000	0.000000	-1.661939
a8	C	1.667081	2.210862	0.000079
	C	0.553944	1.418085	0.000030
	C	-0.929198	1.519630	-0.000068
	C	-1.630092	2.641313	-0.000072
	C	0.841743	0.029071	-0.000016
	C	-0.346115	-0.712978	-0.000015
	C	-0.361979	-2.109557	-0.000021
	C	-1.647022	-2.696506	0.000019
	C	-2.776858	-1.882162	0.000074
	C	-2.721670	-0.468503	0.000079
	C	-1.473215	0.132750	0.000022
	H	-1.761594	-3.775001	0.000016
	H	-3.754237	-2.352072	0.000098
	H	-3.643212	0.102509	0.000093
	O	-2.247613	3.619286	-0.000065
	C	2.970233	1.717027	0.000082
	H	3.811424	2.401957	0.000118
	C	3.204878	0.336863	0.000019
	H	4.225033	-0.032097	0.000020
	C	2.109929	-0.557013	-0.000023
	C	0.941477	-2.734515	-0.000067
	H	1.000157	-3.818043	-0.000079
	C	2.104830	-2.003510	-0.000068
	H	3.055530	-2.526678	-0.000079
H	H	0.000000	0.000000	0.000000
a9	C	4.568534	0.257260	-0.000043
	C	3.488422	-0.277913	-0.000030
	C	2.199158	-0.879590	0.000011
	C	1.029551	-0.117057	-0.000008
	C	0.684068	1.323646	-0.000064
	C	1.519020	2.353091	-0.000114
	H	5.523085	0.723742	0.000279
	C	-0.197610	-0.804724	0.000031
	C	-1.268632	0.097360	0.000005
	C	-2.603382	-0.311268	0.000035
	C	-3.554014	0.734336	0.000002
	C	-3.120755	2.057756	-0.000055
	C	-1.756098	2.433987	-0.000083
	C	-0.804393	1.427340	-0.000052
	H	-4.616396	0.515987	0.000021
	H	-3.864757	2.846802	-0.000079
	H	-1.492231	3.485625	-0.000128
	O	2.207037	3.281396	-0.000159
	C	2.050652	-2.300194	0.000068
	H	2.958458	-2.891727	0.000082
	C	0.822830	-2.946138	0.000107
	H	0.791343	-4.030178	0.000150
	C	-0.373083	-2.189134	0.000088
	C	-2.800459	-1.742844	0.000094
	H	-3.814348	-2.129837	0.000119
	C	-1.748109	-2.628846	0.000119
	H	-1.955650	-3.693977	0.000164
aTS1-5	C	3.821670	-0.378682	0.114108
	C	3.260661	0.925685	0.060613
	C	1.929027	1.267560	-0.019945
	C	0.888486	0.281566	-0.018478
	C	0.782931	-1.090056	0.055770
	C	3.301741	-1.615559	-0.009815
	H	4.892461	-0.462724	0.293118
	H	3.988224	1.728031	0.124182
	C	-0.472109	0.773882	-0.011670
	C	-1.348950	-0.302707	-0.003560
	C	-2.732322	-0.151822	0.009144
	C	-3.465264	-1.369471	0.017273
	C	-2.781538	-2.579520	0.020905
	C	-1.362921	-2.687287	0.024031
	C	-0.611961	-1.524888	0.011590
	H	-4.549997	-1.364221	0.021372
	H	-3.357716	-3.498323	0.026107
	H	-0.903115	-3.668983	0.037246
	O	3.192822	-2.760369	-0.161118
	C	1.495439	2.659763	-0.036116

	H	2.276666	3.413328	-0.045390
	C	0.190127	3.064859	-0.033155
	H	-0.043008	4.124037	-0.041886
	C	-0.881219	2.087692	-0.016427
	C	-3.188822	1.211871	-0.000594
	H	-4.255289	1.413099	-0.003384
	C	-2.306145	2.278804	-0.013616
	H	-2.703794	3.288567	-0.022764
aTS1-6	C	-3.321350	-1.766552	0.000000
	C	-3.472117	-0.457241	0.000000
	C	-2.360613	0.482151	0.000000
	C	-1.064589	-0.018826	0.000000
	C	-0.485291	-1.359032	0.000000
	C	-1.127196	-2.539984	0.000000
	H	-3.891922	-2.679828	0.000000
	H	-4.491444	-0.058087	0.000000
	C	0.000000	0.892088	0.000000
	C	1.217506	0.204356	0.000000
	C	2.448723	0.859571	0.000000
	C	3.578612	0.009707	0.000000
	C	3.398164	-1.371604	0.000000
	C	2.127385	-1.998788	0.000000
	C	1.002520	-1.191114	0.000000
	H	4.582484	0.420490	0.000000
	H	4.276710	-2.007619	0.000000
	H	2.065278	-3.081262	0.000000
	O	-1.296472	-3.698494	0.000000
	C	-2.509368	1.898257	0.000000
	H	-3.515927	2.304595	0.000000
	C	-1.433986	2.780231	0.000000
	H	-1.621942	3.848336	0.000000
	C	-0.105115	2.281341	0.000000
	C	2.364291	2.303540	0.000000
	H	3.284694	2.878829	0.000000
	C	1.161835	2.975521	0.000000
	H	1.167381	4.060746	0.000000
aTS1-3	C	2.435179	-0.954110	-0.798304
	C	2.910047	0.522482	-0.831195
	C	1.891402	1.345959	-0.303315
	C	1.476879	2.730584	-0.272622
	C	0.154743	3.087196	0.006055
	C	-0.884762	2.116853	0.266768
	C	-2.323732	2.190906	0.270593
	C	-3.107040	1.045037	0.245172
	C	-2.559435	-0.296287	0.164064
	C	-3.195254	-1.534533	-0.106678
	C	-2.413343	-2.664158	-0.342100
	C	-0.994032	-2.660368	-0.366274
	C	-0.322477	-1.473596	-0.096560
	C	1.045864	-0.900567	-0.142337
	C	2.972956	-1.485353	0.420673
	C	0.895656	0.467230	0.131304
	C	-0.417797	0.814307	0.356811
	C	-1.169832	-0.356690	0.230631
	H	2.613444	-1.562534	-1.693319
	H	3.903032	0.772643	-1.175470
	H	2.174771	3.517034	-0.537607
	H	-0.103101	4.140463	-0.042595
	H	-2.819680	3.156249	0.247627
	H	-4.185913	1.162968	0.220015
	H	-4.275837	-1.607421	-0.168349
	H	-2.916777	-3.600103	-0.560008
	H	-0.471635	-3.574632	-0.627028
	O	3.463945	-1.796751	1.417576
aTS1-7	C	2.561908	-0.797334	-0.864440
	C	2.912534	0.556930	-0.965319
	C	1.964684	1.378343	-0.250637
	C	1.057693	0.506641	0.320006
	C	-0.269126	0.844216	0.472731
	C	-1.057206	-0.299712	0.216243
	C	-2.443037	-0.204275	0.082986
	C	-3.088961	-1.408513	-0.291065
	C	-2.334657	-2.545099	-0.558401
	C	-0.915406	-2.566974	-0.516564
	C	-0.258087	-1.410650	-0.149854
	C	1.209774	-0.952432	0.000085

	C	2.239191	-1.601449	0.779923
	H	3.000704	-1.605205	-1.434199
	H	3.778300	0.903284	-1.514161
	H	-4.167521	-1.443393	-0.402996
	H	-2.850196	-3.451198	-0.857021
	H	-0.385036	-3.466994	-0.805689
	O	2.506044	-2.580177	1.389785
	C	-0.743348	2.150805	0.363646
	C	1.568586	2.757514	-0.250888
	H	2.254849	3.523627	-0.594479
	C	0.268232	3.126680	0.083607
	H	-0.004417	4.174968	0.014898
	C	-2.984856	1.132827	0.214585
	H	-4.059986	1.265899	0.152956
	C	-2.182305	2.250768	0.315733
	H	-2.648731	3.230710	0.308173
aTS5-3	C	2.980962	-0.459796	-0.517257
	C	2.952443	1.038406	-0.309336
	C	1.693388	1.540997	-0.173904
	C	0.729620	0.490466	-0.174209
	C	-0.651689	0.770869	-0.051663
	C	-1.325273	-0.438402	-0.069382
	C	-2.704180	-0.499488	0.075283
	C	-3.232298	-1.825449	0.058103
	C	-2.363167	-2.896612	-0.079995
	C	-0.941307	-2.771775	-0.202495
	C	-0.382304	-1.511058	-0.198225
	C	0.969309	-0.847112	-0.236346
	C	3.940836	-1.175570	0.172694
	H	2.911217	-0.798299	-1.554917
	H	3.874421	1.603175	-0.272347
	H	-4.297478	-2.005918	0.156002
	H	-2.779118	-3.898375	-0.088840
	H	-0.341122	-3.671318	-0.287679
	O	4.359007	-1.978265	0.907668
	C	-1.211739	2.007806	0.105799
	C	1.122389	2.884222	-0.014389
	H	1.790452	3.738582	-0.001081
	C	-0.225674	3.099918	0.115401
	H	-0.574108	4.121488	0.231582
	C	-3.348407	0.781180	0.228183
	H	-4.427363	0.816713	0.339890
	C	-2.642055	1.980409	0.245545
	H	-3.194075	2.906014	0.373205
aTS5-10	C	-3.349951	-0.470540	0.015502
	C	-3.002023	0.887815	-0.004272
	C	-1.649076	1.261224	-0.047515
	C	-0.643501	0.256194	-0.039469
	C	0.703023	0.696273	-0.015778
	C	1.527110	-0.429839	-0.019095
	C	2.911212	-0.339354	0.013632
	C	3.580182	-1.597223	0.008588
	C	2.833896	-2.768774	-0.014915
	C	1.409173	-2.799731	-0.024687
	C	0.716129	-1.600516	-0.028539
	C	-0.706042	-1.172524	0.042836
	C	-4.550897	-1.019225	0.028566
	H	-2.385680	-1.204830	0.079581
	H	-3.767677	1.656180	0.058186
	H	4.663673	-1.650645	0.025028
	H	3.362860	-3.715662	-0.018710
	H	0.895949	-3.755259	-0.028348
	O	-5.538815	-1.625520	0.013411
	C	1.170311	1.995052	0.007105
	C	-1.194104	2.635194	-0.031237
	H	-1.948432	3.415766	-0.039163
	C	0.133274	2.999315	-0.005861
	H	0.395400	4.051988	0.004122
	C	3.429876	1.006271	0.035821
	H	4.504680	1.157062	0.051117
	C	2.603902	2.117854	0.031587
	H	3.054788	3.104766	0.047294
aTS10-11	C	-2.835990	-0.092181	-0.201631
	C	-2.694236	1.292236	-0.196541
	C	-1.453714	1.776663	0.287960
	C	-0.646027	0.713562	0.704814

C	0.723758	0.789368	0.428289
C	1.218906	-0.512313	0.284350
C	2.519026	-0.761546	-0.145736
C	2.830217	-2.135222	-0.319942
C	1.849923	-3.095649	-0.097080
C	0.514423	-2.783822	0.277919
C	0.172070	-1.455560	0.457657
C	-1.068403	-0.669197	0.796084
C	-3.767028	-0.973891	-0.437182
H	-1.711273	-1.029650	1.589581
H	-3.439459	1.938367	-0.649831
H	3.817873	-2.442923	-0.646846
H	2.105012	-4.138878	-0.247558
H	-0.210256	-3.584870	0.374468
O	-4.487947	-1.889116	-0.568976
C	1.406245	1.926653	0.025682
C	-0.787225	3.025954	0.005333
H	-1.382448	3.904520	-0.220309
C	0.588226	3.107191	-0.093002
H	1.042168	4.054999	-0.362525
C	3.308217	0.417840	-0.415475
H	4.342531	0.298084	-0.721266
C	2.777374	1.693061	-0.351003
H	3.404856	2.534413	-0.626893

aTS3-4	C	2.515006	-0.924263	-0.513875
	C	3.084907	0.480279	-0.291631
	C	2.038704	1.389905	-0.286626
	C	0.909511	0.611624	-0.618631
	C	-0.409882	0.995013	-0.424708
	C	-1.163013	-0.177230	-0.425933
	C	-2.482721	-0.159779	0.008620
	C	-3.083591	-1.446968	0.119787
	C	-2.313684	-2.574275	-0.127531
	C	-0.924984	-2.542715	-0.464369
	C	-0.301513	-1.318707	-0.615872
	C	1.077468	-0.754860	-0.755667
	C	2.699356	-1.792366	1.057858
	H	3.119809	-1.633799	-1.078652
	H	4.130774	0.647461	-0.072417
	H	-4.116932	-1.557973	0.430406
	H	-2.778977	-3.548005	-0.018253
	H	-0.385173	-3.478848	-0.549616
	O	2.141245	-2.775961	1.294457
	C	-0.770270	2.216929	0.089240
	C	1.684409	2.747995	0.122121
	H	2.460225	3.471362	0.347813
	C	0.365767	3.127165	0.290092
	H	0.169578	4.135515	0.640537
	C	-2.964400	1.141479	0.415104
	H	-3.993477	1.232336	0.748254
	C	-2.153979	2.272148	0.476826
	H	-2.578320	3.191401	0.867443

aTS6-8	C	4.568024	-0.324370	0.719445
	C	4.218015	0.222818	-0.305269
	C	2.022225	1.056469	-0.125806
	C	0.959601	0.192897	-0.085241
	C	0.682434	-1.269931	-0.087845
	C	1.573576	-2.246727	-0.121777
	H	4.736166	-0.765618	1.672478
	H	4.236374	0.607628	-1.298322
	C	-0.310549	0.817732	-0.029579
	C	-1.329734	-0.142333	-0.000380
	C	-2.684111	0.194259	0.055224
	C	-3.576507	-0.900787	0.078657
	C	-3.074405	-2.199503	0.046735
	C	-1.693466	-2.502409	-0.009047
	C	-0.796556	-1.446255	-0.033535
	H	-4.648204	-0.739387	0.121402
	H	-3.775527	-3.026754	0.065341
	H	-1.373972	-3.538244	-0.031345
	O	2.332376	-3.119831	-0.150151
	C	1.857226	2.444741	-0.093448
	H	2.730337	3.089312	-0.111799
	C	0.584972	3.023325	-0.037147
	H	0.487373	4.103820	-0.016759
	C	-0.558003	2.192688	-0.004692

	C	-2.958617	1.613247	0.080773
	H	-3.991234	1.944196	0.123847
	C	-1.957128	2.553768	0.053101
	H	-2.222305	3.605923	0.075331
aTS6-9	C	4.334547	0.523666	-0.146102
	C	3.455751	-0.307250	-0.005790
	C	2.165424	-0.930693	0.009464
	C	1.008871	-0.145951	0.008092
	C	0.687086	1.299502	0.012013
	C	1.524200	2.327439	0.021222
	H	5.199955	1.138532	-0.205998
	H	4.538693	-1.733084	0.782948
	C	-0.229990	-0.813159	0.000820
	C	-1.286231	0.106150	0.001182
	C	-2.627582	-0.280044	-0.005463
	C	-3.560673	0.781067	-0.004525
	C	-3.105599	2.097070	0.002377
	C	-1.734897	2.450315	0.008555
	C	-0.800468	1.427780	0.007843
	H	-4.626449	0.580344	-0.009224
	H	-3.836303	2.898352	0.002958
	H	-1.453361	3.497317	0.013549
	O	2.196790	3.267320	0.029347
	C	1.991714	-2.345686	0.002083
	H	2.889168	-2.952209	0.006186
	C	0.753230	-2.970586	-0.007365
	H	0.704328	-4.053846	-0.013398
	C	-0.429387	-2.194254	-0.007139
	C	-2.848709	-1.707991	-0.012715
	H	-3.868866	-2.077988	-0.017980
	C	-1.811469	-2.611248	-0.013604
	H	-2.036393	-3.672735	-0.019508
aTS6-7	C	2.754814	-0.856483	-1.218693
	C	3.150189	0.367610	-0.867477
	C	2.130865	1.157212	-0.143191
	C	1.105473	0.343004	0.273834
	C	-0.176607	0.849374	0.388327
	C	-1.106528	-0.180792	0.155033
	C	-2.469566	0.078854	0.014520
	C	-3.257013	-1.044845	-0.333598
	C	-2.647913	-2.276260	-0.553542
	C	-1.247026	-2.481146	-0.467753
	C	-0.456079	-1.402151	-0.123813
	C	1.063065	-1.143831	0.036727
	C	1.604108	-2.007539	0.978968
	H	3.301319	-1.664119	-1.690015
	H	4.113821	0.792431	-1.145746
	H	-4.330283	-0.948981	-0.458967
	H	-3.269178	-3.118916	-0.835950
	H	-0.830719	-3.455213	-0.697109
	O	2.237846	-2.921730	1.334155
	C	-0.498536	2.207186	0.341735
	C	1.885839	2.556948	-0.100875
	H	2.678852	3.245603	-0.372728
	C	0.616070	3.072652	0.171523
	H	0.470653	4.147540	0.142650
	C	-2.846455	1.471043	0.153026
	H	-3.897168	1.733842	0.086545
	C	-1.917749	2.478245	0.291825
	H	-2.261763	3.507176	0.318611
aTS7-4	C	2.536107	-0.227235	-0.973481
	C	2.730087	1.128662	-0.985390
	C	1.660037	1.804746	-0.213396
	C	0.950650	0.768168	0.342816
	C	-0.413460	0.825025	0.514870
	C	-0.931983	-0.459893	0.236506
	C	-2.300720	-0.659808	0.074381
	C	-2.665756	-1.956369	-0.365549
	C	-1.677604	-2.886527	-0.672043
	C	-0.289319	-2.600916	-0.608023
	C	0.102847	-1.348281	-0.173192
	C	1.409094	-0.574885	-0.057260
	C	2.299654	-1.448037	1.354262
	H	3.172776	-0.951169	-1.463808
	H	3.515981	1.626414	-1.539919
	H	-3.709265	-2.219591	-0.503081

	H	-1.980281	-3.867359	-1.021686
	H	0.426315	-3.348688	-0.930089
	O	2.779424	-2.483555	1.191550
	C	-1.148111	2.003039	0.407452
	C	0.990840	3.062109	-0.239805
	H	1.489364	3.948594	-0.617208
	C	-0.362679	3.160341	0.111118
	H	-0.845071	4.129066	0.028528
	C	-3.119260	0.530325	0.226210
	H	-4.197124	0.430057	0.149708
	C	-2.580332	1.791883	0.355035
	H	-3.248638	2.647024	0.358088
aTS11-12	C	2.301090	-0.691693	-0.120379
	C	2.067981	-2.008913	-0.290193
	C	0.671218	-2.273561	0.146821
	C	0.263155	-1.099603	0.747115
	C	-1.025171	-0.636056	0.561614
	C	-0.973952	0.765402	0.391887
	C	-2.093935	1.482662	-0.032764
	C	-1.857729	2.850974	-0.309349
	C	-0.567921	3.360063	-0.218409
	C	0.561824	2.565498	0.113159
	C	0.362565	1.231484	0.401675
	C	1.273605	0.026401	0.749141
	C	4.650409	0.087174	-0.491126
	H	1.743840	0.187599	1.728351
	H	2.747386	-2.718923	-0.743371
	H	-2.668091	3.496499	-0.631445
	H	-0.404800	4.405755	-0.455251
	H	1.551621	3.007458	0.090708
	O	4.786037	1.186598	-0.252882
	C	-2.071261	-1.428070	0.088000
	C	-0.362506	-3.166855	-0.259436
	H	-0.117190	-4.135709	-0.680636
	C	-1.702089	-2.770761	-0.229151
	H	-2.455876	-3.465772	-0.585431
	C	-3.282408	0.688443	-0.271672
	H	-4.194909	1.195671	-0.567934
	C	-3.269062	-0.688889	-0.243208
	H	-4.165159	-1.227568	-0.534301
b	C	3.278847	-0.991371	0.000006
	C	3.208592	0.471345	-0.000219
	C	1.971671	1.128785	-0.000125
	C	0.860602	0.280124	-0.000071
	C	0.827882	-1.163777	-0.000027
	C	2.030908	-1.795709	0.000044
	C	-0.429641	0.783811	-0.000004
	C	-1.330408	-0.289328	0.000004
	C	-2.704838	-0.080550	0.000060
	C	-3.477614	-1.271757	0.000044
	C	-2.834962	-2.504106	-0.000035
	C	-1.419633	-2.660018	-0.000101
	C	-0.633411	-1.524172	-0.000069
	H	-4.561638	-1.232460	0.000086
	H	-3.442542	-3.402245	-0.000038
	H	-0.997030	-3.658471	-0.000128
	H	2.163838	-2.871334	0.000099
	O	4.384030	-1.564199	0.000156
	C	-0.775945	2.124006	0.000041
	C	1.653214	2.544563	-0.000064
	H	2.470552	3.257702	-0.000093
	C	0.355764	3.019351	0.000011
	H	0.191812	4.091815	0.000039
	C	-2.195851	2.355969	0.000116
	H	-2.574274	3.372805	0.000159
	C	-3.104946	1.309213	0.000131
	H	-4.164061	1.545733	0.000178
	H	4.159716	0.991776	0.000003
b2	C	2.841648	-1.193996	0.699629
	C	2.178315	-1.595647	-0.585421
	C	0.770366	-1.125808	-0.753488
	C	0.852650	0.288210	-0.740440
	C	2.057070	0.896170	-0.479653
	C	3.058733	-0.232543	-0.419521
	C	-0.378859	0.878943	-0.506795
	C	-1.303603	-0.161768	-0.379211

	C	-0.643239	-1.438438	-0.508082
	C	-1.449083	-2.545822	-0.249001
	H	-1.066606	-3.559124	-0.299129
	C	-2.796833	-2.333950	0.138360
	C	-3.365580	-1.076204	0.332707
	C	-2.580972	0.087812	0.103411
	H	2.596231	-2.450465	-1.110431
	H	4.054180	-0.171209	-0.849623
	O	3.071206	-1.478012	1.829151
	H	-3.407968	-3.208018	0.335585
	H	-4.386405	-0.999464	0.691295
	C	1.966367	2.258276	-0.081679
	H	2.859708	2.831625	0.139540
	C	-0.526269	2.174327	-0.046244
	C	-2.845287	1.478433	0.425323
	H	-3.834317	1.744915	0.784719
	C	0.717126	2.883657	0.095559
	H	0.711172	3.916638	0.427578
	C	-1.878533	2.467161	0.377353
	H	-2.139743	3.466325	0.710411
b3	C	2.639573	-0.613724	-0.414727
	C	2.978720	0.870879	-0.120051
	C	1.835746	1.622215	-0.213854
	C	0.819622	0.706350	-0.603416
	C	-0.553334	0.936690	-0.450852
	C	-1.161253	-0.314683	-0.433600
	C	-2.476825	-0.450487	-0.007785
	C	-2.912519	-1.800261	0.147658
	C	-2.001942	-2.828176	-0.038266
	C	-0.619566	-2.630152	-0.349250
	C	-0.157999	-1.344741	-0.550607
	C	1.141182	-0.614711	-0.672929
	C	3.127711	-1.546621	0.718411
	H	3.228843	-0.969112	-1.274380
	H	3.978962	1.179183	0.152506
	H	-3.928400	-2.028452	0.451828
	H	-2.339553	-3.848313	0.109127
	H	0.043533	-3.487383	-0.364967
	O	2.619927	-2.531411	1.112107
	C	-1.067316	2.104281	0.047051
	C	1.301963	2.941285	0.150690
	H	1.977373	3.756191	0.386263
	C	-0.052032	3.154302	0.267496
	H	-0.384540	4.134654	0.594512
	C	-3.122013	0.784756	0.366744
	H	-4.158312	0.755019	0.688092
	C	-2.451926	2.003879	0.418722
	H	-2.984072	2.873002	0.791547
b5	C	1.184926	-0.680743	-0.000022
	C	1.010599	0.799045	0.000216
	C	-0.385063	1.029163	-0.000328
	C	-1.051529	-0.190952	-0.000340
	C	-0.086691	-1.257335	-0.000007
	C	1.816055	1.922466	0.000756
	C	-1.039856	2.256611	-0.000283
	C	-0.179803	3.389325	0.000132
	C	1.194827	3.205067	0.000565
	H	2.899526	1.870952	0.001235
	C	-0.622914	-2.614596	0.000162
	C	0.110724	-3.733916	0.000024
	H	-0.068763	-4.798529	0.000053
	C	2.425576	-1.413265	-0.000035
	C	3.640578	-0.890947	-0.000301
	O	4.717619	-0.459482	-0.000547
	H	2.396274	-2.499694	0.000160
	H	1.837056	4.078854	0.000888
	H	-0.588169	4.394455	0.000134
	C	-2.423650	-0.280320	-0.000167
	C	-2.107262	-2.705613	0.000465
	H	-2.524146	-3.706252	0.000613
	C	-2.474428	2.184213	-0.000461
	H	-3.055146	3.100608	-0.000681
	C	-2.945897	-1.637585	0.000272
	H	-4.018560	-1.803688	0.000897
	C	-3.132991	0.966619	-0.000386
	H	-4.218225	0.955725	-0.000491

	C	-4.441370	-0.560928	-0.000249
	C	-3.164423	-0.890354	0.000337
	C	-2.048049	0.050243	0.000151
	C	-0.728571	-0.393546	0.000144
	C	-0.054583	-1.734925	0.000150
	C	-0.621576	-2.924198	0.000221
	H	-2.960343	-1.956921	0.000669
	C	0.289555	0.573643	0.000157
	C	1.555008	-0.039501	0.000040
	C	2.745991	0.686822	-0.000059
	C	3.923952	-0.098732	-0.000168
	C	3.830719	-1.486261	-0.000206
	C	2.595481	-2.182030	-0.000130
b6	C	1.430844	-1.438141	0.000014
	H	4.900625	0.373544	-0.000242
	H	4.745838	-2.068291	-0.000303
	H	2.591601	-3.266227	-0.000161
	H	-0.336019	-3.964334	0.000232
	O	-5.569533	-0.289265	-0.000547
	C	0.131705	1.957155	0.000103
	C	-2.247228	1.467752	0.000161
	H	-3.267508	1.839068	0.000232
	C	-1.217789	2.393150	0.000102
	H	-1.456113	3.451602	0.000033
	C	1.354678	2.722396	-0.000026
	H	1.293715	3.805999	-0.000112
	C	2.592780	2.123170	-0.000053
	H	3.481725	2.745372	-0.000109
	C	1.652853	-2.053194	-0.370870
	C	2.779285	-0.971639	-0.437720
	C	2.012267	0.364028	-0.498491
	C	0.724821	-0.046877	-0.593926
	C	-0.383124	0.734191	-0.434641
	C	-1.469443	-0.132109	-0.232015
	C	-2.699942	0.383352	0.158155
	C	-3.685373	-0.600986	0.424710
	C	-3.351104	-1.949604	0.334069
	C	-2.049517	-2.426159	0.017202
	C	-1.058675	-1.503246	-0.267574
	C	0.437329	-1.461152	-0.468986
	C	3.786284	-1.112396	0.713158
	H	1.901025	-3.094314	-0.211529
b7	H	3.402296	-1.137376	-1.329862
	H	-4.690284	-0.319385	0.721433
	H	-4.118641	-2.684398	0.550918
	H	-1.858546	-3.493171	0.031509
	O	4.383620	-0.253384	1.254666
	C	-0.315613	2.090292	-0.166807
	C	2.157502	1.765635	-0.292020
	H	3.137415	2.217449	-0.190435
	C	1.026778	2.596878	-0.147739
	H	1.200609	3.650763	0.042675
	C	-2.726947	1.830902	0.313533
	H	-3.665849	2.297093	0.595223
	C	-1.613411	2.640060	0.179961
	H	-1.720810	3.702550	0.372759
	C	3.860645	-0.469105	0.000324
	C	1.690816	3.233050	-0.000678
	C	0.496874	2.540170	-0.000130
	C	-0.775341	3.259563	0.000291
	C	-2.005409	2.661229	0.000359
	C	-2.111776	1.227504	0.000169
	C	-3.282428	0.399204	0.000306
	C	-3.206117	-0.981570	0.000224
	C	-1.941667	-1.670428	0.000039
	C	-1.656262	-3.062093	-0.000061
b8	C	-0.337158	-3.496929	-0.000245
	C	0.774907	-2.611465	-0.000318
	C	0.524465	-1.254408	-0.000201
	C	1.356178	-0.002077	-0.000341
	C	2.703278	0.079596	-0.000460
	C	0.398320	1.111832	-0.000314
	C	-0.895984	0.555141	-0.000114
	C	-0.819440	-0.847471	-0.000055
	H	1.699659	4.316553	-0.000738
	H	-0.718084	4.342977	0.000505

	H	-2.901298	3.273190	0.000650
	H	-4.259710	0.870688	0.000470
	H	-4.124259	-1.559575	0.000301
	H	-2.461090	-3.789466	-0.000006
	H	-0.142295	-4.563506	-0.000343
	H	1.783406	-3.009921	-0.000448
	H	2.637474	2.709757	-0.001235
	O	4.980347	-0.827644	0.001009
b9	C	4.497538	-0.479429	0.000002
	C	3.224703	-0.393036	-0.000018
	C	2.054197	0.355819	-0.000018
	C	0.762281	-0.231027	-0.000015
	C	0.225688	-1.621282	-0.000002
	C	0.929561	-2.763196	0.000012
	H	2.011977	-2.748857	0.000006
	C	-0.340735	0.633144	-0.000009
	C	-1.540223	-0.103310	-0.000008
	C	-2.797668	0.499446	-0.000002
	C	-3.892633	-0.399200	0.000003
	C	-3.656254	-1.769119	0.000003
	C	-2.355226	-2.334137	0.000001
	C	-1.266908	-1.479876	-0.000004
	H	-4.911921	-0.028354	0.000006
	H	-4.506261	-2.442385	0.000006
	H	-2.244625	-3.412909	0.000005
	H	0.432724	-3.726967	0.000026
	O	5.655481	-0.708293	0.000016
	C	-0.323189	2.029419	0.000000
	C	2.092712	1.810069	0.000000
	H	3.076971	2.263179	0.000006
	C	0.978871	2.614860	0.000006
	H	1.094670	3.693533	0.000015
	C	-1.608820	2.665004	0.000008
	H	-1.659341	3.748772	0.000016
	C	-2.785242	1.940213	0.000005
	H	-3.729956	2.474149	0.000011
b10	C	-3.564949	-0.997611	0.139190
	C	-2.750642	1.420950	0.087958
	C	-1.320245	1.940233	-0.101967
	C	-0.552800	3.105162	0.165015
	C	0.858531	3.067236	0.159701
	C	1.594805	1.855861	-0.065260
	C	2.973866	1.472844	0.163374
	C	3.359741	0.144901	0.164879
	C	2.432969	-0.960827	-0.016432
	C	2.609303	-2.356165	0.183154
	C	1.499144	-3.199699	0.137934
	C	0.168312	-2.753954	-0.061122
	C	-0.058081	-1.396032	-0.278642
	C	-1.178760	-0.445761	-0.343664
	C	-2.563794	-0.147223	-0.038391
	C	-0.580941	0.841797	-0.429480
	C	0.796566	0.776047	-0.400225
	C	1.131526	-0.579177	-0.314014
	H	-3.162267	1.684530	1.066549
	H	-1.032321	4.042428	0.427184
	H	1.388839	3.980966	0.407250
	H	3.720177	2.230469	0.379869
	H	4.400208	-0.086064	0.371320
	H	3.587626	-2.770338	0.402329
	H	1.655188	-4.259964	0.305374
	H	-0.642067	-3.472411	-0.006672
	H	-3.443423	1.791836	-0.673836
	O	-4.449908	-1.734119	0.301073
b11	C	1.890893	-1.891311	0.097037
	C	2.773808	-0.583381	-0.003992
	C	1.919362	0.603067	0.199879
	C	0.690867	0.061073	0.513063
	C	-0.503754	0.761228	0.458407
	C	-1.512585	-0.194818	0.312640
	C	-2.798792	0.189794	-0.037819
	C	-3.685955	-0.889406	-0.310272
	C	-3.201425	-2.195542	-0.283317
	C	-1.846265	-2.537121	-0.034266
	C	-0.938844	-1.520204	0.257578
	C	0.510614	-1.323602	0.392020

	C	4.069038	-0.597171	-0.247109
	H	2.263276	-2.554976	0.885163
	H	1.921745	-2.454227	-0.842166
	H	-4.722527	-0.707427	-0.573142
	H	-3.890857	-3.002209	-0.508202
	H	-1.541972	-3.575118	-0.112944
	O	5.210680	-0.609099	-0.466485
	C	-0.584980	2.102443	0.137281
	C	1.907571	2.009993	-0.029876
	H	2.821700	2.545758	-0.260794
	C	0.699957	2.732008	-0.039019
	H	0.750458	3.792329	-0.264318
	C	-2.980084	1.620522	-0.203239
	H	-3.970714	1.990213	-0.448800
	C	-1.937839	2.529935	-0.143323
	H	-2.146069	3.573405	-0.356950
CO	C	0.000000	0.000000	-0.643976
	O	0.000000	0.000000	0.482982
b4	C	1.685666	-2.530321	-0.170025
	C	2.852682	-1.731217	-0.284868
	C	2.535758	-0.325475	0.055551
	C	1.227168	-0.418893	0.452657
	C	0.319821	0.599755	0.448465
	C	-0.954835	0.007122	0.329148
	C	-2.062167	0.792112	0.038436
	C	-3.253870	0.060899	-0.203580
	C	-3.218781	-1.332853	-0.211419
	C	-2.036574	-2.094350	-0.031348
	C	-0.846805	-1.426859	0.231737
	C	0.607910	-1.714710	0.264387
	H	1.651434	-3.579222	-0.430640
	H	3.807423	-2.106115	-0.632514
	H	-4.187021	0.571857	-0.416597
	H	-4.140726	-1.867838	-0.411372
	H	-2.078807	-3.172629	-0.135208
	C	0.659720	1.908126	0.131484
	C	2.966138	1.013198	-0.184549
	H	3.984887	1.228776	-0.489762
	C	2.059374	2.090851	-0.119436
	H	2.436315	3.080878	-0.354655
	C	-0.505809	2.745755	-0.077624
	H	-0.384258	3.807124	-0.269301
	C	-1.781381	2.215436	-0.097504
	H	-2.613344	2.885717	-0.289029
b12	C	-3.013773	-1.765495	0.177024
	C	-2.552658	-0.306625	-0.036657
	C	-2.969888	1.047238	0.105851
	C	-2.038818	2.108566	0.067116
	C	-0.630219	1.894216	-0.085051
	C	0.547984	2.732868	0.041523
	C	1.821332	2.193519	0.054728
	C	2.098215	0.766126	-0.025323
	C	3.305435	0.039059	0.122800
	C	3.271675	-1.353972	0.129626
	C	2.080960	-2.122187	0.024515
	C	0.878365	-1.455339	-0.135731
	C	-0.594513	-1.760498	-0.142391
	C	-1.667746	-2.527467	0.110704
	C	-1.221446	-0.441423	-0.264165
	C	-0.297026	0.563520	-0.275656
	C	0.970672	-0.029138	-0.199031
	H	-3.491109	-1.921262	1.149976
	H	-4.010569	1.297503	0.283854
	H	-2.417872	3.115419	0.208450
	H	0.441114	3.806881	0.155585
	H	2.661455	2.871100	0.170621
	H	4.253744	0.550089	0.252376
	H	4.207184	-1.888953	0.251634
	H	2.136681	-3.202334	0.093545
	H	-3.711941	-2.126243	-0.585335
b13	C	-2.911661	-1.626458	0.343628
	C	-2.590397	-0.346181	0.006870
	C	-3.013261	1.048572	0.152333
	C	-2.107084	2.080824	0.085688
	C	-0.660926	1.878948	-0.119067
	C	0.474127	2.737194	0.089040

	C	1.768771	2.228164	0.093142
	C	2.060060	0.822510	-0.058754
	C	3.268425	0.101605	0.171608
	C	3.231356	-1.284085	0.194427
	C	2.040179	-2.058898	0.033262
	C	0.846159	-1.410904	-0.219066
	C	-0.619289	-1.706505	-0.287003
	C	-1.750681	-2.621614	0.181819
	C	-1.222061	-0.488236	-0.399635
	C	-0.316361	0.585253	-0.404977
	C	0.952492	0.024225	-0.318186
	H	-1.533090	-3.100769	1.143141
	H	-4.050896	1.276498	0.367724
	H	-2.472617	3.089053	0.253021
	H	0.331006	3.794238	0.288308
	H	2.589392	2.912783	0.282787
	H	4.200739	0.619848	0.368531
	H	4.153814	-1.820395	0.389847
	H	2.099300	-3.135467	0.153269
	H	-2.016740	-3.422260	-0.517414
bTS1-2	C	-3.390797	-0.908444	-0.251467
	C	-2.987140	0.197607	0.624463
	C	-1.874336	1.101879	0.213420
	C	-1.575605	2.485781	0.340689
	C	-0.273353	2.974079	0.125083
	C	0.827440	2.108912	-0.188296
	C	2.263937	2.297126	-0.139573
	C	3.130672	1.222445	-0.150455
	C	2.678691	-0.158999	-0.161951
	C	3.399029	-1.362677	0.074092
	C	2.705289	-2.561684	0.223801
	C	1.291049	-2.665585	0.196027
	C	0.542768	-1.517452	-0.048806
	C	-0.858077	-1.076777	0.005421
	C	-2.197024	-1.445622	0.460889
	C	-0.831086	0.324572	-0.223432
	C	0.459709	0.789972	-0.390241
	C	1.309123	-0.323208	-0.297814
	H	-3.663379	0.445893	1.438153
	H	-2.339013	3.188283	0.656367
	H	-0.097720	4.033201	0.282619
	H	2.675202	3.297431	-0.050729
	H	4.196451	1.416926	-0.085811
	H	4.479324	-1.354140	0.172445
	H	3.275074	-3.464125	0.416128
	H	0.825602	-3.623126	0.400918
	H	-2.391299	-2.274531	1.135999
	O	-4.335247	-1.319672	-0.854650
bTS1-5	C	3.398065	-1.449546	-0.007902
	C	3.182935	1.126132	0.074746
	C	1.879722	1.436326	0.029981
	C	0.879145	0.399733	-0.040459
	C	0.938646	-0.993258	0.011417
	C	2.107000	-1.803742	0.111391
	C	-0.489728	0.797361	-0.075810
	C	-1.291974	-0.339335	-0.062049
	C	-2.680191	-0.283098	-0.040572
	C	-3.321146	-1.552942	0.004901
	C	-2.552104	-2.707255	0.041566
	C	-1.126001	-2.705037	0.043920
	C	-0.470230	-1.490817	-0.004682
	H	-4.403347	-1.627997	0.018102
	H	-3.057485	-3.666012	0.078672
	H	-0.599925	-3.653058	0.088516
	H	2.008578	-2.862640	0.342224
	O	4.550948	-1.482542	-0.165594
	C	-0.995268	2.074877	-0.034295
	C	1.344148	2.817506	0.080552
	H	2.069253	3.621032	0.138691
	C	0.016243	3.118794	0.038100
	H	-0.287942	4.160596	0.063829
	C	-2.428320	2.169441	-0.029296
	H	-2.894967	3.149083	-0.008799
	C	-3.236224	1.044252	-0.038381
	H	-4.313848	1.169438	-0.029745
	H	4.143794	1.613551	0.014497

	C	-3.743969	-0.755201	0.030657
	C	-3.321778	0.516246	-0.092354
	C	-1.976193	1.035148	-0.044831
	C	-0.866794	0.208453	0.003570
	C	-0.734820	-1.261903	-0.029411
	C	-1.796208	-2.039740	-0.078937
	C	0.412809	0.758363	0.037953
	C	1.373400	-0.266622	0.025578
	C	2.740604	-0.001430	0.028281
	C	3.565531	-1.153477	0.004570
	C	2.987996	-2.418428	-0.026683
	C	1.585393	-2.637918	-0.042358
	C	0.756974	-1.533094	-0.016886
	H	4.646331	-1.059021	0.007020
bTS1-6	H	3.639543	-3.285077	-0.046703
	H	1.202920	-3.651594	-0.079223
	H	-2.114015	-3.068678	-0.065379
	O	-4.512900	-1.631662	0.174162
	C	0.728262	2.111041	0.029775
	C	-1.692279	2.441510	-0.054324
	H	-2.531189	3.128852	-0.090562
	C	-0.408398	2.967417	-0.014334
	H	-0.282707	4.045100	-0.025101
	C	2.142885	2.400107	0.041452
	H	2.470542	3.434782	0.043850
	C	3.093001	1.402059	0.045598
	H	4.142684	1.676651	0.056588
	H	-4.149409	1.197102	-0.277680
	C	2.669164	-1.323328	0.793335
	C	3.016781	0.288863	-0.334004
	C	1.978599	1.236279	-0.394526
	C	1.689920	2.597490	0.020301
	C	0.386334	3.030752	0.206141
	C	-0.775767	2.159294	0.038249
	C	-2.143225	2.267396	0.478470
	C	-2.987934	1.164949	0.473097
	C	-2.556762	-0.158429	0.081567
	C	-3.188894	-1.422337	0.256906
	C	-2.463898	-2.581732	0.013907
	C	-1.090721	-2.600493	-0.370237
	C	-0.436714	-1.397257	-0.575908
	C	0.943368	-0.877800	-0.793967
bTS2-3	C	2.429695	-1.149171	-0.631949
	C	0.835400	0.494915	-0.722144
	C	-0.471127	0.923153	-0.478874
	C	-1.256849	-0.224482	-0.405608
	H	4.080720	0.444072	-0.219961
	H	2.498684	3.284898	0.241530
	H	0.234581	4.045580	0.559783
	H	-2.519960	3.208559	0.865405
	H	-4.000148	1.292317	0.843748
	H	-4.210936	-1.491595	0.613469
	H	-2.953720	-3.536812	0.169563
	H	-0.581746	-3.555012	-0.447395
	H	2.954306	-1.803711	-1.339454
	O	3.129250	-2.057084	1.598097
	C	3.034733	-1.212357	0.800831
	C	2.975179	-0.597677	-0.532218
	C	2.099808	0.658024	-0.563604
	C	2.132118	2.046533	-0.256106
	C	0.938786	2.772860	-0.050881
	C	-0.356093	2.157767	-0.093873
	C	-1.685894	2.578314	0.299698
	C	-2.729263	1.673559	0.391728
	C	-2.589595	0.247095	0.142695
	C	-3.486315	-0.829019	0.364597
bTS2-7	C	-3.038972	-2.138981	0.190035
	C	-1.712949	-2.487176	-0.173933
	C	-0.798103	-1.469004	-0.419118
	C	0.658404	-1.294479	-0.660572
	C	1.961141	-1.820150	-0.654415
	C	0.846555	0.131781	-0.670271
	C	-0.319570	0.819587	-0.449704
	C	-1.327479	-0.137906	-0.294555
	H	3.890179	-0.666063	-1.121405
	H	3.073094	2.572919	-0.141981

	H	1.027652	3.823776	0.203579
	H	-1.874135	3.613727	0.564434
	H	-3.696922	2.043363	0.716560
	H	-4.504777	-0.650945	0.692937
	H	-3.738347	-2.946883	0.376325
	H	-1.436530	-3.534316	-0.224050
	H	2.316108	-2.808007	-0.909625
	O	3.166092	-1.005024	1.952654
bTS5-3	C	1.127364	-0.595993	-0.507364
	C	-0.120443	-1.405983	-0.395851
	C	-1.176271	-0.445212	-0.245829
	C	-0.646292	0.835104	-0.251557
	C	0.747443	0.710534	-0.414146
	C	-0.521879	-2.725372	-0.311063
	C	-2.512294	-0.668864	0.060482
	C	-2.878543	-2.045536	0.122886
	C	-1.902442	-3.011921	-0.070030
	H	0.176856	-3.550831	-0.395186
	C	1.644168	1.810611	-0.238990
	C	2.926548	1.391339	-0.312156
	H	3.878422	1.899280	-0.207137
	C	2.617098	-0.707848	-0.556592
	C	3.229700	-1.558711	0.345205
	O	3.887067	-1.885264	1.250130
	H	3.100143	-0.749979	-1.535554
	H	-2.192386	-4.055382	-0.009482
	H	-3.898227	-2.345222	0.339473
	C	-1.299436	1.986287	0.098785
	C	0.945594	3.076996	0.066789
	H	1.536911	3.977873	0.187745
	C	-3.269515	0.524250	0.344131
	H	-4.325420	0.431608	0.577630
	C	-0.415623	3.157212	0.213222
	H	-0.852315	4.122393	0.450211
	C	-2.695214	1.792135	0.376757
	H	-3.320291	2.638208	0.643188
bTS6-7	C	4.100838	-0.503682	0.335043
	C	3.029314	-0.513741	-0.534090
	C	1.979458	0.564627	-0.378001
	C	1.994006	1.983350	-0.267149
	C	0.811565	2.725965	-0.105844
	C	-0.468696	2.095814	-0.039537
	C	-1.818153	2.579186	0.176158
	C	-2.892016	1.714388	0.264724
	C	-2.771087	0.269492	0.163421
	C	-3.740390	-0.758353	0.276646
	C	-3.343100	-2.089289	0.176863
	C	-1.998711	-2.503758	-0.026891
	C	-1.021464	-1.532407	-0.147850
	C	0.483795	-1.443316	-0.322124
	C	1.621360	-2.131446	-0.419904
	C	0.745313	-0.005425	-0.325561
	C	-0.411375	0.717403	-0.168731
	C	-1.476693	-0.187412	-0.059559
	H	3.356193	-0.725490	-1.553612
	H	2.937561	2.517379	-0.300179
	H	0.893368	3.804181	-0.018405
	H	-1.999911	3.643947	0.280290
	H	-3.877991	2.136655	0.431765
	H	-4.785925	-0.523822	0.446797
	H	-4.100895	-2.859711	0.269805
	H	-1.770562	-3.562624	-0.073859
	H	1.874914	-3.184222	-0.438527
	O	4.816182	-0.891834	1.171280
bTS5-8	C	3.771226	-0.383663	-0.026613
	C	1.803107	3.057250	-0.025971
	C	0.514233	2.535341	0.013268
	C	-0.752677	3.268081	-0.029287
	C	-1.991439	2.673887	-0.033365
	C	-2.118711	1.235006	0.006343
	C	-3.285430	0.394067	-0.018140
	C	-3.191493	-0.986971	-0.013181
	C	-1.922803	-1.672766	0.010545
	C	-1.620244	-3.061626	-0.018141
	C	-0.293937	-3.475227	-0.020533
	C	0.811029	-2.578315	0.000036

	C	0.554695	-1.219829	0.033340
	C	1.326504	0.051657	0.045573
	C	2.692685	0.373904	0.000108
	C	0.371951	1.116414	0.056483
	C	-0.918019	0.553291	0.055715
	C	-0.811286	-0.840500	0.046984
	H	1.885899	4.144778	0.094063
	H	-0.689911	4.351090	-0.061062
	H	-2.882413	3.292720	-0.063460
	H	-4.269120	0.850840	-0.048816
	H	-4.105156	-1.571865	-0.038449
	H	-2.412831	-3.801791	-0.043556
	H	-0.083671	-4.538557	-0.045483
	H	1.818184	-2.980602	-0.015825
	H	2.791790	1.562553	-0.049939
	O	4.788861	-0.943645	-0.028306
bTS6-9	C	-4.376856	-0.526758	-0.000137
	C	-3.077879	-0.511834	-0.000092
	C	-1.995878	0.442523	-0.000053
	C	-0.735199	-0.114699	-0.000018
	C	-0.340998	-1.537805	-0.000017
	C	-1.309245	-2.443988	-0.000051
	H	-2.515842	-1.683768	-0.000082
	C	0.400877	0.673505	0.000025
	C	1.537494	-0.151306	0.000053
	C	2.822834	0.380633	0.000087
	C	3.857954	-0.588012	0.000099
	C	3.537659	-1.942056	0.000074
	C	2.205473	-2.435154	0.000037
	C	1.172221	-1.517534	0.000028
	H	4.899932	-0.285705	0.000125
	H	4.346645	-2.664221	0.000081
	H	2.033020	-3.505403	0.000017
	H	-1.404408	-3.519800	-0.000056
	O	-5.540227	-0.635696	-0.000177
	C	0.425027	2.060662	0.000034
	C	-2.027766	1.875512	-0.000043
	H	-2.989219	2.376989	-0.000069
	C	-0.871584	2.653988	-0.000002
	H	-0.977614	3.733893	0.000001
	C	1.756805	2.623714	0.000075
	H	1.878771	3.702088	0.000086
	C	2.884397	1.829297	0.000100
	H	3.858500	2.307388	0.000129
bTS8-10	C	3.586048	-1.154483	-0.205926
	C	2.723529	1.843630	0.107341
	C	1.296362	2.023786	0.138893
	C	0.457414	3.131050	-0.230779
	C	-0.931362	3.048483	-0.236051
	C	-1.617725	1.813600	0.034160
	C	-2.992015	1.419760	-0.178664
	C	-3.375765	0.093535	-0.153107
	C	-2.430139	-0.987348	0.033816
	C	-2.594774	-2.386940	-0.145602
	C	-1.482626	-3.220880	-0.111895
	C	-0.152716	-2.749342	0.058857
	C	0.044317	-1.395678	0.267256
	C	1.191227	-0.439280	0.303831
	C	2.535901	-0.419358	-0.007132
	C	0.607737	0.858099	0.447127
	C	-0.781554	0.770633	0.388472
	C	-1.128870	-0.587285	0.312864
	H	3.335030	2.372458	-0.619175
	H	0.918635	4.079305	-0.485103
	H	-1.500379	3.931873	-0.506886
	H	-3.737437	2.175587	-0.403595
	H	-4.416126	-0.150860	-0.341889
	H	-3.574836	-2.809256	-0.340821
	H	-1.629059	-4.284050	-0.266936
	H	0.673395	-3.448160	-0.009731
	H	3.230483	1.592958	1.029463
	O	4.621295	-1.678969	-0.374512
bTS9-11	C	1.696198	-2.093817	0.420775
	C	2.917589	-0.314510	-0.093890
	C	1.920229	0.638373	0.212081
	C	0.710782	0.051335	0.579890

C	-0.494761	0.747618	0.470350
C	-1.510356	-0.198010	0.278039
C	-2.795998	0.184474	-0.086139
C	-3.674857	-0.894448	-0.380037
C	-3.195698	-2.199600	-0.352194
C	-1.843218	-2.535816	-0.075019
C	-0.954743	-1.513875	0.226400
C	0.498471	-1.350826	0.476675
C	4.166326	-0.479593	-0.380731
H	2.371697	-2.038287	1.266286
H	1.778250	-3.010426	-0.158299
H	-4.707042	-0.708656	-0.657409
H	-3.879358	-3.005720	-0.594481
H	-1.530175	-3.571791	-0.142858
O	5.269968	-0.773097	-0.652482
C	-0.606990	2.089165	0.159320
C	1.862877	2.071436	0.021871
H	2.777708	2.612508	-0.190006
C	0.661606	2.763091	0.012788
H	0.682935	3.828388	-0.193737
C	-2.992893	1.609393	-0.231838
H	-3.981800	1.977358	-0.485177
C	-1.951329	2.515336	-0.139232
H	-2.151368	3.563037	-0.339114

bTS3-4	C	2.515006	-0.924263	-0.513875
	C	3.084907	0.480279	-0.291631
	C	2.038704	1.389905	-0.286626
	C	0.909511	0.611624	-0.618631
	C	-0.409882	0.995013	-0.424708
	C	-1.163013	-0.177230	-0.425933
	C	-2.482721	-0.159779	0.008620
	C	-3.083591	-1.446968	0.119787
	C	-2.313684	-2.574275	-0.127531
	C	-0.924984	-2.542715	-0.464369
	C	-0.301513	-1.318707	-0.615872
	C	1.077468	-0.754860	-0.755667
	C	2.699356	-1.792366	1.057858
	H	3.119809	-1.633799	-1.078652
	H	4.130774	0.647461	-0.072417
	H	-4.116932	-1.557973	0.430406
	H	-2.778977	-3.548005	-0.018253
	H	-0.385173	-3.478848	-0.549616
	O	2.141245	-2.775961	1.294457
	C	-0.770270	2.216929	0.089240
	C	1.684409	2.747995	0.122121
	H	2.460225	3.471362	0.347813
	C	0.365767	3.127165	0.290092
	H	0.169578	4.135515	0.640537
	C	-2.964400	1.141479	0.415104
	H	-3.993477	1.232336	0.748254
	C	-2.153979	2.272148	0.476826
	H	-2.578320	3.191401	0.867443

bTS7-4	C	4.067624	-0.787761	0.496716
	C	2.786295	-0.528472	-0.883059
	C	1.998581	0.671171	-0.433112
	C	1.943850	2.094109	-0.511127
	C	0.750769	2.788605	-0.226955
	C	-0.471219	2.120082	0.121084
	C	-1.860373	2.532350	0.186666
	C	-2.884859	1.606378	0.259669
	C	-2.674744	0.165727	0.235785
	C	-3.595957	-0.903307	0.095385
	C	-3.120487	-2.200398	-0.080935
	C	-1.742586	-2.535147	-0.171025
	C	-0.803569	-1.528038	-0.020929
	C	0.669567	-1.313903	-0.221044
	C	1.851094	-1.705775	-0.800255
	C	0.849638	0.100197	0.025863
	C	-0.326555	0.749516	0.265043
	C	-1.341020	-0.224041	0.243628
	H	3.458744	-0.468069	-1.730982
	H	2.800614	2.672965	-0.839252
	H	0.757068	3.867216	-0.344538
	H	-2.118040	3.585605	0.141280
	H	-3.905924	1.974089	0.281460
	H	-4.665696	-0.722159	0.095393

	H	-3.843226	-3.000823	-0.195703
	H	-1.459851	-3.560083	-0.382778
	H	2.126010	-2.679702	-1.183048
	O	3.784251	-1.034601	1.583722
bTS10-12	C	4.266649	1.506097	0.219592
	C	2.566580	-1.610140	-0.044987
	C	1.096591	-2.071487	-0.147824
	C	0.239800	-3.182856	0.095176
	C	-1.162282	-3.027039	0.151826
	C	-1.804644	-1.754520	0.002288
	C	-3.153549	-1.263744	0.219225
	C	-3.439667	0.089159	0.215304
	C	-2.437192	1.128630	0.029189
	C	-2.520148	2.538108	0.152306
	C	-1.361516	3.305897	0.055117
	C	-0.061390	2.764538	-0.134227
	C	0.066177	1.393528	-0.275250
	C	1.155833	0.358582	-0.331010
	C	2.415352	-0.070909	-0.146758
	C	0.428584	-0.911208	-0.370859
	C	-0.922745	-0.728047	-0.291161
	C	-1.157045	0.653080	-0.232811
	H	3.031181	-1.884818	0.907635
	H	0.644017	-4.172634	0.280138
	H	-1.757712	-3.907980	0.368216
	H	-3.960690	-1.961608	0.417695
	H	-4.464180	0.394918	0.402959
	H	-3.469480	3.027438	0.343540
	H	-1.449064	4.381748	0.160466
	H	0.797056	3.425749	-0.140301
	H	3.210365	-1.999443	-0.840552
	O	5.265772	0.998827	0.388673
bTS11-13	C	-1.887439	-1.757704	-0.223543
	C	-2.640238	-0.420372	-0.095440
	C	-1.854590	0.671201	-0.311983
	C	-0.588185	0.069162	-0.606881
	C	0.630715	0.750481	-0.460790
	C	1.606704	-0.226655	-0.301866
	C	2.888654	0.117735	0.109095
	C	3.737113	-0.992416	0.393777
	C	3.216353	-2.274921	0.317306
	C	1.853501	-2.570753	0.000094
	C	0.995892	-1.533127	-0.310732
	C	-0.465449	-1.286740	-0.524322
	C	-5.037773	-0.066328	0.450776
	H	-2.337689	-2.387659	-0.999056
	H	-1.955674	-2.317340	0.716315
	H	4.765197	-0.845291	0.706726
	H	3.866921	-3.109714	0.555088
	H	1.519033	-3.601476	0.051050
	O	-5.616713	-1.024873	0.621629
	C	0.731045	2.071460	-0.116028
	C	-1.778750	2.119512	-0.107332
	H	-2.689684	2.689453	0.033201
	C	-0.567469	2.765116	-0.023561
	H	-0.573464	3.830957	0.181677
	C	3.092178	1.529208	0.332745
	H	4.074866	1.871641	0.641172
	C	2.065137	2.463964	0.250467
	H	2.279793	3.495475	0.510102
c	C	-2.864572	-1.878045	0.000005
	C	-3.247453	-0.445532	0.000052
	C	-2.123453	0.513984	-0.000015
	C	-0.871871	-0.060187	-0.000099
	C	-0.500086	-1.452302	-0.000092
	C	-1.565296	-2.368476	-0.000049
	H	-3.706578	-2.560840	0.000040
	C	0.274242	0.728824	-0.000115
	C	1.391406	-0.111744	-0.000095
	C	2.680477	0.398868	-0.000017
	C	3.700507	-0.592061	0.000063
	C	3.351304	-1.939352	0.000090
	C	2.010053	-2.409893	0.000049
	C	0.983356	-1.477127	-0.000053
	H	4.748565	-0.312023	0.000120
	H	4.146340	-2.676628	0.000153

CO	H	1.824179	-3.478109	0.000084
	C	-2.158100	1.942760	0.000039
	H	-3.125377	2.431695	0.000099
	C	-1.000158	2.715835	0.000029
	H	-1.093984	3.796683	0.000083
	C	0.301859	2.109262	-0.000038
	C	2.758392	1.846151	0.000010
	H	3.737668	2.313751	0.000062
	C	1.640306	2.658300	0.000005
	H	1.778289	3.734474	0.000051
	H	-1.396266	-3.440317	-0.000029
	O	-4.434791	-0.110535	0.000090
c3	C	-1.965140	-1.586153	0.465685
	C	-2.865607	-0.310963	0.559384
	C	-1.909047	0.850130	0.217524
	C	-0.758753	0.198881	-0.068361
	C	0.473594	0.763359	-0.212925
	C	1.409035	-0.280702	-0.181948
	C	2.766839	0.012337	-0.148378
	C	3.602735	-1.128069	-0.036739
	C	3.027637	-2.392094	0.069396
	C	1.625848	-2.630760	0.102282
	C	0.768492	-1.550945	-0.016866
	C	-0.705512	-1.237544	0.100759
	C	-4.140864	-0.354271	-0.299730
	H	-2.369150	-2.561319	0.703023
	H	-3.250070	-0.208754	1.584259
	H	4.683023	-1.030243	-0.013268
	H	3.686472	-3.248759	0.159805
	H	1.264818	-3.643779	0.238591
	O	-4.654895	-1.288740	-0.799924
	C	0.699924	2.123266	-0.108288
	C	-1.765018	2.266477	0.278026
	H	-2.614176	2.908984	0.483683
	C	-0.503457	2.876455	0.106709
	H	-0.454837	3.957362	0.186778
	C	3.075266	1.435847	-0.155029
	H	4.119619	1.731802	-0.147357
	C	2.117843	2.434422	-0.123445
	H	2.450564	3.466591	-0.084471
c5	C	3.478802	0.178794	-0.000023
	C	4.755232	-0.172164	-0.000014
	C	0.884541	2.242902	-0.000007
	C	0.494497	0.931930	-0.000005
	C	1.080274	-0.434334	-0.000010
	C	2.392460	-0.768300	-0.000018
	H	3.282954	1.247086	-0.000004
	C	-0.917165	0.775867	0.000004
	C	-1.242770	-0.589591	0.000004
	C	-2.560872	-1.045702	0.000011
	C	-2.705612	-2.453145	0.000009
	C	-1.572019	-3.260893	0.000000
	C	-0.250793	-2.750883	-0.000007
	C	-0.074038	-1.375971	-0.000005
	H	-3.690693	-2.907390	0.000015
	H	-1.703406	-4.337560	-0.000001
	H	0.583762	-3.443780	-0.000014
	C	0.005801	3.327460	0.000000
	H	0.388942	4.342254	-0.000001
	C	-1.375761	3.112068	0.000009
	H	-2.049766	3.962441	0.000015
	C	-1.877037	1.787616	0.000011
	C	-3.569760	-0.010909	0.000020
	H	-4.615740	-0.300157	0.000026
	C	-3.247410	1.325155	0.000020
	H	-4.045883	2.060069	0.000026
	H	2.655521	-1.821667	-0.000021
	O	5.875512	-0.465087	-0.000004
CO	C	0.000000	0.000000	-0.643977
	O	0.000000	0.000000	0.482983
c4	C	1.685666	-2.530321	-0.170025
	C	2.852682	-1.731217	-0.284868
	C	2.535758	-0.325475	0.055551
	C	1.227168	-0.418893	0.452657
	C	0.319821	0.599755	0.448465
	C	-0.954835	0.007122	0.329148

	C	-2.062167	0.792112	0.038436
	C	-3.253870	0.060899	-0.203580
	C	-3.218781	-1.332853	-0.211419
	C	-2.036574	-2.094350	-0.031348
	C	-0.846805	-1.426859	0.231737
	C	0.607910	-1.714710	0.264387
	H	1.651434	-3.579222	-0.430640
	H	3.807423	-2.106115	-0.632514
	H	-4.187021	0.571857	-0.416597
	H	-4.140726	-1.867838	-0.411372
	H	-2.078807	-3.172629	-0.135208
	C	0.659720	1.908126	0.131484
	C	2.966138	1.013198	-0.184549
	H	3.984887	1.228776	-0.489762
	C	2.059374	2.090851	-0.119436
	H	2.436315	3.080878	-0.354655
	C	-0.505809	2.745755	-0.077624
	H	-0.384258	3.807124	-0.269301
	C	-1.781381	2.215436	-0.097504
	H	-2.613344	2.885717	-0.289029
cTS1-5	C	-3.039278	-1.881125	-0.000284
	C	-3.677803	-0.688940	-0.000193
	C	-1.974568	0.884049	-0.000161
	C	-0.885677	0.076098	-0.000099
	C	-0.619610	-1.355059	-0.000100
	C	-1.650668	-2.238482	-0.000201
	H	-3.773177	-2.683931	-0.000456
	C	0.346642	0.766348	-0.000009
	C	1.382652	-0.176383	0.000058
	C	2.721206	0.209372	0.000181
	C	3.645855	-0.863027	0.000255
	C	3.174866	-2.173212	0.000206
	C	1.798662	-2.516011	0.000087
	C	0.862308	-1.493866	0.000009
	H	4.714228	-0.675378	0.000355
	H	3.898846	-2.980910	0.000265
	H	1.514045	-3.562456	0.000063
	C	-1.920487	2.279330	-0.000102
	H	-2.827706	2.872160	-0.000136
	C	-0.670553	2.913493	-0.000009
	H	-0.633431	3.997743	0.000021
	C	0.525855	2.144004	0.000045
	C	2.944419	1.639584	0.000230
	H	3.965965	2.006101	0.000323
	C	1.914292	2.553781	0.000168
	H	2.151902	3.612490	0.000214
	H	-1.451296	-3.304932	-0.000240
	O	-4.603508	0.029923	-0.000111
cTS5-3	C	1.919126	-1.740759	-0.393885
	C	3.038480	-0.710564	-0.544435
	C	1.869428	1.020932	-0.283338
	C	0.760402	0.252155	-0.200989
	C	-0.506582	0.782273	-0.062389
	C	-1.424772	-0.275518	-0.001359
	C	-2.784324	-0.028382	0.147988
	C	-3.585913	-1.197552	0.196303
	C	-2.985023	-2.449422	0.097678
	C	-1.585220	-2.646813	-0.052651
	C	-0.766485	-1.532817	-0.104416
	C	0.694684	-1.203560	-0.242639
	C	4.163827	-0.890692	0.234076
	H	2.159328	-2.795398	-0.436098
	H	3.323314	-0.483170	-1.574337
	H	-4.663085	-1.130312	0.308258
	H	-3.618651	-3.328641	0.137542
	H	-1.196692	-3.656694	-0.121068
	O	4.981687	-0.616688	1.020154
	C	-0.792734	2.134209	0.010549
	C	1.656617	2.424976	-0.230596
	H	2.490449	3.116457	-0.294830
	C	0.365550	2.966664	-0.079842
	H	0.265526	4.046720	-0.031164
	C	-3.138260	1.378588	0.226635
	H	-4.185161	1.640702	0.342027
	C	-2.209991	2.399564	0.162914
	H	-2.561378	3.424151	0.230818

cTS1-3	C	-2.700179	-1.172940	0.681154
	C	-3.451771	-0.667880	-0.448041
	C	-2.095314	0.262798	0.116677
	C	-0.809100	-0.133793	-0.222115
	C	-0.427730	-1.502030	-0.024306
	C	-1.530674	-2.134350	0.461545
	H	-3.222580	-1.252798	1.641835
	C	0.274241	0.696134	-0.309198
	C	1.424049	-0.117955	-0.279580
	C	2.684600	0.452061	-0.142132
	C	3.741560	-0.486128	-0.017545
	C	3.452963	-1.846289	0.028552
	C	2.133320	-2.374542	-0.002965
	C	1.075272	-1.496839	-0.150293
	H	4.771246	-0.155418	0.069172
	H	4.275869	-2.544656	0.133498
	H	1.987004	-3.442234	0.115099
	C	-2.199567	1.689147	0.382142
	H	-3.160347	2.117855	0.642724
	C	-1.097576	2.531995	0.272322
	H	-1.249471	3.584959	0.487502
	C	0.228859	2.057731	-0.045535
	C	2.692082	1.901008	-0.036267
	H	3.647898	2.407307	0.050562
	C	1.535945	2.661277	0.035707
	H	1.629370	3.730880	0.194055
	H	-1.634143	-3.167500	0.768181
	O	-4.578841	-0.399354	-0.737919
cTS3-4	C	4.067624	-0.787761	0.496716
	C	2.786295	-0.528472	-0.883059
	C	1.998581	0.671171	-0.433112
	C	1.943850	2.094109	-0.511127
	C	0.750769	2.788605	-0.226955
	C	-0.471219	2.120082	0.121084
	C	-1.860373	2.532350	0.186666
	C	-2.884859	1.606378	0.259669
	C	-2.674744	0.165727	0.235785
	C	-3.595957	-0.903307	0.095385
	C	-3.120487	-2.200398	-0.080935
	C	-1.742586	-2.535147	-0.171025
	C	-0.803569	-1.528038	-0.020929
	C	0.669567	-1.313903	-0.221044
	C	1.851094	-1.705775	-0.800255
	C	0.849638	0.100197	0.025863
	C	-0.326555	0.749516	0.265043
	C	-1.341020	-0.224041	0.243628
	H	3.458744	-0.468069	-1.730982
	H	2.800614	2.672965	-0.839252
	H	0.757068	3.867216	-0.344538
	H	-2.118040	3.585605	0.141280
	H	-3.905924	1.974089	0.281460
	H	-4.665696	-0.722159	0.095393
	H	-3.843226	-3.000823	-0.195703
	H	-1.459851	-3.560083	-0.382778
	H	2.126010	-2.679702	-1.183048
	O	3.784251	-1.034601	1.583722
d	C	2.441707	2.604398	-0.000016
	C	3.042648	1.344116	-0.000018
	C	2.225316	0.199202	-0.000056
	C	0.866447	0.434684	-0.000081
	C	0.209486	1.689546	-0.000073
	C	1.037517	2.801900	-0.000042
	H	3.078929	3.481738	0.000006
	H	4.121491	1.245271	0.000001
	C	-0.084090	-0.608304	-0.000059
	C	-1.352538	-0.044445	-0.000052
	C	-2.501505	-0.832630	0.000017
	C	-3.714935	-0.100812	0.000038
	C	-3.672920	1.289918	0.000002
	C	-2.466830	2.051136	-0.000045
	C	-1.262597	1.377227	-0.000071
	H	-4.673373	-0.608485	0.000087
	H	-4.611653	1.832850	0.000022
	H	-2.528056	3.133689	-0.000051
	C	2.634248	-1.243359	-0.000070
	C	1.570847	-2.278814	0.000044

	H	1.938890	-3.298860	0.000116
	C	0.192311	-1.969818	0.000019
	C	-2.261619	-2.262080	0.000083
	H	-3.114678	-2.932632	0.000139
	C	-0.994162	-2.806175	0.000090
	H	-0.884698	-3.885130	0.000150
	H	0.645980	3.813235	-0.000031
	O	3.821399	-1.581977	0.000162
d3	C	-1.822716	2.869765	0.465913
	C	-2.555335	1.666479	0.592844
	C	-1.931283	0.483603	0.183622
	C	-0.686783	0.670001	-0.370534
	C	0.167930	1.775909	-0.358833
	C	-0.472287	2.951726	0.054253
	H	-2.306138	3.786732	0.785106
	H	-3.540257	1.690709	1.045242
	C	0.029861	-0.536880	-0.440072
	C	1.380279	-0.256552	-0.457912
	C	2.274445	-1.247385	-0.050301
	C	3.609040	-0.778294	0.126259
	C	3.867341	0.580185	0.011703
	C	2.863387	1.574819	-0.212408
	C	1.564389	1.168681	-0.439038
	H	4.410724	-1.454470	0.403479
	H	4.883161	0.923942	0.174395
	H	3.140506	2.620697	-0.136981
	C	-3.173926	-1.814254	-0.268793
	C	-2.045770	-1.067314	0.452789
	H	-2.243865	-1.244495	1.517093
	C	-0.608720	-1.603949	0.101308
	C	1.659201	-2.497010	0.332871
	H	2.299635	-3.319196	0.635372
	C	0.273918	-2.670831	0.453511
	H	-0.094183	-3.604895	0.863868
	H	0.041065	3.903890	0.132648
	O	-4.118561	-1.364389	-0.810416
d5	C	2.590536	3.139639	-0.000032
	C	1.261976	3.594585	-0.000159
	C	0.267747	2.642310	-0.000165
	C	0.473697	1.286957	-0.000056
	C	1.842683	0.845088	0.000073
	C	2.879159	1.772063	0.000083
	H	3.398741	3.862986	-0.000024
	H	1.042482	4.656296	-0.000247
	C	-0.394002	0.102925	-0.000037
	C	0.469655	-1.017416	0.000103
	C	0.039430	-2.349865	0.000164
	C	1.052908	-3.342005	0.000306
	C	2.387127	-2.971896	0.000377
	C	2.796244	-1.614182	0.000313
	C	1.831201	-0.626916	0.000175
	H	0.781866	-4.392507	0.000359
	H	3.148919	-3.743389	0.000485
	H	3.854524	-1.376756	0.000373
	C	-4.009639	0.925758	-0.000347
	C	-2.693695	1.025271	-0.000272
	H	-2.304713	2.038741	-0.000304
	C	-1.766897	-0.100120	-0.000125
	C	-1.373530	-2.540839	0.000075
	H	-1.783392	-3.545289	0.000115
	C	-2.224401	-1.460857	-0.000063
	H	-3.294497	-1.644029	-0.000129
	H	3.911623	1.440356	0.000180
	O	-5.167092	0.855072	-0.000411
CO	C	0.000000	0.000000	-0.643976
	O	0.000000	0.000000	0.482982
d4	C	-3.263688	-1.236654	-0.404380
	C	-3.339133	0.171941	-0.388680
	C	-2.221987	0.886244	0.087531
	C	-1.214937	0.060748	0.595936
	C	-0.981392	-1.299397	0.402241
	C	-2.106060	-1.986170	-0.082911
	H	-4.122375	-1.781436	-0.781919
	H	-4.209820	0.658308	-0.815116
	C	-0.012429	0.788240	0.677474
	C	1.044535	-0.076204	0.519890

	C	2.262374	0.427037	0.046530
	C	3.200137	-0.577385	-0.316148
	C	2.804750	-1.910131	-0.304927
	C	1.473225	-2.349088	-0.019686
	C	0.539540	-1.419832	0.387530
	H	4.195054	-0.318278	-0.662626
	H	3.525115	-2.661325	-0.610361
	H	1.218243	-3.388210	-0.198169
	C	-1.573487	2.201357	-0.120198
	H	-2.049080	3.063404	-0.570622
	C	-0.144816	2.072385	0.185240
	C	2.269192	1.852573	-0.221778
	H	3.195364	2.308690	-0.556582
	C	1.122053	2.644493	-0.203266
	H	1.198634	3.668214	-0.554413
	H	-2.098395	-3.050318	-0.292596
dTS1-5	C	-2.248442	2.880752	-0.051492
	C	-2.977424	1.676575	-0.058229
	C	-2.229289	0.518855	-0.066848
	C	-0.872058	0.503447	-0.016712
	C	-0.124546	1.725644	0.004684
	C	-0.842862	2.915284	-0.013612
	H	-2.798680	3.815184	-0.075771
	H	-4.060432	1.680166	-0.070799
	C	0.021350	-0.608037	0.008479
	C	1.320792	-0.095824	0.036504
	C	2.453160	-0.912762	0.018869
	C	3.694657	-0.225553	0.024126
	C	3.714763	1.162079	0.032981
	C	2.536121	1.958265	0.030519
	C	1.308266	1.326152	0.035980
	H	4.629091	-0.776792	0.015750
	H	4.673237	1.669090	0.037032
	H	2.627994	3.038932	0.023367
	C	-2.778526	-1.687415	0.039586
	C	-1.632201	-2.407174	-0.075243
	H	-1.847239	-3.455169	-0.270661
	C	-0.263371	-1.955373	-0.037604
	C	2.181378	-2.320461	-0.026015
	H	3.009885	-3.021065	-0.042070
	C	0.890299	-2.813847	-0.058750
	H	0.741275	-3.887891	-0.095905
	H	-0.338497	3.875166	0.005437
	O	-3.943629	-1.597659	0.188786
dTS5-3	C	1.798057	3.146995	0.115688
	C	2.642088	2.036513	-0.116423
	C	2.034465	0.810280	-0.393885
	C	0.672333	0.825756	-0.440715
	C	-0.229201	1.869352	-0.153104
	C	0.386691	3.091513	0.121259
	H	2.269148	4.099458	0.337362
	H	3.716563	2.166675	-0.048582
	C	-0.009645	-0.402624	-0.525099
	C	-1.353324	-0.193594	-0.292036
	C	-2.199074	-1.277065	-0.064885
	C	-3.524238	-0.900071	0.303766
	C	-3.822366	0.444032	0.469819
	C	-2.873765	1.507404	0.328854
	C	-1.586802	1.198622	-0.058285
	H	-4.290190	-1.646096	0.486597
	H	-4.831351	0.711899	0.764583
	H	-3.186294	2.519629	0.561110
	C	2.966631	-1.960450	0.381477
	C	2.165413	-1.283656	-0.551138
	H	2.617019	-1.351895	-1.542538
	C	0.662416	-1.578984	-0.499160
	C	-1.554842	-2.563832	-0.122586
	H	-2.150853	-3.456938	0.033299
	C	-0.177037	-2.719677	-0.310100
	H	0.242131	-3.719438	-0.283628
	H	-0.174380	3.985925	0.369289
	O	3.725176	-1.951538	1.270229
dTS1-3	C	-2.077900	2.622092	0.525524
	C	-2.736906	1.382434	0.555244
	C	-2.033517	0.256512	0.073164
	C	-0.755045	0.526011	-0.393114

C	-0.008456	1.707613	-0.326854
C	-0.732183	2.816715	0.126658
H	-2.625796	3.485938	0.886588
H	-3.752315	1.313623	0.925647
C	0.080700	-0.597957	-0.455815
C	1.399749	-0.182705	-0.463431
C	2.398553	-1.074701	-0.069691
C	3.675477	-0.470366	0.121023
C	3.789481	0.908857	0.039603
C	2.682293	1.791059	-0.163994
C	1.438245	1.250828	-0.411954
H	4.542891	-1.066235	0.384066
H	4.762424	1.355988	0.211902
H	2.840446	2.859141	-0.061348
C	-2.903044	-1.235620	-0.520318
C	-1.881220	-1.513881	0.453268
H	-2.217002	-1.902841	1.420925
C	-0.424608	-1.746107	0.072644
C	1.929259	-2.387692	0.296820
H	2.655970	-3.136480	0.594533
C	0.573301	-2.710180	0.413532
H	0.305629	-3.681608	0.814226
H	-0.284454	3.796261	0.250029
O	-4.089111	-1.385157	-0.582554

dTSts3-4	C	1.864886	2.874377	-0.548562
	C	2.563141	1.673659	-0.808252
	C	1.969309	0.473271	-0.394503
	C	0.792979	0.643901	0.319041
	C	-0.046048	1.755219	0.423743
	C	0.563811	2.945212	0.000992
	H	2.320892	3.801425	-0.878768
	H	3.486608	1.711338	-1.375537
	C	0.063651	-0.559537	0.346466
	C	-1.278972	-0.267098	0.453258
	C	-2.209527	-1.200750	-0.012772
	C	-3.540733	-0.701377	-0.089792
	C	-3.773529	0.645229	0.154038
	C	-2.742246	1.601920	0.413040
	C	-1.443103	1.159735	0.551056
	H	-4.362495	-1.339650	-0.396806
	H	-4.789142	1.015207	0.064254
	H	-3.000750	2.655268	0.427139
	C	3.287329	-1.804200	0.499334
	C	2.015030	-1.008026	-0.750733
	H	2.482373	-1.311605	-1.679192
	C	0.654129	-1.559321	-0.377825
	C	-1.636254	-2.409443	-0.561497
	H	-2.307231	-3.184875	-0.916823
	C	-0.266194	-2.579652	-0.784436
	H	0.061161	-3.460930	-1.325667
	H	0.051073	3.900934	0.007319
	O	3.128945	-1.735729	1.634812

e	C	-2.378971	-2.856904	0.000028
	C	-3.058626	-1.646603	0.000023
	C	-2.318301	-0.427495	-0.000010
	C	-0.929834	-0.595006	-0.000045
	C	-0.201217	-1.804941	-0.000030
	C	-0.959599	-2.967116	0.000006
	H	-2.957186	-3.774129	0.000055
	H	-4.142797	-1.635216	0.000048
	C	-0.047964	0.506143	-0.000056
	C	1.255654	0.014609	-0.000048
	C	2.353242	0.871273	-0.000010
	C	3.611880	0.206372	0.000026
	C	3.651509	-1.179991	0.000032
	C	2.490157	-2.010942	0.000010
	C	1.250468	-1.407174	-0.000032
	H	4.538491	0.770185	0.000054
	H	4.619799	-1.668268	0.000063
	H	2.614388	-3.088199	0.000030
	C	-2.757432	0.924310	0.000007
	H	-3.812702	1.174817	0.000031
	C	-1.854036	2.099121	0.000009
	C	-0.383924	1.831616	-0.000021
	C	2.031484	2.275314	0.000009
	H	2.839533	2.999396	0.000034

	C	0.721592	2.738583	0.000006
	H	0.528952	3.804982	0.000031
	H	-0.507459	-3.952586	0.000022
	O	-2.322189	3.242750	0.000027
e3	C	-1.822716	2.869765	0.465913
	C	-2.555335	1.666479	0.592844
	C	-1.931283	0.483603	0.183622
	C	-0.686783	0.670001	-0.370534
	C	0.167930	1.775909	-0.358833
	C	-0.472287	2.951726	0.054253
	H	-2.306138	3.786732	0.785106
	H	-3.540257	1.690709	1.045242
	C	0.029861	-0.536880	-0.440072
	C	1.380279	-0.256552	-0.457912
	C	2.274445	-1.247385	-0.050301
	C	3.609040	-0.778294	0.126259
	C	3.867341	0.580185	0.011703
	C	2.863387	1.574819	-0.212408
	C	1.564389	1.168681	-0.439038
	H	4.410724	-1.454470	0.403479
	H	4.883161	0.923942	0.174395
	H	3.140506	2.620697	-0.136981
	C	-3.173926	-1.814254	-0.268793
	C	-2.045770	-1.067314	0.452789
	H	-2.243865	-1.244495	1.517093
	C	-0.608720	-1.603949	0.101308
	C	1.659201	-2.497010	0.332871
	H	2.299635	-3.319196	0.635372
	C	0.273918	-2.670831	0.453511
	H	-0.094183	-3.604895	0.863868
	H	0.041065	3.903890	0.132648
	O	-4.118561	-1.364389	-0.810416
e5	C	-1.844183	2.826653	0.000000
	C	-0.481988	3.099239	0.000000
	C	0.477608	2.066336	0.000000
	C	0.000000	0.750952	0.000000
	C	-1.398488	0.475975	0.000000
	C	-2.321279	1.511396	0.000000
	H	-2.547052	3.652125	0.000000
	H	-0.152368	4.133305	0.000000
	C	0.716041	-0.533040	0.000000
	C	-0.283828	-1.553732	0.000000
	C	-0.017107	-2.929813	0.000000
	C	-1.156117	-3.782180	0.000000
	C	-2.428612	-3.242526	0.000000
	C	-2.662193	-1.842042	0.000000
	C	-1.580135	-0.987065	0.000000
	H	-1.023928	-4.858795	0.000000
	H	-3.283382	-3.909661	0.000000
	H	-3.681649	-1.471713	0.000000
	C	1.918251	2.324242	0.000000
	H	2.614612	1.491862	0.000000
	C	2.473788	3.519481	0.000000
	C	1.992790	-1.001501	0.000000
	C	1.352605	-3.321187	0.000000
	H	1.618977	-4.373072	0.000000
	C	2.349184	-2.356261	0.000000
	H	3.392485	-2.652167	0.000000
	H	-3.386923	1.313536	0.000000
	O	2.976401	4.565626	0.000000
CO	C	0.000000	0.000000	-0.643976
	O	0.000000	0.000000	0.482982
e4	C	-3.263688	-1.236654	-0.404380
	C	-3.339133	0.171941	-0.388680
	C	-2.221987	0.886244	0.087531
	C	-1.214937	0.060748	0.595936
	C	-0.981392	-1.299397	0.402241
	C	-2.106060	-1.986170	-0.082911
	H	-4.122375	-1.781436	-0.781919
	H	-4.209820	0.658308	-0.815116
	C	-0.012429	0.788240	0.677474
	C	1.044535	-0.076204	0.519890
	C	2.262374	0.427037	0.046530
	C	3.200137	-0.577385	-0.316148
	C	2.804750	-1.910131	-0.304927
	C	1.473225	-2.349088	-0.019686

	C	0.539540	-1.419832	0.387530
	H	4.195054	-0.318278	-0.662626
	H	3.525115	-2.661325	-0.610361
	H	1.218243	-3.388210	-0.198169
	C	-1.573487	2.201357	-0.120198
	H	-2.049080	3.063404	-0.570622
	C	-0.144816	2.072385	0.185240
	C	2.269192	1.852573	-0.221778
	H	3.195364	2.308690	-0.556582
	C	1.122053	2.644493	-0.203266
	H	1.198634	3.668214	-0.554413
	H	-2.098395	-3.050318	-0.292596
eTS1-5	C	-2.170841	-2.985139	-0.014230
	C	-2.924755	-1.813212	-0.045973
	C	-2.289410	-0.551707	-0.032570
	C	-0.901799	-0.589572	-0.001082
	C	-0.109289	-1.762059	0.026093
	C	-0.763333	-2.986940	0.022184
	H	-2.692385	-3.935900	-0.020524
	H	-4.007328	-1.874916	-0.071502
	C	-0.051696	0.559338	-0.031493
	C	1.286236	0.100714	-0.014566
	C	2.383627	0.962552	-0.023178
	C	3.650791	0.313200	0.006262
	C	3.714241	-1.069264	0.043049
	C	2.561633	-1.905997	0.054413
	C	1.314141	-1.317902	0.027646
	H	4.565731	0.895668	0.001568
	H	4.688713	-1.544463	0.065329
	H	2.689957	-2.982576	0.083297
	C	-2.980966	0.720843	-0.059220
	H	-4.054088	0.726529	-0.237796
	C	-2.512756	1.987566	0.047347
	C	-0.266968	1.888825	-0.082312
	C	2.088900	2.364199	-0.053807
	H	2.900340	3.084429	-0.071277
	C	0.776200	2.828661	-0.072157
	H	0.574688	3.892977	-0.100169
	H	-0.222867	-3.926296	0.037522
	O	-2.658314	3.149989	0.191891
eTS5-3	C	1.993927	2.917810	0.074557
	C	2.737369	1.737481	-0.134137
	C	2.035033	0.550728	-0.376689
	C	0.671356	0.689579	-0.397996
	C	-0.136243	1.804085	-0.132216
	C	0.583028	2.979481	0.099188
	H	2.544382	3.833456	0.260248
	H	3.819810	1.769702	-0.085871
	C	-0.083294	-0.495016	-0.460915
	C	-1.410388	-0.168220	-0.235415
	C	-2.352788	-1.175718	-0.044855
	C	-3.650144	-0.687118	0.286558
	C	-3.843172	0.678885	0.438428
	C	-2.809817	1.659760	0.311152
	C	-1.540405	1.240726	-0.030705
	H	-4.481481	-1.365741	0.445906
	H	-4.835196	1.029936	0.701498
	H	-3.047803	2.698856	0.511519
	C	3.344054	-1.433714	0.375394
	C	2.396885	-0.936613	-0.534892
	H	2.667469	-1.235879	-1.549006
	C	0.472215	-1.722798	-0.470713
	C	-1.824566	-2.513454	-0.123434
	H	-2.499994	-3.353228	0.009511
	C	-0.463215	-2.790219	-0.316924
	H	-0.148023	-3.828123	-0.319051
	H	0.101622	3.924216	0.326867
	O	3.645025	-2.185900	1.217507
eTS1-3	C	-1.912015	2.938355	-0.478743
	C	-2.632340	1.746244	-0.731284
	C	-2.058550	0.544395	-0.319439
	C	-0.847863	0.662994	0.343901
	C	0.003696	1.775951	0.432760
	C	-0.601431	2.977413	0.040430
	H	-2.363838	3.875517	-0.784858
	H	-3.568798	1.795676	-1.275099

	C	-0.131283	-0.544072	0.413213
	C	1.220650	-0.240486	0.460600
	C	2.155692	-1.150102	-0.045349
	C	3.469634	-0.646490	-0.169145
	C	3.712582	0.704040	0.087914
	C	2.686395	1.640786	0.379945
	C	1.387462	1.185710	0.540089
	H	4.277452	-1.276240	-0.526815
	H	4.723806	1.077752	-0.029043
	H	2.931410	2.697277	0.401675
	C	-2.175409	-0.972323	-0.649652
	H	-2.566958	-1.286117	-1.614661
	C	-2.373537	-1.914166	0.441934
	C	-0.733081	-1.614272	-0.258355
	C	1.583668	-2.363841	-0.618505
	H	2.264249	-3.109272	-1.018225
	C	0.231086	-2.568572	-0.793157
	H	-0.104620	-3.454729	-1.319772
	H	-0.072203	3.924221	0.050943
	O	-2.929081	-2.151684	1.456613
eTS3-4	C	1.864886	2.874377	-0.548562
	C	2.563141	1.673659	-0.808252
	C	1.969309	0.473271	-0.394503
	C	0.792979	0.643901	0.319041
	C	-0.046048	1.755219	0.423743
	C	0.563811	2.945212	0.000992
	H	2.320892	3.801425	-0.878768
	H	3.486608	1.711338	-1.375537
	C	0.063651	-0.559537	0.346466
	C	-1.278972	-0.267098	0.453258
	C	-2.209527	-1.200750	-0.012772
	C	-3.540733	-0.701377	-0.089792
	C	-3.773529	0.645229	0.154038
	C	-2.742246	1.601920	0.413040
	C	-1.443103	1.159735	0.551056
	H	-4.362495	-1.339650	-0.396806
	H	-4.789142	1.015207	0.064254
	H	-3.000750	2.655268	0.427139
	C	3.287329	-1.804200	0.499334
	C	2.015030	-1.008026	-0.750733
	H	2.482373	-1.311605	-1.679192
	C	0.654129	-1.559321	-0.377825
	C	-1.636254	-2.409443	-0.561497
	H	-2.307231	-3.184875	-0.916823
	C	-0.266194	-2.579652	-0.784436
	H	0.061161	-3.460930	-1.325667
	H	0.051073	3.900934	0.007319
	O	3.128945	-1.735729	1.634812
f	C	3.456923	0.357260	-0.322189
	C	3.018414	1.674294	-0.308097
	C	1.675121	2.027582	0.077961
	C	0.939987	0.980642	0.613419
	C	1.390059	-0.362849	0.601160
	C	2.595953	-0.744591	0.047435
	H	4.450416	0.150025	-0.706718
	H	3.684953	2.443528	-0.684339
	C	-0.465657	0.968212	0.647621
	C	-0.896821	-0.396908	0.664429
	C	-2.111545	-0.826588	0.195441
	C	-2.181162	-2.211018	-0.165027
	C	-1.046063	-3.015280	-0.195853
	C	0.258857	-2.494913	0.121133
	C	0.255971	-1.210694	0.639704
	H	-3.127556	-2.613910	-0.506923
	H	-1.142227	-4.032947	-0.560101
	C	0.896563	3.205816	-0.238831
	H	1.402042	4.096258	-0.598291
	C	-0.485696	3.202597	-0.201397
	H	-1.018097	4.088490	-0.530559
	C	-1.241606	2.013198	0.150782
	C	-3.090005	0.263430	-0.124315
	C	-2.582885	1.662238	-0.138746
	H	-3.301615	2.388015	-0.503624
	C	2.677103	-2.148398	-0.295272
	C	1.569300	-2.978290	-0.259436
	H	3.611105	-2.550282	-0.674623

	H	1.677235	-3.998624	-0.612928
	O	-4.254140	0.029376	-0.460179
f3	C	3.355845	-1.002037	0.120612
	C	2.649616	-2.184593	0.205764
	C	1.241504	-2.243498	-0.118935
	C	0.753575	-1.128781	-0.801434
	C	1.465319	0.117200	-0.836297
	C	2.724775	0.239508	-0.271748
	H	4.379442	-0.981476	0.481101
	H	3.136589	-3.052938	0.637810
	C	-0.613108	-0.815084	-0.747642
	C	-0.758124	0.613727	-0.735944
	C	-1.765186	1.014402	0.098577
	C	-1.592081	2.301592	0.678745
	C	-0.369084	2.973451	0.547744
	C	0.774546	2.372213	-0.077948
	C	0.518028	1.194709	-0.781774
	H	-2.351134	2.738104	1.319151
	H	-0.245953	3.910985	1.080655
	C	0.242767	-3.073104	0.493550
	H	0.552149	-3.976942	1.008701
	C	-1.089871	-2.662435	0.634669
	H	-1.745863	-3.251930	1.266235
	C	-1.516978	-1.426000	0.076937
	C	-3.932334	-0.510427	0.000732
	C	-2.508222	-0.295522	0.538098
	H	-2.605509	-0.330777	1.628345
	C	3.094984	1.574340	0.145714
	C	2.165962	2.589628	0.250480
	H	4.102022	1.752074	0.509528
	H	2.469311	3.529316	0.700881
	O	-4.592832	0.220981	-0.643977
f5	C	-1.969085	2.880983	0.000134
	C	-0.633756	3.252067	0.000081
	C	0.444108	2.293082	-0.000001
	C	0.047047	0.962729	-0.000034
	C	-1.304219	0.612862	0.000017
	C	-2.365469	1.494576	0.000109
	H	-2.726568	3.657799	0.000200
	H	-0.390997	4.309943	0.000107
	C	0.858359	-0.201304	-0.000082
	C	-0.091901	-1.355828	-0.000057
	C	-0.143800	-2.719276	-0.000050
	C	-1.328969	-3.470898	0.000012
	C	-2.575415	-2.841826	0.000079
	C	-2.637450	-1.421931	0.000079
	C	-1.405465	-0.778087	0.000003
	H	-1.280001	-4.554507	0.000012
	H	-3.478107	-3.443998	0.000132
	C	1.857089	2.469520	-0.000041
	H	2.295247	3.462085	-0.000027
	C	2.690084	1.365380	-0.000101
	H	3.761889	1.538982	-0.000135
	C	2.234078	0.000150	-0.000118
	C	4.478592	-1.023368	-0.000138
	C	3.162467	-1.124803	-0.000171
	H	2.775967	-2.138369	-0.000223
	C	-3.656300	0.847657	0.000177
	C	-3.778095	-0.530496	0.000162
	H	-4.558976	1.449852	0.000247
	H	-4.773893	-0.961962	0.000220
	O	5.635505	-0.948372	-0.000110
CO	C	0.000000	0.000000	-0.643976
	O	0.000000	0.000000	0.482982
f4	C	-1.294097	2.727136	-0.295812
	C	-2.397172	1.894527	-0.331457
	C	-2.319111	0.523191	0.107890
	C	-1.168392	0.207031	0.835439
	C	0.000000	1.046660	0.818337
	C	0.000000	2.261847	0.151274
	H	-1.373933	3.713636	-0.741494
	H	-3.300816	2.250830	-0.815912
	C	-0.718478	-1.115232	0.901735
	C	0.718478	-1.115232	0.901735
	C	1.192293	-2.139778	0.086507
	C	2.482034	-1.884322	-0.490897

	C	3.035043	-0.604674	-0.433708
	C	2.319111	0.523191	0.107890
	C	1.168392	0.207031	0.835439
	H	2.987800	-2.635813	-1.088181
	H	3.964811	-0.428256	-0.965341
	C	-3.035043	-0.604674	-0.433708
	H	-3.964811	-0.428256	-0.965341
	C	-2.482033	-1.884323	-0.490897
	H	-2.987799	-2.635813	-1.088181
	C	-1.192293	-2.139778	0.086507
	C	0.000000	-2.875307	-0.349091
	H	0.000000	-3.694526	-1.057627
	C	1.294097	2.727136	-0.295812
	C	2.397172	1.894527	-0.331457
	H	1.373933	3.713636	-0.741495
	H	3.300815	2.250831	-0.815912
fTS1-5	C	-3.394756	-0.971572	-0.173954
	C	-2.715897	-2.182227	-0.169697
	C	-1.301467	-2.273449	0.096202
	C	-0.712771	-1.084778	0.506856
	C	-1.411502	0.140088	0.499839
	C	-2.721300	0.279141	0.083935
	H	-4.445266	-0.968019	-0.445970
	H	-3.260746	-3.078955	-0.447385
	C	0.670121	-0.821558	0.496282
	C	0.832602	0.614715	0.483735
	C	1.850094	1.413000	0.083792
	C	1.649713	2.774753	-0.213360
	C	0.349865	3.292689	-0.257125
	C	-0.779795	2.468894	0.047033
	C	-0.472712	1.187161	0.479270
	H	2.486581	3.417178	-0.463285
	H	0.210344	4.321373	-0.573660
	C	-0.360043	-3.312131	-0.211948
	H	-0.713165	-4.295547	-0.505049
	C	1.003755	-3.063549	-0.236544
	H	1.669362	-3.864200	-0.541899
	C	1.572745	-1.769303	0.052802
	C	3.517625	-0.148986	-0.105690
	C	2.926989	-1.379993	-0.229304
	H	3.589630	-2.075357	-0.739857
	C	-3.107775	1.643914	-0.200720
	C	-2.189506	2.679481	-0.213726
	H	-4.134101	1.860237	-0.479444
	H	-2.530602	3.668984	-0.500415
	O	4.486506	0.512069	-0.026137
fTS5-3	C	3.157857	-1.554780	0.108305
	C	2.246613	-2.590280	0.179341
	C	0.843535	-2.384271	-0.106433
	C	0.547633	-1.164774	-0.709736
	C	1.479565	-0.086570	-0.748503
	C	2.761991	-0.208120	-0.242278
	H	4.177437	-1.738488	0.432288
	H	2.578249	-3.550646	0.560845
	C	-0.739997	-0.600988	-0.643277
	C	-0.618998	0.835508	-0.650175
	C	-1.526407	1.581955	0.031015
	C	-1.065835	2.824511	0.543258
	C	0.290214	3.172365	0.461979
	C	1.271142	2.280386	-0.081059
	C	0.757049	1.142545	-0.698303
	H	-1.735485	3.499435	1.066526
	H	0.611979	4.098588	0.929099
	C	-0.283615	-3.079833	0.441343
	H	-0.140993	-4.055841	0.893889
	C	-1.534768	-2.470044	0.569170
	H	-2.311244	-2.988329	1.121208
	C	-1.755680	-1.146876	0.087642
	C	-4.009766	-0.104540	0.046276
	C	-2.713048	-0.038871	0.557644
	H	-2.729392	0.091682	1.640855
	C	3.395707	1.037327	0.129619
	C	2.686012	2.219475	0.213749
	H	4.429896	1.027514	0.458857
	H	3.184775	3.097457	0.611902
	O	-4.900055	0.316734	-0.581616

fTS1-3	C	3.393048	-0.753090	-0.024989
	C	2.792601	-1.986932	0.111423
	C	1.372925	-2.159041	-0.106393
	C	0.748318	-1.092427	-0.753583
	C	1.352048	0.202156	-0.844001
	C	2.635091	0.431174	-0.366922
	H	4.436274	-0.647582	0.255620
	H	3.377666	-2.812795	0.503196
	C	-0.637518	-0.894830	-0.630628
	C	-0.910879	0.509287	-0.658846
	C	-1.946928	0.874591	0.218157
	C	-1.777756	2.168549	0.854334
	C	-0.619645	2.897957	0.673307
	C	0.532151	2.381457	-0.041438
	C	0.317945	1.191686	-0.738931
	H	-2.550767	2.560025	1.505906
	H	-0.524361	3.842075	1.200949
	C	0.497900	-3.069633	0.571397
	H	0.919152	-3.939465	1.065171
	C	-0.854543	-2.775536	0.793274
	H	-1.415123	-3.413207	1.468482
	C	-1.438562	-1.607555	0.236110
	C	-3.470643	-0.027680	-0.208196
	C	-2.500320	-0.581464	0.716369
	H	-2.803543	-0.580818	1.760932
	C	2.920836	1.784362	0.035289
	C	1.906593	2.711030	0.213675
	H	3.927783	2.046348	0.343468
	H	2.148622	3.664521	0.672541
	O	-4.173961	-0.242935	-1.134090
fTS3-4	C	3.216411	-1.293100	-0.025009
	C	2.400778	-2.394476	0.140286
	C	0.975484	-2.313626	-0.082048
	C	0.552297	-1.167889	-0.759535
	C	1.383331	-0.000053	-0.871376
	C	2.685824	-0.000107	-0.398164
	H	4.260103	-1.370982	0.262637
	H	2.826287	-3.299566	0.561912
	C	-0.767532	-0.717573	-0.621980
	C	-0.767467	0.717662	-0.621990
	C	-1.657252	1.203084	0.313564
	C	-1.316031	2.472026	0.867926
	C	-0.051214	3.022238	0.631354
	C	0.975692	2.313571	-0.082091
	C	0.552402	1.167860	-0.759555
	H	-1.970471	2.973410	1.573131
	H	0.207012	3.941426	1.147600
	C	-0.051484	-3.022187	0.631411
	H	0.206660	-3.941387	1.147676
	C	-1.316253	-2.471857	0.867971
	H	-1.970736	-2.973169	1.573187
	C	-1.657361	-1.202897	0.313582
	C	-4.117006	0.000291	-0.177375
	C	-2.436518	0.000129	0.801034
	H	-2.824722	0.000143	1.812089
	C	3.216527	1.292846	-0.025034
	C	2.400993	2.394299	0.140240
	H	4.260226	1.370640	0.262609
	H	2.826583	3.299359	0.561847
	O	-4.143834	-0.000165	-1.325243
g	C	0.523613	2.160029	0.664543
	C	-0.891541	2.015479	0.674010
	C	-1.469048	0.746642	0.973497
	C	-0.635954	-0.259026	1.449501
	C	0.754251	-0.111067	1.447282
	C	1.352574	1.047251	0.959695
	C	-0.931418	-1.641379	1.231748
	C	0.284488	-2.348969	1.102539
	C	0.402247	-3.496117	0.298540
	C	1.725581	-3.770717	-0.193895
	C	2.759038	-2.816670	-0.107380
	C	2.507530	-1.547448	0.531964
	C	1.327351	-1.401212	1.221533
	C	-2.738917	0.367022	0.441153
	C	-3.040018	-1.023690	0.235243
	C	-2.063332	-2.030376	0.552653

C	-0.838874	-4.039871	-0.184626
C	-2.047928	-3.323657	-0.088234
C	2.674940	0.934717	0.418473
C	3.253200	-0.358916	0.209951
C	-4.170994	-1.396712	-0.517513
C	-3.558109	1.372520	-0.130845
C	-4.765459	0.960876	-0.755676
C	-5.062085	-0.376465	-0.938902
H	-5.960543	-0.653765	-1.480161
C	-3.052175	2.714935	-0.198052
C	-1.747613	3.026966	0.128903
C	-1.150880	4.356408	-0.213428
C	1.137189	3.341814	0.093012
C	0.307221	4.424779	-0.238199
H	0.725652	5.351124	-0.616093
C	2.520165	3.296627	-0.212814
C	3.276694	2.094022	-0.147011
C	4.555522	1.936841	-0.756922
H	5.062492	2.814076	-1.144758
C	4.443293	-0.493751	-0.537680
C	5.114920	0.689896	-0.944660
H	6.057254	0.602765	-1.475223
C	4.033057	-2.914627	-0.782483
C	4.837378	-1.820780	-0.948326
C	-3.276707	-3.684548	-0.760396
C	-4.286543	-2.780687	-0.926742
H	2.982461	4.178303	-0.645040
H	5.774441	-1.928865	-1.484703
H	-5.182544	-3.077930	-1.461785
H	-3.666649	3.495680	-0.633883
H	-3.375583	-4.681464	-1.177073
H	-0.828925	-4.955914	-0.767817
H	4.334640	-3.868659	-1.202071
H	1.903515	-4.670307	-0.775535
H	-5.431797	1.716342	-1.158293
O	-1.846296	5.322224	-0.535040
C	3.184770	-0.453584	0.217355
C	2.630798	0.864688	0.371994
C	1.376053	1.016442	1.030745
C	0.723621	-0.102821	1.564086
C	1.256216	-1.413616	1.351040
C	2.425838	-1.607011	0.640601
C	-0.679782	-0.205192	1.560857
C	-1.015294	-1.579456	1.346076
C	-2.141625	-1.940181	0.630609
C	-2.157024	-3.257210	0.034240
C	-0.978121	-4.024007	0.000295
C	0.268992	-3.506014	0.487310
C	0.181684	-2.331578	1.254270
C	0.565331	2.110652	0.690498
C	-0.841720	2.008972	0.688826
C	-1.486059	0.808435	1.026402
C	-3.057234	-0.908564	0.203148
C	-2.701754	0.476114	0.360602
C	2.635246	-2.907963	0.045985
C	1.580481	-3.838089	0.007226
C	-1.413470	2.979512	-0.174000
C	0.998082	3.153329	-0.168848
C	-0.281851	5.310205	0.154321
C	-0.274884	3.942647	-0.581270
H	-0.273601	4.167236	-1.649248
C	2.287060	3.121573	-0.640545
C	3.121269	1.954669	-0.404678
C	4.334004	1.742003	-1.111033
C	4.309745	-0.649128	-0.608256
C	4.918100	0.491356	-1.190041
H	5.812324	0.360364	-1.790499
C	4.686055	-2.005439	-0.942220
C	3.884238	-3.072646	-0.663838
C	-3.365343	-3.601273	-0.681767
C	-4.137226	-1.264992	-0.628944
C	-4.311895	-2.661426	-0.963947
C	-3.339155	1.483262	-0.421271
C	-4.503256	1.096834	-1.135728
H	-5.050917	1.849661	-1.693339
C	-4.900229	-0.224999	-1.216400

g3 (row label at left of second block)

g4	C	-2.680557	2.757955	-0.654569
	H	5.595070	-2.155694	-1.515436
	H	-5.187093	-2.941180	-1.541300
	H	-5.761882	-0.484605	-1.822647
	H	-3.155425	3.449279	-1.343453
	H	2.659538	3.878026	-1.323506
	H	4.771247	2.566941	-1.664097
	O	-0.927931	5.640496	1.080001
	H	-3.487708	-4.615549	-1.047080
	H	-0.988849	-4.959109	-0.551860
	H	1.730085	-4.761810	-0.543849
	H	4.154036	-4.058270	-1.028494
g5	C	3.334334	0.517755	0.169863
	C	2.427566	1.613021	0.401055
	C	1.119844	1.360149	0.939995
	C	0.862664	0.073975	1.394038
	C	1.766930	-1.010636	1.165211
	C	2.942291	-0.829201	0.478643
	C	-0.431327	-0.443765	1.400461
	C	-0.335246	-1.854120	1.181631
	C	-1.317967	-2.545250	0.516290
	C	-0.955527	-3.788426	-0.120910
	C	0.403459	-4.144770	-0.225607
	C	1.449683	-3.279256	0.249647
	C	1.025193	-2.205475	1.051332
	C	-0.001392	2.243658	0.718323
	C	-1.348835	1.709519	0.732450
	C	-1.517840	0.304066	0.958594
	C	-2.539025	-1.848953	0.226983
	C	-2.638059	-0.432823	0.453630
	C	3.531195	-1.982352	-0.159696
	C	2.796705	-3.181211	-0.245523
	C	-2.543485	2.425587	0.330552
	C	0.430872	3.517057	0.279446
	C	-3.290544	4.609730	-0.533563
	C	-2.504589	3.890738	0.243388
	H	-1.785007	4.458058	0.822905
	C	1.677581	3.889487	-0.086393
	C	2.727310	2.891826	-0.122951
	C	3.984133	3.087623	-0.746721
	C	4.517083	0.713227	-0.570225
	C	4.850812	2.032571	-0.962857
	H	5.778476	2.205003	-1.498717
	C	5.259537	-0.458283	-0.988318
	C	4.786293	-1.728825	-0.831424
	C	-2.048385	-4.476361	-0.771625
	C	-3.542808	-2.528757	-0.489860
	C	-3.273221	-3.887950	-0.909301
	C	-3.744709	0.288778	-0.042598
	C	-4.805445	-0.444366	-0.637662
	H	-5.684562	0.089284	-0.983707
	C	-4.705571	-1.804976	-0.856477
	C	-3.688992	1.717665	0.008151
	H	6.192939	-0.301480	-1.519247
	H	-4.063588	-4.423969	-1.424941
	H	-5.507816	-2.322622	-1.372187
	H	-4.578600	2.268318	-0.282490
	H	1.895702	4.899857	-0.419172
	H	4.240419	4.075134	-1.115865
	O	-3.973476	5.254707	-1.214829
	H	-1.875926	-5.461877	-1.191407
	H	0.661288	-5.025400	-0.806504
	H	3.213281	-3.998641	-0.826634
	H	5.338100	-2.563373	-1.251237
CO	C	0.000000	0.000000	-0.643976
	O	0.000000	0.000000	0.482982
g4	C	3.125555	-0.362098	0.234446
	C	2.671670	0.976721	0.470576
	C	1.431340	1.182783	1.150379
	C	0.704971	0.083363	1.625157
	C	1.139939	-1.247133	1.328847
	C	2.289669	-1.483065	0.599698
	C	-0.704953	0.083368	1.625147
	C	-1.139963	-1.247167	1.328870
	C	-2.289621	-1.483037	0.599554
	C	-2.402003	-2.758188	-0.071706

	C	-1.283184	-3.606263	-0.157211
	C	-0.000015	-3.208198	0.348768
	C	-0.000024	-2.076369	1.182054
	C	0.699599	2.343850	0.879660
	C	-0.699527	2.343757	0.879458
	C	-1.431284	1.182736	1.150293
	C	-3.125507	-0.362121	0.234288
	C	-2.671612	0.976709	0.470463
	C	2.402002	-2.758135	-0.071651
	C	1.283170	-3.606214	-0.157262
	C	-1.169952	3.404584	0.025539
	C	1.170002	3.404789	0.025707
	C	0.000061	4.132159	-0.411958
	H	-0.000005	4.963538	-1.103324
	C	2.486279	3.299839	-0.434217
	C	3.232744	2.076185	-0.253366
	C	4.428975	1.815929	-0.976016
	C	4.232749	-0.591532	-0.611538
	C	4.921312	0.533611	-1.130347
	H	5.801897	0.373155	-1.743686
	C	4.508081	-1.948359	-1.025063
	C	3.632177	-2.970495	-0.801101
	C	-3.632133	-2.970445	-0.801264
	C	-4.232748	-0.591573	-0.611618
	C	-4.508008	-1.948344	-1.025165
	C	-3.232774	2.076216	-0.253307
	C	-4.429191	1.815947	-0.975662
	H	-4.922672	2.637433	-1.484991
	C	-4.921533	0.533630	-1.129991
	C	-2.486250	3.299772	-0.434272
	H	5.400787	-2.130143	-1.614652
	H	-5.400464	-2.130190	-1.615124
	H	-5.802248	0.373291	-1.743191
	H	-2.908534	4.050063	-1.095542
	H	2.908723	4.050066	-1.095452
	H	4.922251	2.637422	-1.485519
	H	-3.827915	-3.949677	-1.225482
	H	-1.363971	-4.504269	-0.762477
	H	1.364053	-4.504097	-0.762679
	H	3.828032	-3.949869	-1.225008
gTS1-5	C	3.107867	-0.909925	0.178933
	C	2.753505	0.477401	0.332492
	C	1.465943	0.825720	0.859238
	C	0.680215	-0.196383	1.371175
	C	1.036443	-1.572601	1.215877
	C	2.179079	-1.943297	0.547966
	C	-0.712231	-0.109375	1.362521
	C	-1.226732	-1.436154	1.215419
	C	-2.407654	-1.678063	0.555559
	C	-2.607067	-2.991419	-0.009499
	C	-1.529769	-3.897744	-0.058889
	C	-0.215908	-3.534801	0.400852
	C	-0.144988	-2.340732	1.139194
	C	0.821765	2.076353	0.550705
	C	-0.612935	2.173657	0.534809
	C	-1.373046	1.001467	0.843221
	C	-3.211695	-0.545448	0.191189
	C	-2.694459	0.787399	0.337681
	C	2.219937	-3.268544	-0.023175
	C	1.045024	-4.044554	-0.067091
	C	-1.342136	3.303613	0.001070
	C	1.732624	3.017124	0.039402
	C	0.491393	5.087076	-0.036696
	C	-0.729017	4.597230	-0.256761
	H	-1.357464	5.355801	-0.720337
	C	3.023307	2.830337	-0.309030
	C	3.555889	1.481272	-0.261882
	C	4.773725	1.091273	-0.871792
	C	4.256446	-1.273749	-0.551275
	C	5.112472	-0.242314	-1.010026
	H	6.022073	-0.508502	-1.538400
	C	4.429522	-2.670211	-0.895024
	C	3.461296	-3.608431	-0.682392
	C	-3.884291	-3.185161	-0.659166
	C	-4.400851	-0.773167	-0.528377
	C	-4.737448	-2.139232	-0.867879

gTS1-3	C	-3.363825	1.881046	-0.255174
	C	-4.630890	1.636491	-0.850484
	H	-5.185105	2.470483	-1.268503
	C	-5.130533	0.355293	-0.981608
	C	-2.680947	3.135244	-0.327854
	H	5.338291	-2.953506	-1.416097
	H	-5.676352	-2.315929	-1.382747
	H	-6.071643	0.200732	-1.499318
	H	-3.217571	3.977587	-0.752741
	H	3.639321	3.641448	-0.683600
	H	5.419659	1.853696	-1.294119
	O	1.395987	5.814579	0.097108
	H	-1.670282	-4.835078	-0.589053
	H	1.073766	-4.990749	-0.599422
	H	3.603730	-4.619626	-1.049038
	H	-4.146503	-4.173129	-1.022848
gTS5-3	C	3.258666	-0.192715	0.205867
	C	2.595045	1.074557	0.366580
	C	1.298253	1.115750	0.963951
	C	0.756235	-0.060911	1.482955
	C	1.408700	-1.319717	1.292133
	C	2.596817	-1.411208	0.598576
	C	-0.625979	-0.291732	1.483188
	C	-0.833328	-1.695019	1.294935
	C	-1.927654	-2.172742	0.605775
	C	-1.825024	-3.487818	0.016815
	C	-0.576330	-4.136209	-0.031578
	C	0.620662	-3.499396	0.443284
	C	0.426066	-2.333486	1.203874
	C	0.398972	2.162403	0.629954
	C	-1.002016	1.916002	0.610784
	C	-1.516178	0.641213	0.947242
	C	-2.950602	-1.238235	0.210333
	C	-2.729652	0.175720	0.358060
	C	2.927654	-2.688406	0.008810
	C	1.959515	-3.709089	-0.035255
	C	-1.806382	2.835597	-0.118248
	C	0.883522	3.299552	-0.043692
	C	-1.418060	5.261490	0.030719
	C	-1.043442	4.080484	-0.550092
	H	-0.869002	4.190378	-1.619038
	C	2.179407	3.374824	-0.465278
	C	3.059135	2.223458	-0.327993
	C	4.306805	2.120498	-0.994674
	C	4.424336	-0.284090	-0.580046
	C	4.971621	0.912830	-1.105383
	H	5.892999	0.862976	-1.676560
	C	4.913472	-1.602135	-0.925280
	C	4.198130	-2.737438	-0.680466
	C	-3.012856	-3.949162	-0.666701
	C	-4.026663	-1.704865	-0.569675
	C	-4.062085	-3.111150	-0.909279
	C	-3.541998	1.108568	-0.338271
	C	-4.695768	0.606050	-0.994982
	H	-5.364659	1.302498	-1.490017
	C	-4.935184	-0.751470	-1.095453
	C	-3.070160	2.463650	-0.514178
	H	5.845486	-1.668988	-1.477265
	H	-4.923409	-3.480593	-1.456305
	H	-5.793853	-1.099807	-1.660004
	H	-3.685214	3.148751	-1.088357
	H	2.561698	4.241740	-0.997444
	H	4.712234	2.997848	-1.488294
	O	-1.385533	6.235076	0.669562
	H	-3.044269	-4.969442	-1.034665
	H	-0.503250	-5.071363	-0.578914
	H	2.194812	-4.617199	-0.582514
	H	4.558778	-3.691329	-1.050971
gTS1-3	C	2.829790	-1.367018	0.191380
	C	2.707443	0.047329	0.380247
	C	1.556637	0.566257	1.055578
	C	0.596651	-0.317676	1.563539
	C	0.708364	-1.723595	1.325898
	C	1.761541	-2.247471	0.602510
	C	-0.774448	0.004662	1.575366
	C	-1.508247	-1.201340	1.344216

C	-2.695584	-1.197308	0.636126
C	-3.109675	-2.439267	0.024265
C	-2.215641	-3.524459	-0.032349
C	-0.867092	-3.410185	0.445126
C	-0.592957	-2.275126	1.227601
C	1.113344	1.863607	0.757619
C	-0.252659	2.171775	0.729541
C	-1.233996	1.216996	1.054127
C	-3.257561	0.067643	0.228502
C	-2.497600	1.277086	0.396265
C	1.568330	-3.542530	-0.011148
C	0.282628	-4.112539	-0.051292
C	-0.520798	3.285734	-0.111752
C	1.902467	2.794201	-0.010341
C	1.709920	4.500027	0.403409
C	0.801545	3.899969	-0.551454
H	0.851628	4.280601	-1.575077
C	3.114826	2.319815	-0.555838
C	3.515997	0.955519	-0.376167
C	4.613809	0.391519	-1.087686
C	3.847351	-1.885105	-0.642794
C	4.780552	-0.974176	-1.199600
H	5.596736	-1.361526	-1.800723
C	3.793594	-3.281445	-1.000149
C	2.706724	-4.063898	-0.731969
C	-4.370954	-2.392633	-0.681437
C	-4.401585	0.066511	-0.595069
C	-4.992438	-1.207146	-0.942455
C	-2.808081	2.440478	-0.364777
C	-4.038942	2.435602	-1.070921
H	-4.337387	3.326850	-1.613206
C	-4.817610	1.296378	-1.162363
C	-1.796710	3.460314	-0.587733
H	4.613067	-3.689896	-1.582618
H	-5.915396	-1.202062	-1.513131
H	-5.721679	1.318441	-1.762055
H	-2.039066	4.270352	-1.267646
H	3.732334	2.965035	-1.170762
H	5.291414	1.055188	-1.614502
O	2.433695	5.434558	0.529869
H	-4.796146	-3.317437	-1.057211
H	-2.510528	-4.404732	-0.595801
H	0.145512	-5.029848	-0.616141
H	2.666334	-5.078456	-1.114217
gTS3-4			
C	3.124501	-0.665077	0.194852
C	2.668343	0.691751	0.318402
C	1.434322	0.952011	0.985763
C	0.704174	-0.105034	1.545697
C	1.138928	-1.455722	1.360657
C	2.288713	-1.750729	0.652498
C	-0.704176	-0.105034	1.545696
C	-1.138929	-1.455722	1.360656
C	-2.288713	-1.750729	0.652496
C	-2.401366	-3.077762	0.089991
C	-1.282546	-3.930075	0.076745
C	0.000000	-3.491877	0.549449
C	-0.000001	-2.295076	1.286250
C	0.703410	2.092077	0.624383
C	-0.703411	2.092077	0.624382
C	-1.434323	0.952011	0.985761
C	-3.124501	-0.665077	0.194849
C	-2.668343	0.691751	0.318398
C	2.401366	-3.077762	0.089994
C	1.282546	-3.930075	0.076747
C	-1.188301	3.077505	-0.286616
C	1.188301	3.077505	-0.286615
C	0.000000	5.422379	0.417786
C	0.000000	3.897948	-0.699087
H	0.000001	4.365067	-1.675865
C	2.474729	2.935004	-0.765742
C	3.224530	1.722375	-0.497863
C	4.412957	1.404008	-1.206798
C	4.226963	-0.962795	-0.632478
C	4.908829	0.114484	-1.251523
H	5.786156	-0.096651	-1.854066
C	4.504903	-2.350253	-0.930436

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C   3.631340   -3.350231   -0.619733
C  -3.631340   -3.350231   -0.619737
C  -4.226963   -0.962795   -0.632483
C  -4.504902   -2.350253   -0.930441
C  -3.224529    1.722376   -0.497867
C  -4.412955    1.404008   -1.206803
H  -4.900075    2.179488   -1.789026
C  -4.908828    0.114484   -1.251529
C  -2.474728    2.935004   -0.765745
H   5.397292   -2.579388   -1.503744
H  -5.397290   -2.579388   -1.503751
H  -5.786154   -0.096651   -1.854073
H  -2.892550    3.636862   -1.480435
H   2.892552    3.636862   -1.480432
H   4.900077    2.179488   -1.789020
O  -0.000001    5.316400    1.566266
H  -3.827993   -4.361915   -0.958921
H  -1.363182   -4.875879   -0.450815
H   1.363182   -4.875879   -0.450813
H   3.827994   -4.361915   -0.958916
```

Table S3. Rate coefficients (units: s-1) of product formation from oxyradical a.

T(K)	Reaction	P(atm)						k_∞
		0.1		1		10		
		Eigenvalue	1/e time	Eigenvalue	1/e time	Eigenvalue	1/e time	
1500	Ra1	1.80E+03	1.80E+03	4.40E+03	4.40E+03	7.00E+03	7.00E+03	8.80E+03
	Ra2	6.10E+02	6.10E+02	1.40E+03	1.40E+03	2.10E+03	2.10E+03	2.60E+03
	Ra3	4.70E+02	4.80E+02	7.60E+02	7.60E+02	9.40E+02	9.40E+02	1.00E+03
	Ra4	2.40E+03	2.40E+03	3.90E+03	3.90E+03	4.80E+03	4.80E+03	4.90E+03
	Total	5.30E+03	5.30E+03	1.00E+04	1.00E+04	1.50E+04	1.50E+04	1.70E+04
1600	Ra1	6.10E+03	6.20E+03	2.00E+04	2.00E+04	4.20E+04	4.20E+04	6.80E+04
	Ra2	2.00E+03	2.10E+03	6.20E+03	6.20E+03	1.20E+04	1.20E+04	1.90E+04
	Ra3	1.30E+03	1.40E+03	2.70E+03	2.70E+03	4.10E+03	4.10E+03	5.10E+03
	Ra4	6.80E+03	6.90E+03	1.40E+04	1.40E+04	2.10E+04	2.10E+04	2.90E+04
	Total	1.60E+04	1.70E+04	4.30E+04	4.30E+04	7.90E+04	7.90E+04	1.20E+05
1700	Ra1	1.50E+04	1.60E+04	6.20E+04	6.30E+04	1.70E+05	1.70E+05	4.20E+05
	Ra2	4.80E+03	5.20E+03	1.90E+04	1.90E+04	4.90E+04	4.90E+04	1.10E+05
	Ra3	2.80E+03	3.00E+03	7.10E+03	7.30E+03	1.30E+04	1.30E+04	2.10E+04
	Ra4	1.40E+04	1.60E+04	3.60E+04	3.70E+04	6.60E+04	6.70E+04	1.10E+05
	Total	3.70E+04	4.00E+04	1.20E+05	1.30E+05	3.00E+05	3.00E+05	6.60E+05
1800	Ra1	2.90E+04	3.60E+04	1.40E+05	1.50E+05	5.10E+05	5.20E+05	2.10E+06
	Ra2	9.20E+03	1.20E+04	4.30E+04	4.60E+04	1.40E+05	1.40E+05	5.40E+05
	Ra3	4.70E+03	5.90E+03	1.40E+04	1.50E+04	3.30E+04	3.40E+04	7.50E+04
	Ra4	2.40E+04	3.00E+04	7.20E+04	7.80E+04	1.60E+05	1.70E+05	3.90E+05
	Total	6.60E+04	8.40E+04	2.70E+05	2.90E+05	8.50E+05	8.60E+05	3.10E+06
1900	Ra1	4.90E+04	8.20E+04	2.70E+05	3.30E+05	1.20E+06	1.20E+06	8.60E+06
	Ra2	1.50E+04	2.50E+04	7.90E+04	9.60E+04	3.20E+05	3.40E+05	2.20E+06
	Ra3	6.70E+03	1.10E+04	2.40E+04	2.90E+04	6.60E+04	6.90E+04	2.30E+05
	Ra4	3.40E+04	5.70E+04	1.20E+05	1.40E+05	3.20E+05	3.40E+05	1.20E+06
	Total	1.00E+05	1.80E+05	4.90E+05	6.00E+05	1.90E+06	2.00E+06	1.20E+07
2000	Ra1	7.50E+04	2.10E+05	4.40E+05	6.70E+05	2.20E+06	2.50E+06	3.10E+07
	Ra2	2.30E+04	6.30E+04	1.30E+05	1.90E+05	5.90E+05	6.70E+05	7.50E+06

T(K)	Reaction							
	Ra3	8.50E+03	2.40E+04	3.40E+04	5.20E+04	1.10E+05	1.30E+05	6.60E+05
	Ra4	4.30E+04	1.20E+05	1.70E+05	2.60E+05	5.40E+05	6.10E+05	3.20E+06
	Total	1.50E+05	4.20E+05	7.80E+05	1.20E+06	3.40E+06	3.90E+06	4.20E+07
	Ra1	1.10E+05	6.70E+05	6.60E+05	1.50E+06	3.50E+06	4.70E+06	9.70E+07
	Ra2	3.10E+04	1.90E+05	1.90E+05	4.20E+05	9.40E+05	1.30E+06	2.30E+07
2100	Ra3	9.70E+03	6.10E+04	4.40E+04	9.80E+04	1.60E+05	2.20E+05	1.70E+06
	Ra4	4.90E+04	3.00E+05	2.20E+05	4.80E+05	7.70E+05	1.00E+06	7.70E+06
	Total	2.00E+05	1.20E+06	1.10E+06	2.50E+06	5.40E+06	7.30E+06	1.30E+08
	Ra1	1.40E+05	2.60E+06	9.20E+05	3.80E+06	5.20E+06	9.30E+06	2.70E+08
	Ra2	4.10E+04	7.20E+05	2.50E+05	1.10E+06	1.40E+06	2.50E+06	6.30E+07
2200	Ra3	1.00E+04	1.80E+05	5.10E+04	2.10E+05	2.10E+05	3.80E+05	3.90E+06
	Ra4	5.10E+04	9.10E+05	2.50E+05	1.00E+06	1.00E+06	1.80E+06	1.70E+07
	Total	2.50E+05	4.40E+06	1.50E+06	6.10E+06	7.80E+06	1.40E+07	3.50E+08
	Ra1	1.90E+05	1.00E+07	1.20E+06	1.20E+07	7.20E+06	2.00E+07	6.70E+08
	Ra2	5.00E+04	2.70E+06	3.20E+05	3.10E+06	1.90E+06	5.20E+06	1.50E+08
2300	Ra3	1.00E+04	5.60E+05	5.60E+04	5.40E+05	2.50E+05	7.10E+05	8.40E+06
	Ra4	5.10E+04	2.80E+06	2.70E+05	2.60E+06	1.20E+06	3.30E+06	3.60E+07
	Total	3.00E+05	1.60E+07	1.90E+06	1.80E+07	1.10E+07	2.90E+07	8.60E+08
	Ra1	2.30E+05	3.60E+07	1.50E+06	3.80E+07	9.30E+06	4.90E+07	1.50E+09
	Ra2	6.00E+04	9.50E+06	4.00E+05	1.00E+07	2.40E+06	1.20E+07	3.40E+08
2400	Ra3	1.00E+04	1.60E+06	5.80E+04	1.50E+06	2.90E+05	1.50E+06	1.70E+07
	Ra4	4.80E+04	7.60E+06	2.70E+05	6.90E+06	1.30E+06	6.90E+06	7.00E+07
	Total	3.50E+05	5.50E+07	2.30E+06	5.70E+07	1.30E+07	7.00E+07	1.90E+09
	Ra1	2.70E+05	1.20E+08	1.90E+06	1.20E+08	1.20E+07	1.30E+08	3.10E+09
	Ra2	7.00E+04	3.00E+07	4.70E+05	3.00E+07	2.90E+06	3.30E+07	6.90E+08
2500	Ra3	9.40E+03	4.00E+06	5.70E+04	3.70E+06	3.10E+05	3.50E+06	3.10E+07
	Ra4	4.40E+04	1.90E+07	2.70E+05	1.70E+07	1.40E+06	1.60E+07	1.30E+08
	Total	4.00E+05	1.70E+08	2.60E+06	1.70E+08	1.60E+07	1.80E+08	3.90E+09

Table S4. Rate coefficients (units: s-1) of product formation from oxyradical b.

T(K)	Reaction	P(atm)						
		0.1		1		10		
		Eigenvalue	1/e time	Eigenvalue	1/e time	Eigenvalue	1/e time	k_∞
	Rb1	1.8E+03	1.8E+03	2.4E+03	2.4E+03	2.6E+03	2.6E+03	2.7E+03
1500	Rb2	1.5E+03	1.5E+03	2.0E+03	2.0E+03	2.2E+03	2.2E+03	2.3E+03
	Total	3.3E+03	3.3E+03	4.5E+03	4.5E+03	4.8E+03	4.8E+03	4.9E+03
	Rb1	5.7E+03	5.8E+03	9.9E+03	9.9E+03	1.2E+04	1.2E+04	1.2E+04
1600	Rb2	4.7E+03	4.8E+03	7.9E+03	7.9E+03	9.2E+03	9.2E+03	9.8E+03
	Total	1.0E+04	1.1E+04	1.8E+04	1.8E+04	2.1E+04	2.1E+04	2.2E+04
	Rb1	1.4E+04	1.4E+04	3.1E+04	3.1E+04	4.3E+04	4.3E+04	4.7E+04
1700	Rb2	1.1E+04	1.2E+04	2.3E+04	2.3E+04	3.2E+04	3.2E+04	3.5E+04
	Total	2.5E+04	2.6E+04	5.4E+04	5.4E+04	7.4E+04	7.4E+04	8.2E+04
	Rb1	2.6E+04	3.0E+04	7.4E+04	7.6E+04	1.3E+05	1.3E+05	1.5E+05
1800	Rb2	2.1E+04	2.4E+04	5.5E+04	5.6E+04	8.9E+04	8.9E+04	1.1E+05
	Total	4.7E+04	5.4E+04	1.3E+05	1.3E+05	2.2E+05	2.2E+05	2.6E+05

1900	Rb1	4.4E+04	5.9E+04	1.5E+05	1.6E+05	3.1E+05	3.2E+05	4.4E+05
	Rb2	3.4E+04	4.5E+04	1.1E+05	1.1E+05	2.1E+05	2.1E+05	2.9E+05
	Total	7.7E+04	1.0E+05	2.5E+05	2.7E+05	5.2E+05	5.3E+05	7.3E+05
2000	Rb1	6.5E+04	1.2E+05	2.5E+05	2.9E+05	6.6E+05	6.7E+05	1.1E+06
	Rb2	4.8E+04	8.8E+04	1.8E+05	2.0E+05	4.2E+05	4.3E+05	7.0E+05
	Total	1.1E+05	2.1E+05	4.3E+05	5.0E+05	1.1E+06	1.1E+06	1.9E+06
2100	Rb1	8.9E+04	2.6E+05	3.9E+05	5.3E+05	1.2E+06	1.3E+06	2.7E+06
	Rb2	6.4E+04	1.8E+05	2.6E+05	3.6E+05	7.3E+05	7.8E+05	1.6E+06
	Total	1.5E+05	4.4E+05	6.5E+05	8.9E+05	1.9E+06	2.0E+06	4.3E+06
2200	Rb1	1.2E+05	6.0E+05	5.5E+05	9.8E+05	1.9E+06	2.2E+06	5.9E+06
	Rb2	8.0E+04	4.1E+05	3.6E+05	6.3E+05	1.2E+06	1.3E+06	3.2E+06
	Total	2.0E+05	1.0E+06	9.1E+05	1.6E+06	3.1E+06	3.5E+06	9.1E+06
2300	Rb1	1.5E+05	1.5E+06	7.3E+05	1.9E+06	2.9E+06	3.6E+06	1.2E+07
	Rb2	9.5E+04	9.4E+05	4.6E+05	1.2E+06	1.7E+06	2.1E+06	6.1E+06
	Total	2.4E+05	2.4E+06	1.2E+06	3.1E+06	4.5E+06	5.7E+06	1.8E+07
2400	Rb1	1.8E+05	3.3E+06	9.3E+05	3.8E+06	4.0E+06	6.1E+06	2.3E+07
	Rb2	1.1E+05	2.1E+06	5.6E+05	2.3E+06	2.2E+06	3.4E+06	1.1E+07
	Total	2.9E+05	5.4E+06	1.5E+06	6.1E+06	6.2E+06	9.4E+06	3.4E+07
2500	Rb1	2.1E+05	7.2E+06	1.2E+06	7.7E+06	5.2E+06	1.0E+07	4.1E+07
	Rb2	1.2E+05	4.2E+06	6.5E+05	4.3E+06	2.8E+06	5.5E+06	1.8E+07
	Total	3.3E+05	1.1E+07	1.8E+06	1.2E+07	8.0E+06	1.6E+07	5.9E+07

Table S5. Rate coefficients (units: s-1) of product formation from oxyradical c.

	P(atm)						
	0.1		1		10		
T(K)	Eigenvalue	1/e time	Eigenvalue	1/e time	Eigenvalue	1/e time	k_∞
1500	7.4E+02	7.4E+02	9.0E+02	9.0E+02	9.4E+02	9.4E+02	9.6E+02
1600	3.1E+03	3.1E+03	4.6E+03	4.6E+03	5.2E+03	5.2E+03	5.4E+03
1700	9.3E+03	9.4E+03	1.8E+04	1.8E+04	2.3E+04	2.3E+04	2.5E+04
1800	2.1E+04	2.2E+04	5.2E+04	5.3E+04	8.2E+04	8.2E+04	9.6E+04
1900	4.0E+04	4.5E+04	1.2E+05	1.2E+05	2.4E+05	2.4E+05	3.2E+05
2000	6.4E+04	8.7E+04	2.3E+05	2.5E+05	5.6E+05	5.6E+05	9.6E+05
2100	9.4E+04	1.7E+05	3.9E+05	4.6E+05	1.1E+06	1.2E+06	2.6E+06
2200	1.3E+05	3.6E+05	5.8E+05	8.2E+05	2.0E+06	2.1E+06	6.3E+06
2300	1.6E+05	8.6E+05	8.0E+05	1.5E+06	3.1E+06	3.6E+06	1.4E+07
2400	2.0E+05	2.2E+06	1.0E+06	2.9E+06	4.4E+06	6.0E+06	3.0E+07
2500	2.4E+05	5.3E+06	1.3E+06	6.1E+06	5.9E+06	1.0E+07	5.9E+07

Table S6. Rate coefficients (units: s-1) of product formation from oxyradical d.

T(K)	P(atm) 0.1 Eigenvalue	0.1 1/e time	1 Eigenvalue	1 1/e time	10 Eigenvalue	10 1/e time	k_∞
1500	5.4E+02	5.4E+02	6.3E+02	6.3E+02	6.5E+02	6.5E+02	6.6E+02
1600	2.3E+03	2.3E+03	3.3E+03	3.3E+03	3.6E+03	3.6E+03	3.7E+03
1700	7.3E+03	7.4E+03	1.3E+04	1.3E+04	1.6E+04	1.6E+04	1.7E+04
1800	1.7E+04	1.8E+04	4.0E+04	4.0E+04	5.8E+04	5.8E+04	6.5E+04
1900	3.4E+04	3.7E+04	9.5E+04	9.7E+04	1.7E+05	1.7E+05	2.2E+05
2000	5.6E+04	7.1E+04	1.9E+05	2.0E+05	4.2E+05	4.2E+05	6.4E+05
2100	8.2E+04	1.4E+05	3.2E+05	3.7E+05	8.7E+05	8.9E+05	1.7E+06
2200	1.1E+05	2.8E+05	4.9E+05	6.5E+05	1.6E+06	1.7E+06	4.2E+06
2300	1.5E+05	6.2E+05	7.0E+05	1.2E+06	2.5E+06	2.9E+06	9.4E+06
2400	1.8E+05	1.5E+06	9.2E+05	2.2E+06	3.7E+06	4.7E+06	2.0E+07
2500	2.2E+05	3.7E+06	1.2E+06	4.4E+06	5.1E+06	7.8E+06	3.9E+07

Table S7. Rate coefficients (units: s-1) of product formation from oxyradical e.

T(K)	P(atm) 0.1 Eigenvalue	0.1 1/e time	1 Eigenvalue	1 1/e time	10 Eigenvalue	10 1/e time	k_∞
1500	9.3E+02	9.3E+02	1.2E+03	1.2E+03	1.2E+03	1.2E+03	1.2E+03
1600	3.7E+03	3.8E+03	5.7E+03	5.7E+03	6.4E+03	6.4E+03	6.6E+03
1700	1.1E+04	1.1E+04	2.1E+04	2.1E+04	2.7E+04	2.7E+04	2.9E+04
1800	2.4E+04	2.5E+04	6.0E+04	6.0E+04	9.4E+04	9.4E+04	1.1E+05
1900	4.4E+04	5.1E+04	1.4E+05	1.4E+05	2.6E+05	2.6E+05	3.6E+05
2000	7.0E+04	9.7E+04	2.5E+05	2.8E+05	6.1E+05	6.2E+05	1.0E+06
2100	1.0E+05	1.9E+05	4.2E+05	5.0E+05	1.2E+06	1.3E+06	2.7E+06
2200	1.4E+05	4.2E+05	6.2E+05	8.9E+05	2.1E+06	2.3E+06	6.4E+06
2300	1.7E+05	1.0E+06	8.5E+05	1.7E+06	3.2E+06	3.8E+06	1.4E+07
2400	2.1E+05	2.5E+06	1.1E+06	3.2E+06	4.6E+06	6.4E+06	2.9E+07
2500	2.5E+05	6.0E+06	1.4E+06	6.7E+06	6.2E+06	1.1E+07	5.7E+07

Table S8. Rate coefficients (units: s-1) of product formation from oxyradical f.

T(K)	P(atm)						k_∞
	0.1		1		10		
	Eigenvalue	1/e time	Eigenvalue	1/e time	Eigenvalue	1/e time	
1500	9.7E+02	9.7E+02	1.1E+03	1.2E+03	1.2E+03	1.2E+03	1.2E+03
1600	3.9E+03	3.9E+03	5.5E+03	5.6E+03	5.9E+03	6.1E+03	6.3E+03
1700	1.2E+04	1.2E+04	2.1E+04	2.1E+04	2.4E+04	2.6E+04	2.7E+04
1800	2.6E+04	2.7E+04	6.0E+04	6.0E+04	8.2E+04	8.8E+04	1.0E+05
1900	4.7E+04	5.4E+04	1.4E+05	1.4E+05	2.3E+05	2.5E+05	3.2E+05
2000	7.6E+04	1.1E+05	2.6E+05	2.8E+05	5.4E+05	5.9E+05	9.1E+05
2100	1.1E+05	2.1E+05	4.3E+05	5.1E+05	1.1E+06	1.2E+06	2.4E+06
2200	1.5E+05	4.7E+05	6.4E+05	9.3E+05	1.9E+06	2.2E+06	5.6E+06
2300	1.9E+05	1.1E+06	8.8E+05	1.7E+06	3.0E+06	3.8E+06	1.2E+07
2400	2.3E+05	2.8E+06	1.1E+06	3.4E+06	4.3E+06	6.3E+06	2.4E+07
2500	2.7E+05	6.4E+06	1.4E+06	7.0E+06	5.8E+06	1.1E+07	4.6E+07

Table S9. Rate coefficients (units: s-1) of product formation from oxyradical g.

T(K)	P(atm)						k_∞
	0.1		1		10		
	Eigenvalue	1/e time	Eigenvalue	1/e time	Eigenvalue	1/e time	
1500	1.4E+04	1.4E+04	2.0E+04	2.0E+04	2.1E+04	2.1E+04	2.2E+04
1600	3.9E+04	4.2E+04	7.5E+04	7.5E+04	9.2E+04	9.2E+04	9.8E+04
1700	8.2E+04	1.1E+05	2.1E+05	2.1E+05	3.2E+05	3.2E+05	3.7E+05
1800	1.4E+05	2.7E+05	4.5E+05	5.1E+05	8.8E+05	8.9E+05	1.2E+06
1900	2.1E+05	7.6E+05	7.9E+05	1.1E+06	2.0E+06	2.1E+06	3.3E+06
2000	2.9E+05	2.2E+06	1.2E+06	2.6E+06	3.7E+06	4.2E+06	8.5E+06
2100	3.7E+05	5.7E+06	1.7E+06	6.1E+06	6.1E+06	8.4E+06	2.0E+07
2200	4.5E+05	1.4E+07	2.3E+06	1.4E+07	9.0E+06	1.7E+07	4.3E+07
2300	5.4E+05	3.1E+07	2.9E+06	3.1E+07	1.2E+07	3.4E+07	8.6E+07
2400	6.2E+05	6.5E+07	3.5E+06	6.5E+07	1.6E+07	6.7E+07	1.6E+08
2500	7.0E+05	1.3E+08	4.0E+06	1.3E+08	2.0E+07	1.3E+08	2.9E+08
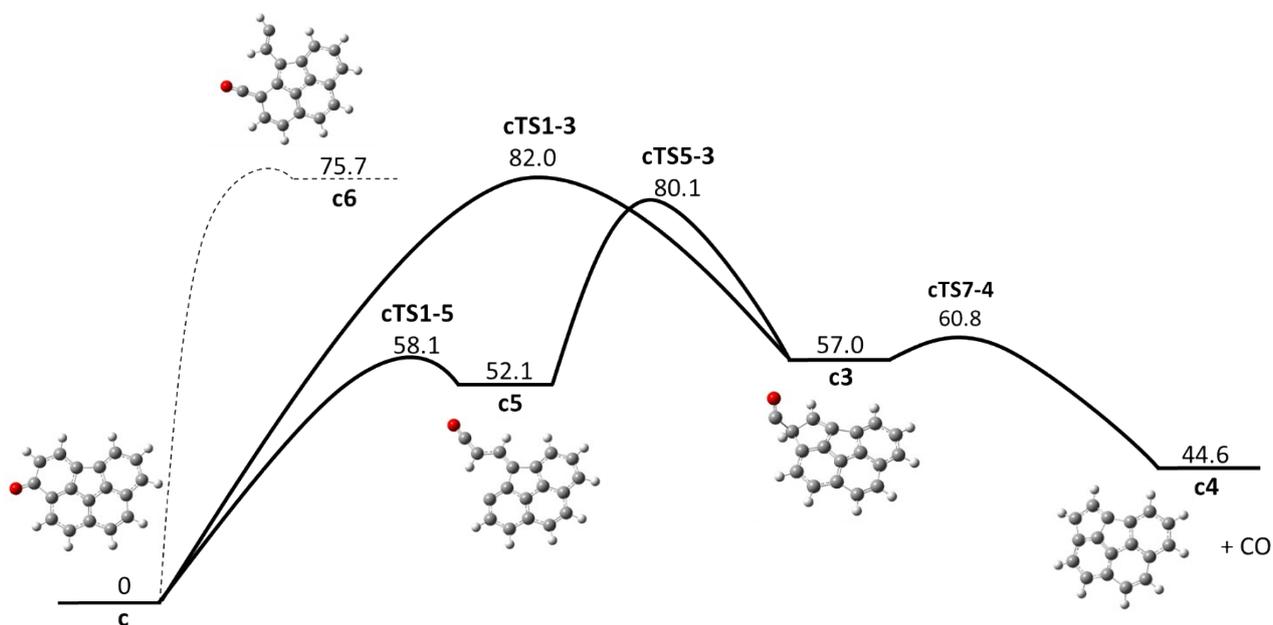
Figure S1 Potential energy surface of oxyradical c calculated at B3LYP/6-311G(d,p) level at 0 K (units: kcal/mol).
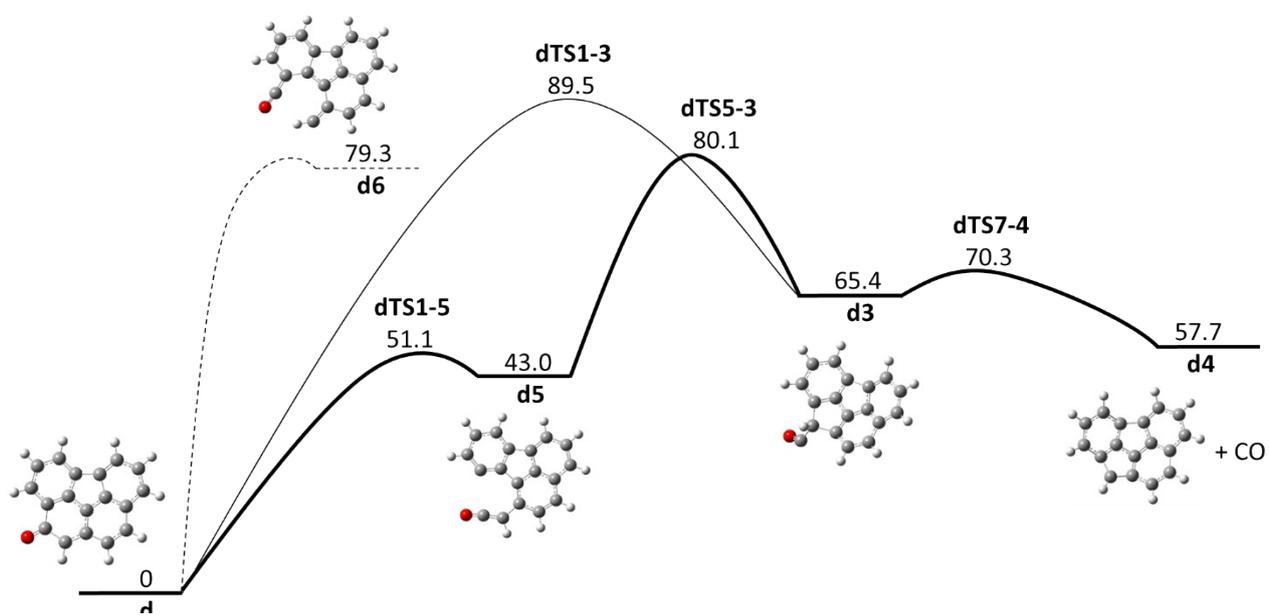
Figure S2 Potential energy surface of oxyradical d calculated at B3LYP/6-311G(d,p) level at 0 K (units: kcal/mol).
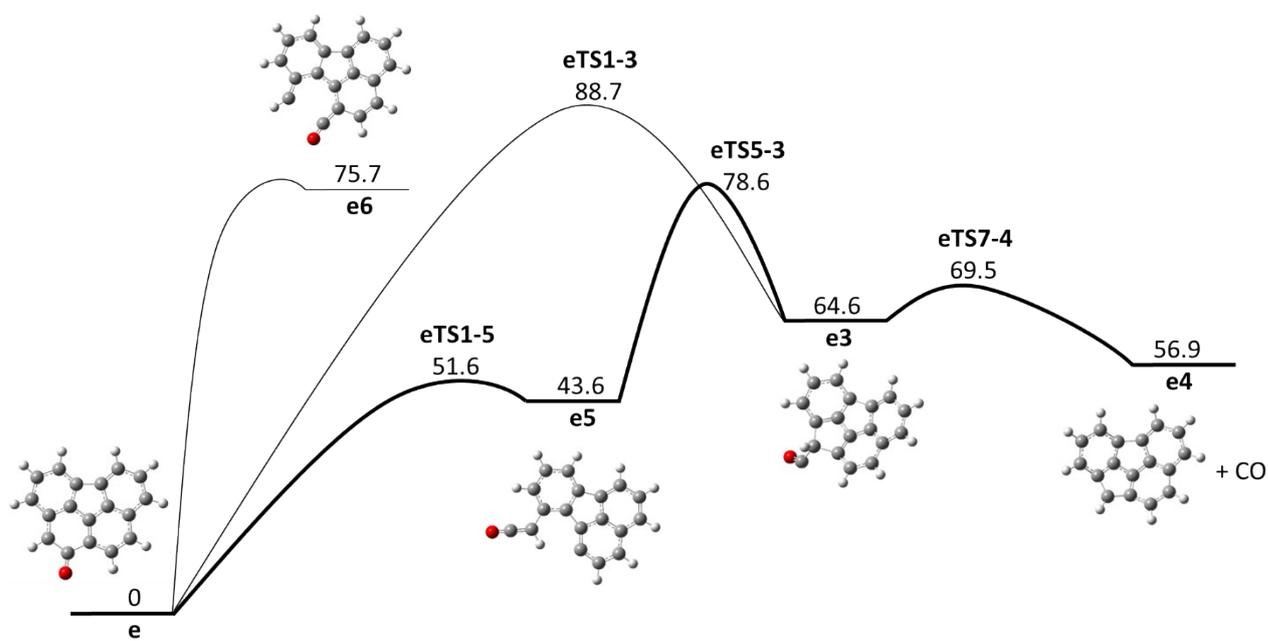
Figure S3 Potential energy surface of oxyradical e calculated at B3LYP/6-311G(d,p) level at 0 K (units: kcal/mol).
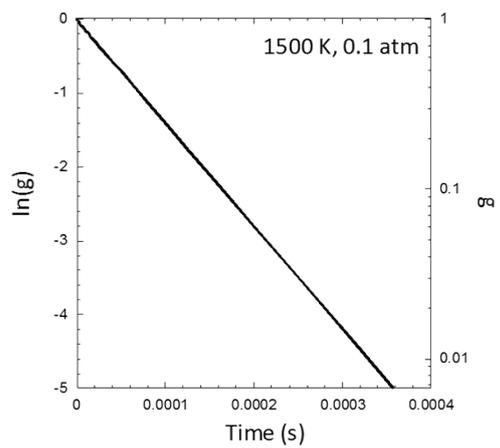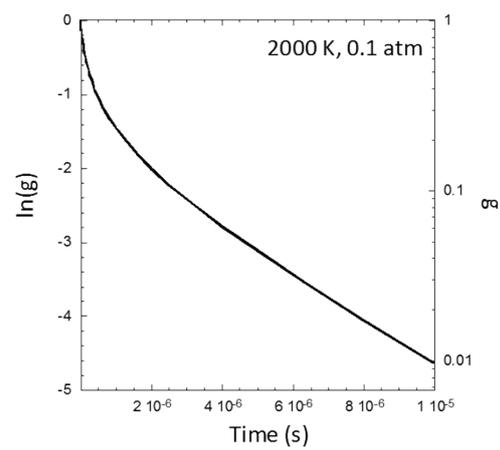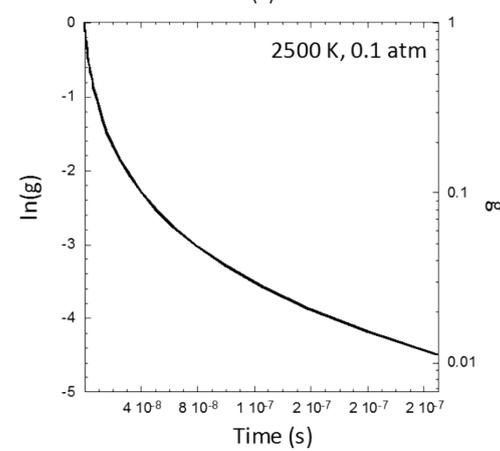
Figure S4 ln (concentration fraction)s as functions of time for oxyradical g at 0.1 atm, (a) 1500 K, (b) 2000 K, (c) 2500 K.

By solving the master equations, we obtain the eigenvalues and the species concentration profiles, from which the effective decomposition rate coefficients of oxyradical g can be determined using three different methods:

a) **Fitting method:** the effective rate constant is the slope from fitting ln[g] vs. time, where [g] is the concentration of the reactant. Fig S5 shows such a fit for [g] over the range 0.95 to 0.05;

b) **Eigenvalue method:** use the modulus of the lowest magnitude eigenvalue as the rate constant;

c) **1/e time method:** use the reciprocal of time at [g] equal to 1/e as the rate constant.
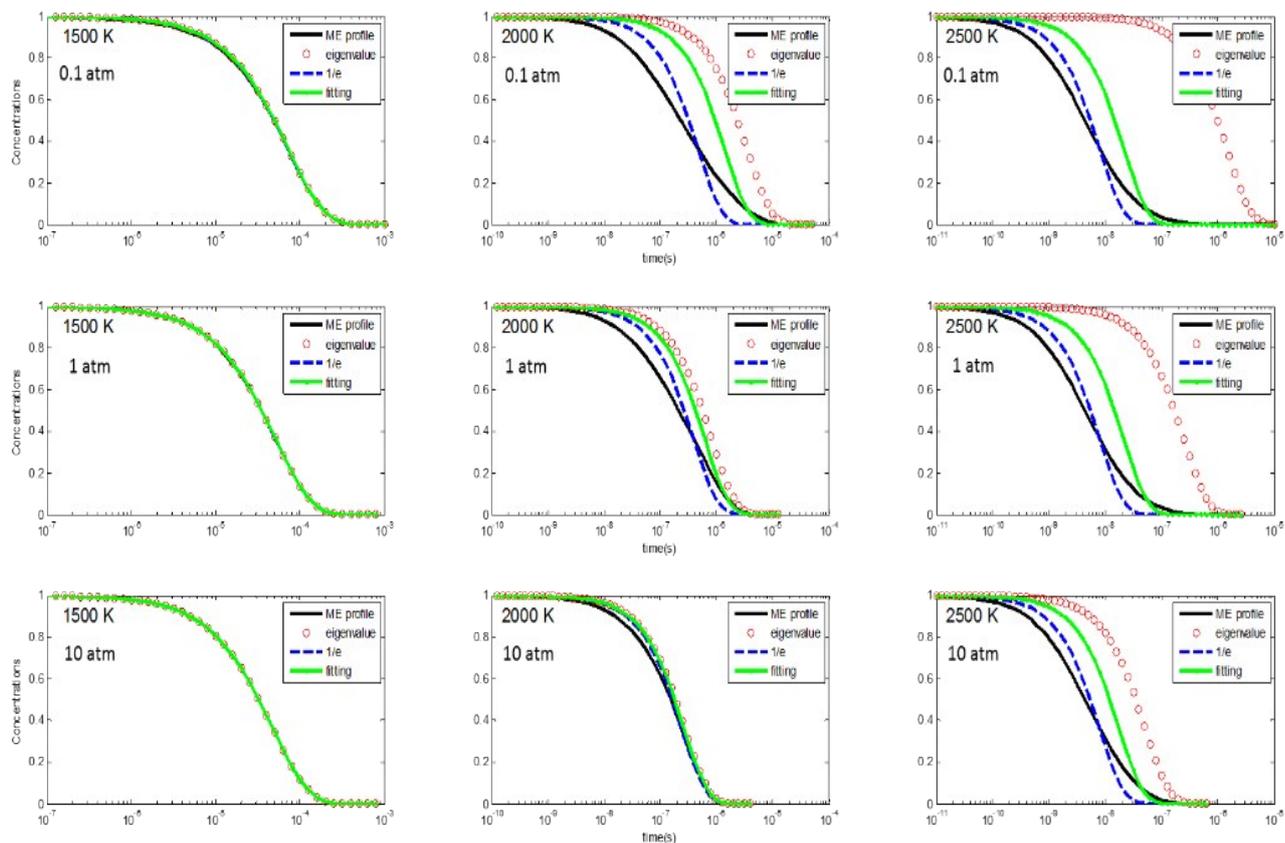
Figure S5 Comparison of concentration profiles of the reactant (oxyradical g) from the master equation modelling with those from the fitting formula e^{-kt}, where k is the effective rate constant derived from three different methods.

Figure S5 shows the comparison of concentration profiles of the reactant (oxyradical g) from the master equation modelling with those from the fitting formula e^{-kt}, using three different k over 1500-2500 K and 0.1-10 atm, where k is the effective rate constant. As can be seen that, at 1500 K, the species profiles from the fitting formulas e^{-kt} are almost identical to those from the master equation modelling, while they differ from each other at 2000 and 2500 K. Among the three methods, the 1/e time method produces concentration profile the closest to the master equation modelling results. The problem of providing a reasonable measure of the rate constant for use in combustion models will be discussed in a future publication.
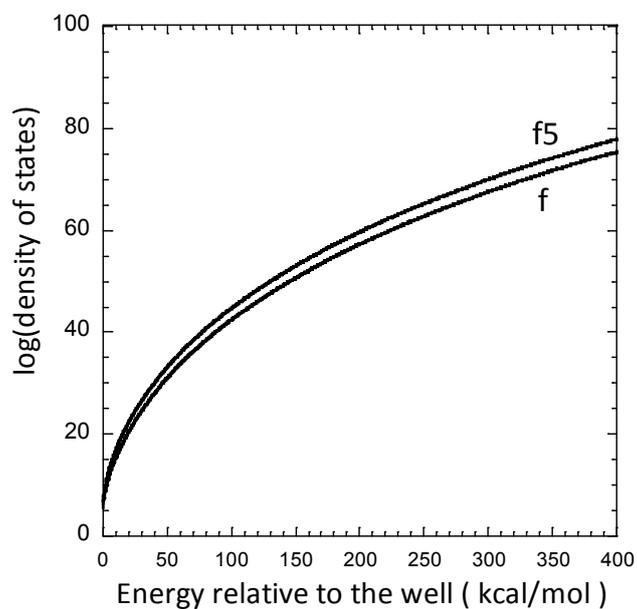
Figure S6 Densities of states as functions of energy, (a) f, (b) f5.
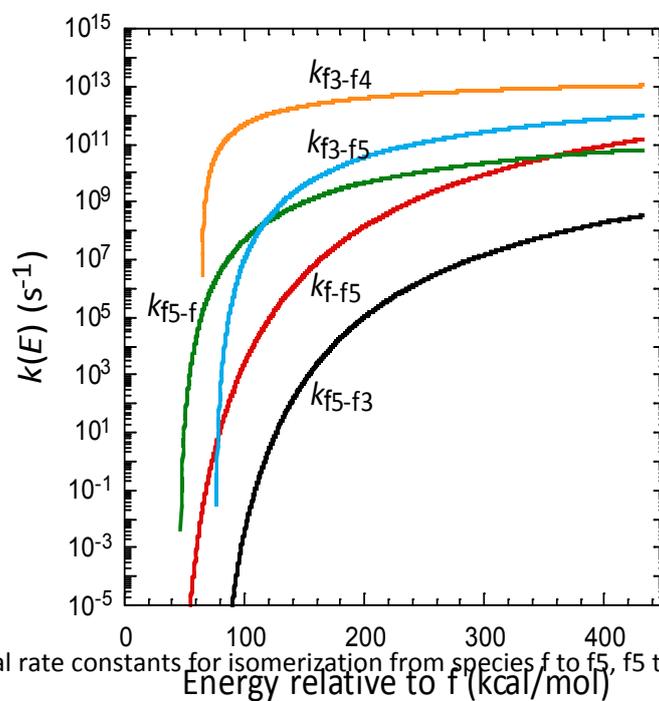
Figure S7 Microcanonical rate constants for isomerization from species f to f5, f5 to f, f5 to f3, and f3-f4.
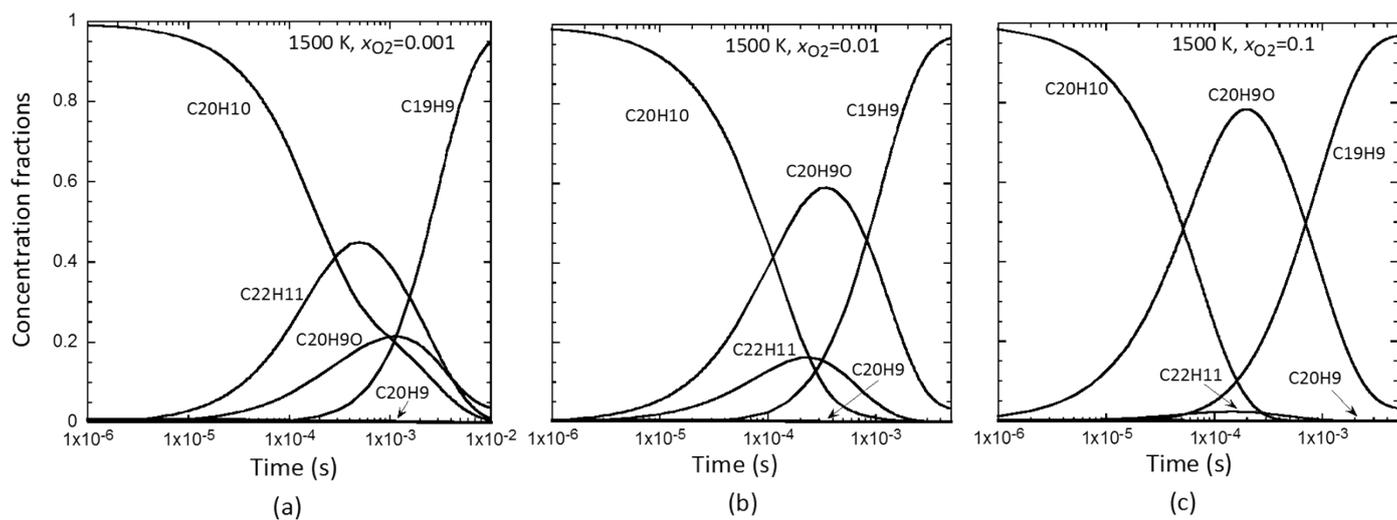
Figure S8 Concentration profiles from the kinetic modelling at 1500 K, (a) x_{O2}=0.001, (b) x_{O2}=0.01, (c) x_{O2}=0.1.
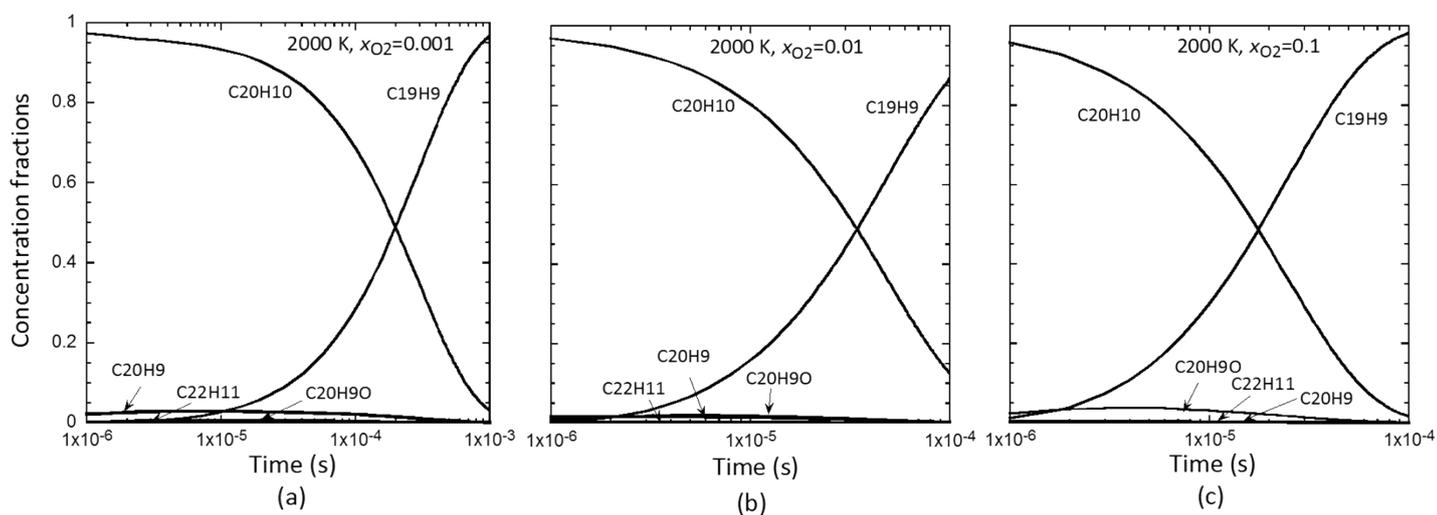

Figure S9 Concentration profiles from the kinetic modelling at 2000 K, (a) x_{O2}=0.001, (b) x_{O2}=0.01, (c) x_{O2}=0.1.
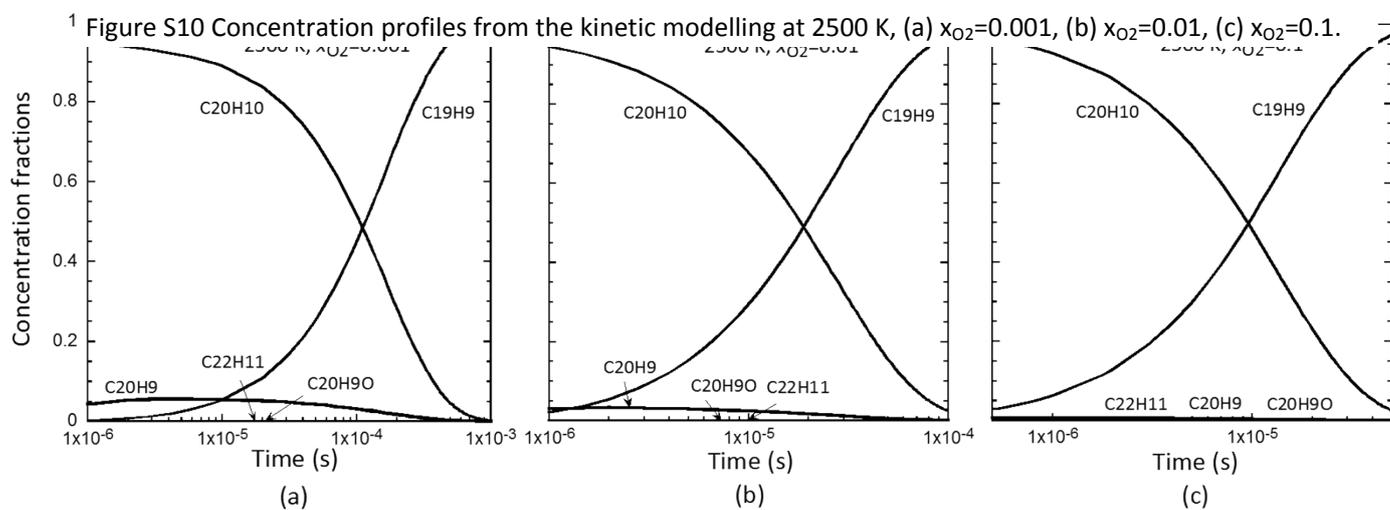
Figure S10 Concentration profiles from the kinetic modelling at 2500 K, (a) x_{O2}=0.001, (b) x_{O2}=0.01, (c) x_{O2}=0.1.
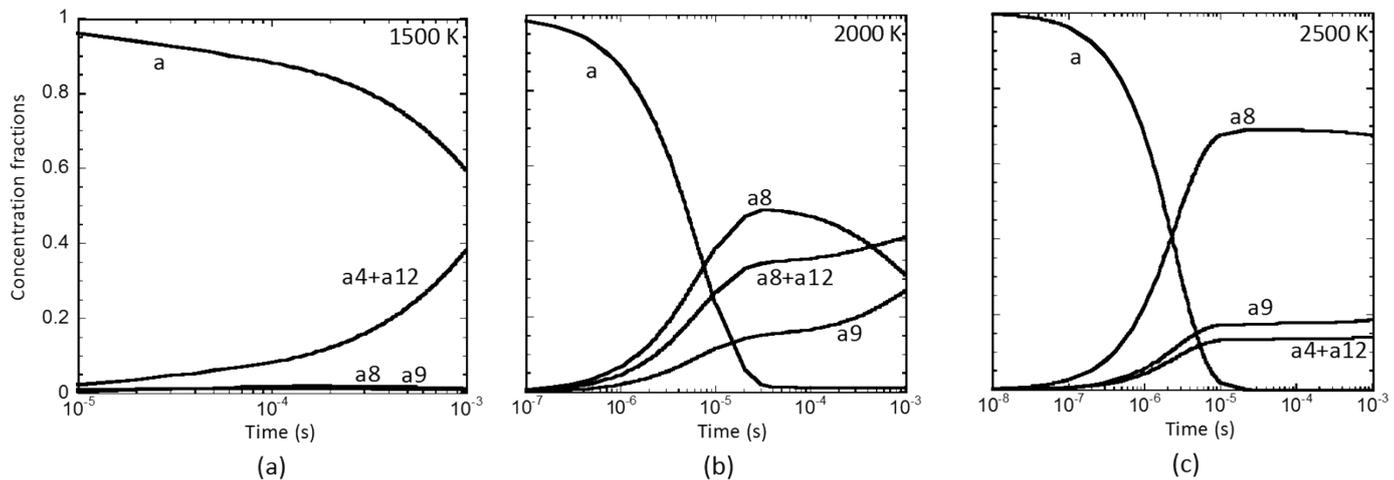
Figure S11 Concentration profiles from the kinetic modelling of oxyradical a at 0.1 atm, (a) 1500 K, (b) 2500 K, (c) 2500 K.
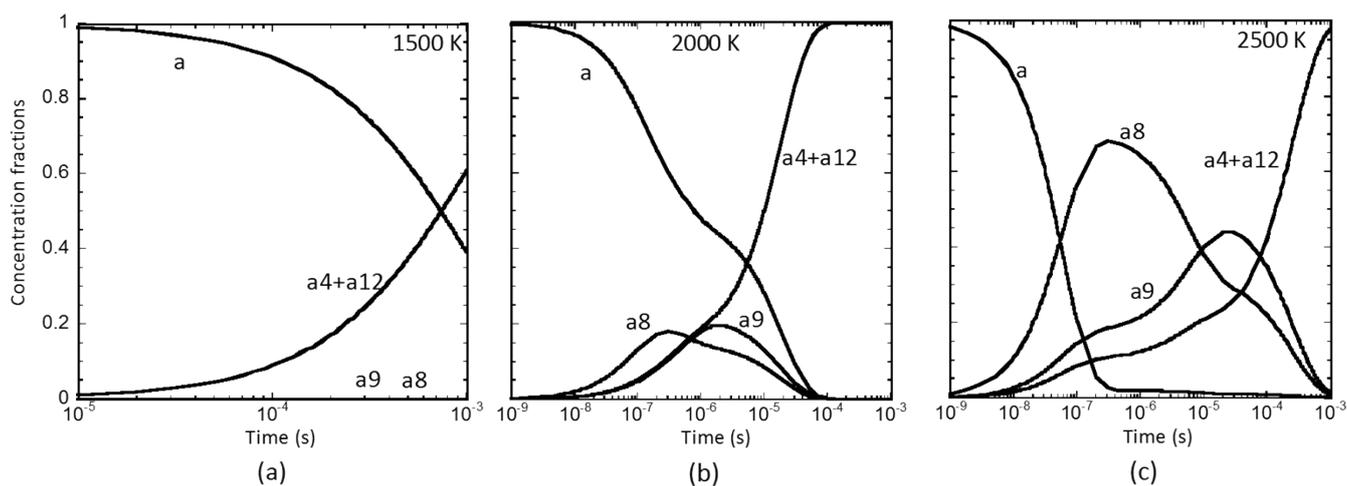

Figure S12 Concentration profiles from the kinetic modelling of oxyradical a at 10 atm, (a) 1500 K, (b) 2500 K, (c) 2500 K.