The Gas-Phase Ozonolysis of b-Caryophyllene ($C_{15}H_{24}$): A Theoretical Study

*** Supporting Information ***

T. L. Nguyen,[a] R. Winterhalter,[b] G. Moortgat,[b] B. Kanawati,[b] J. Peeters,[a] and L. Vereecken[a,*]

a) Department of Chemistry, University of Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium.

b) Max-Planck Institute, Atmospheric Chemistry Division, P.O. Box 3060, D-55020 Mainz, Germany

[*] *Email: Luc.Vereecken@chem.kuleuven.be, Fax: +32-16-327992*

Table of contents:

Figures 1-6 and Table 1 can be found in the main text.

Energetics of a- and b-pinene ozonolysis

Table S1: Calculated ZPE-corrected relative energies (kcal/mol) relative to the primary ozonides for selected structures in the α-pinene + O_3 reaction, at different levels of theory.

Structure	B3LYP[a)]	MPW1B95 [b)]	CBS-QB3	Adapted B3LYP[c)]
α-pinene + O_3	51.3	61.3	61.2	61.2
POZ-1	0.0	0.0	0.0	0.0
POZ-2	1.2	1.3	0.1	1.2
TS1 (POZ-1 → CI-1a)	15.6	21.6	16.7	15.6
TS2 (POZ-2 → CI-1b)	19.2	24.7	20.4	19.2
TS3 (POZ-1 → CI-2a)	16.2	22.1	17.4	16.2
TS4 (POZ-2 → CI-2b)	17.3	23.1	17.9	17.3

a) B3LYP/6-311++G(3df,3pd) // B3LYP/6-311G(d,p)
b) MPW1B95/6-311++G(3df,3pd) // MPW1B95/6-31+G(d,p)
c) B3LYP data with the energy for the singlet open-shell O_3 reactant shifted upwards by 9.9 kcal/mol; this matches the relative energy of the reactants with its CBS-QB3 value of 61.2 kcal/mol (see main text).

Table S2: Calculated ZPE-corrected relative energies (kcal/mol) relative to the initial reactants for selected structures in the β-pinene + O_3 reaction, at different levels of theory.

Structure	B3LYP[a)]	MPW1B95 [b)]	CBS-QB3	Adapted B3LYP[c)]
β-pinene + O_3	48.2	58.5	57.0	57.0
POZ-1	0.2	1.1	0.6	0.2
POZ-2	0.0	0.0	0.0	0.0
TS1 (POZ-1 → HCHO + C_9 CI)	13.5	18.7	14.3	13.5
TS2 (POZ-2 → HCHO + C_9 CI)	12.9	18.0	13.5	12.9
TS3 (POZ-1 → H_2COO + nopinone)	17.9	24.5	19.1	17.9
TS4 (POZ-2 → H_2COO + nopinone)	17.9	24.7	19.1	17.9

a) B3LYP/6-311++G(3df,3pd) // B3LYP/6-311G(d,p)
b) MPW1B95/6-311++G(3df,3pd) // MPW1B95/6-31+G(d,p)
c) B3LYP data with the energy for the singlet open-shell O_3 reactant shifted upwards by 8.8 kcal/mol; this matches the relative energy of the reactants with its CBS-QB3 value of 57.0 kcal/mol (see main text).

Energetics of simplified analogues of b-caryophyllene + O_3 intermediates

Table S3: Relative energies of various structures in the reaction of acetaldehyde carbonyl oxide (CH_3CHOO), at different levels of theory. The transition states correspond to the following CH_3CHOO isomerisation reactions:

syn-CH_3CHOO ↔ TS1 ↔ anti-CH_3CHOO (O-rotation out of the plane of symmetry)
syn-CH_3CHOO ↔ TS2 ↔ anti-CH_3CHOO (O-pseudo-rotation in the plane of symmetry)
syn-CH_3CHOO ↔ TS3 ↔ CH_2CHOOH (1,4-H-shift)
syn-CH_3CHOO ↔ TS4 ↔ dioxirane (ring closure/breaking)
anti-CH_3CHOO ↔ TS5 ↔ dioxirane (ring closure/breaking)

Structure	B3LYP [a]	CIPT2+Q [b]	CCSD(T) [c]	MRCI+Q [d]
Syn-CH_3CHOO	0.0	0.0	0.0	0.0
Anti-CH_3CHOO	3.0	4.1	3.7	2.2
TS1 [e]	29.4	34.3	32.6	30.5; 33.0
TS2	37.0	40.8	41.3	
TS3	15.6	12.6	15.7	21.2
TS4	24.3	23.2	23.3	28.4
TS5	19.7	20.8	19.2	22.8

a) B3LYP/cc-pVTZ
b) CIPT2+Q/cc-pVTZ // B3LYP/cc-pVTZ
c) CCSD(T)/cc-pVTZ // B3LYP/cc-pVTZ
d) From Anglada et al., *J. Am. Chem. Soc.* **1996**, *118*, 4636.
e) Geometry optimized using UB3LYP, to accommodate singlet biradical character of TS1.

Table S4: O–O bond dissociation energy (kcal/mol) in a-unsaturated hydroperoxides: >C=C(OOH)– → $^{\bullet}$OH + >C$^{\bullet}$–C(=O)–. The structures correspond to the hydroperoxide intermediates found in the β-caryophyllene ozonolysis, but with large alkyl substituents replaced by methyl substituents.

Species	B3LYP [a]	MPW1B95 [b]	CBS-QB3
ROOH-1a, $CH_3CH=C(CH_3)OOH$	9.2	13.6	16.7
ROOH-1b, $CH_2=C(CH_3)OOH$	14.0	18.4	20.5
ROOH-2b, trans-$CH_3CH=CHOOH$	10.5	14.5	17.5
ROOH-2b, cis-$CH_3CH=CHOOH$	7.0	10.6	13.7

a) B3LYP/6-311++G(3df,3pd) // B3LYP/6-311G(d,p)
b) MPW1B95/6-311++G(3df,3pd) // MPW1B95/6-31+G(d,p)

Table S5: Calculated barrier height (kcal/mol) for the $CH_3C(O)OCH_3 \rightarrow C_2H_6 + CO_2$ decomposition using B3LYP/cc-pVDZ and CBS-QB3 levels of theory

Structure	B3LYP	CBS-QB3
Ester $CH_3C(O)OCH_3$	0.0	0.0
TS of CO_2-elimination	98.8	96.7

Table S6: Calculated thermal unimolecular rate coefficients at 298 K of the Criegee intermediates for formation of secondary ozonides (SOZ) or via the ester and hydroperoxide (HP) channels.

Species	Rate to SOZ	Rate via ester/HP channels
CI-2a	1.1×10^{4} s^{-1}	5.3 s^{-1}
CI-1b	486 s^{-1}	42 s^{-1}
CI-1a	5.3 s^{-1}	0.57 s^{-1}
CI-2b	7.4 s^{-1}	1.6 s^{-1}

Relative energies of b-caryophyllene + O_3 intermediates and TS

Table S7: Calculated ZPE-corrected relative potential energies (kcal/mol) for various structures in the β-caryophyllene ozonolysis, at different levels of theory.

Structure	B3LYP [a)]	MPW1B95 [b)]	Adapted B3LYP [c)]
O_3 + β-caryophyllene	0.0	0.0	0.0
POZ-1	-55.5	-64.2	-64.2
POZ-2	-54.7	-63.3	-63.4
POZ-3	-48.7	-59.2	-57.4
POZ-4	-47.3	-57.7	-56.0
CI-1a	-87.1		-95.8
CI-2a	-80.7		-89.4
CI-1b	-85.9		-94.6
CI-2b	-83.1		-91.8
Dioxirane-1	-102.4		-111.1
Dioxirane-2	-99.9		-108.6
ROOH-1a	-97.8		-106.5
ROOH-1b	-100.4		-109.1
ROOH-2b	-103.3		-112.0
Rad-1a + OH	-93.9		-102.6
Rad-1b + OH	-84.0		-92.7
Rad-2b + OH	-91.1		-99.8
Acid	-194.5		-203.2
Ester	-182.6		-191.3
SOZ-1	-106.1		-114.8
SOZ-2	-106.8		-115.5
TS1			-1.2
TS2			-0.4
TS3			0.4
TS4			0.6
TS5	-36.9		-45.6
TS6	-37.2		-45.9
TS7	-37.1		-45.8
TS8	-33.0		-41.7
TS9	-68.5		-77.2
TS10	-69.3		-78.0
TS11	-64.4		-73.1
TS12	-64.5		-73.2
TS13	-64.7		-73.4
TS14	-64.8		-73.5
TS15	-59.1		-67.8
TS16	-47.7		-56.4
TS17	-76.4		-85.1
TS18	-53.1		-61.8
TS19	-77.9		-86.6
TS20	-74.8		-83.5
TS21	-75.3		-84.0
TS22	-72.6		-81.3
TS23	-69.8		-78.5

a) B3LYP/6-311++G(3df,3pd) // B3LYP/6-311G(d,p)

b) MPW1B95/6-311++G(3df,3pd) // MPW1B95/6-31+G(d,p)

c) Relative energies based on the B3LYP values[a)], after correcting the energy for O_3 by 8.7 kcal/mol, to bring the addition energies of **POZ-1** and **POZ-2** in line with the MPW1B95 values. (see main text). TS1, TS2, TS3 and TS4 are the B3LYP[a)] energies at the position of the kinetic bottleneck along the barrierless O_3 addition path, at 300K.

Triplet bis(oxy) biradical decomposition

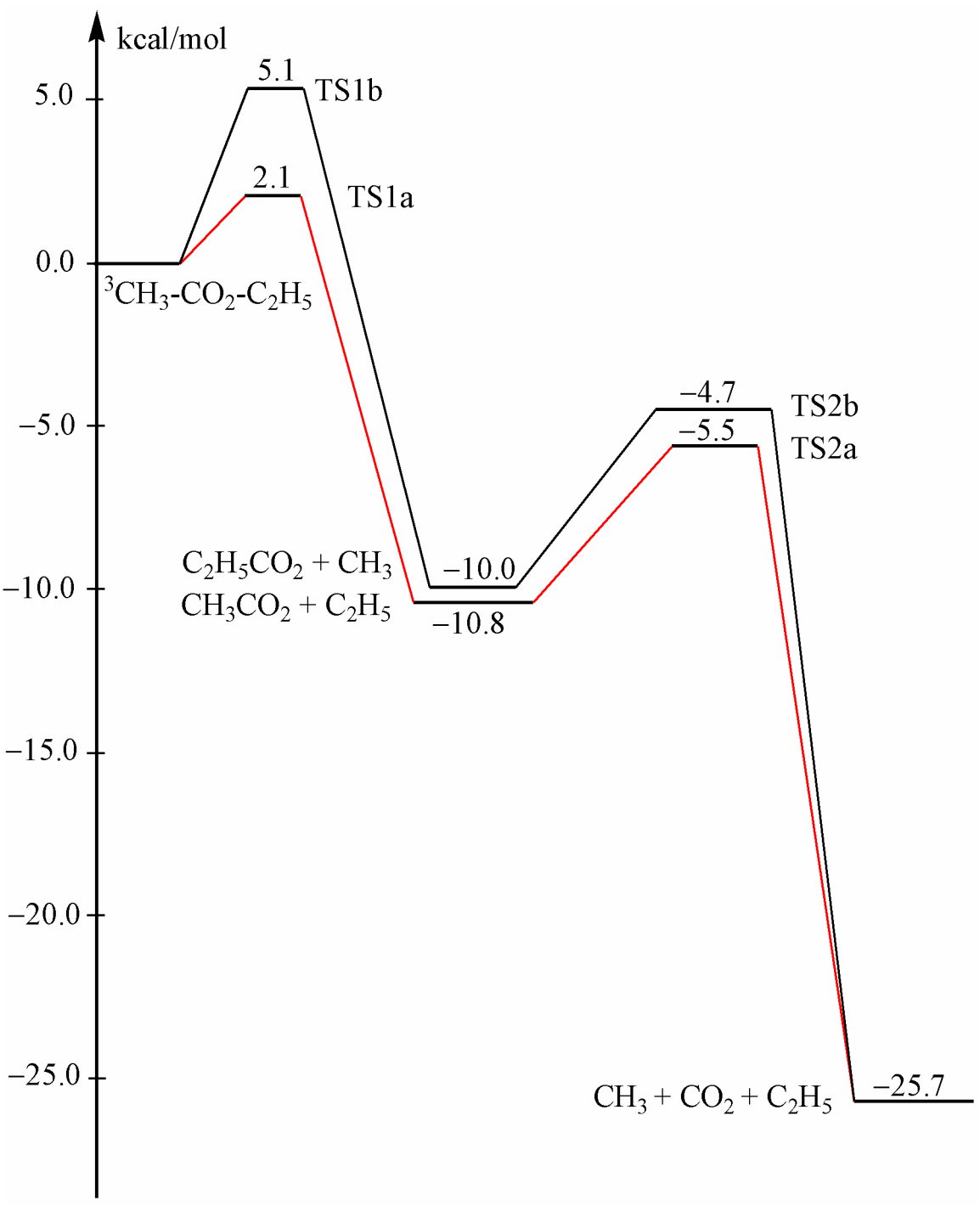


Figure S1: Triplet PES for decomposition of triplet methyl ethyl bis(oxy) computed at the CBS-QB3 level of theory.

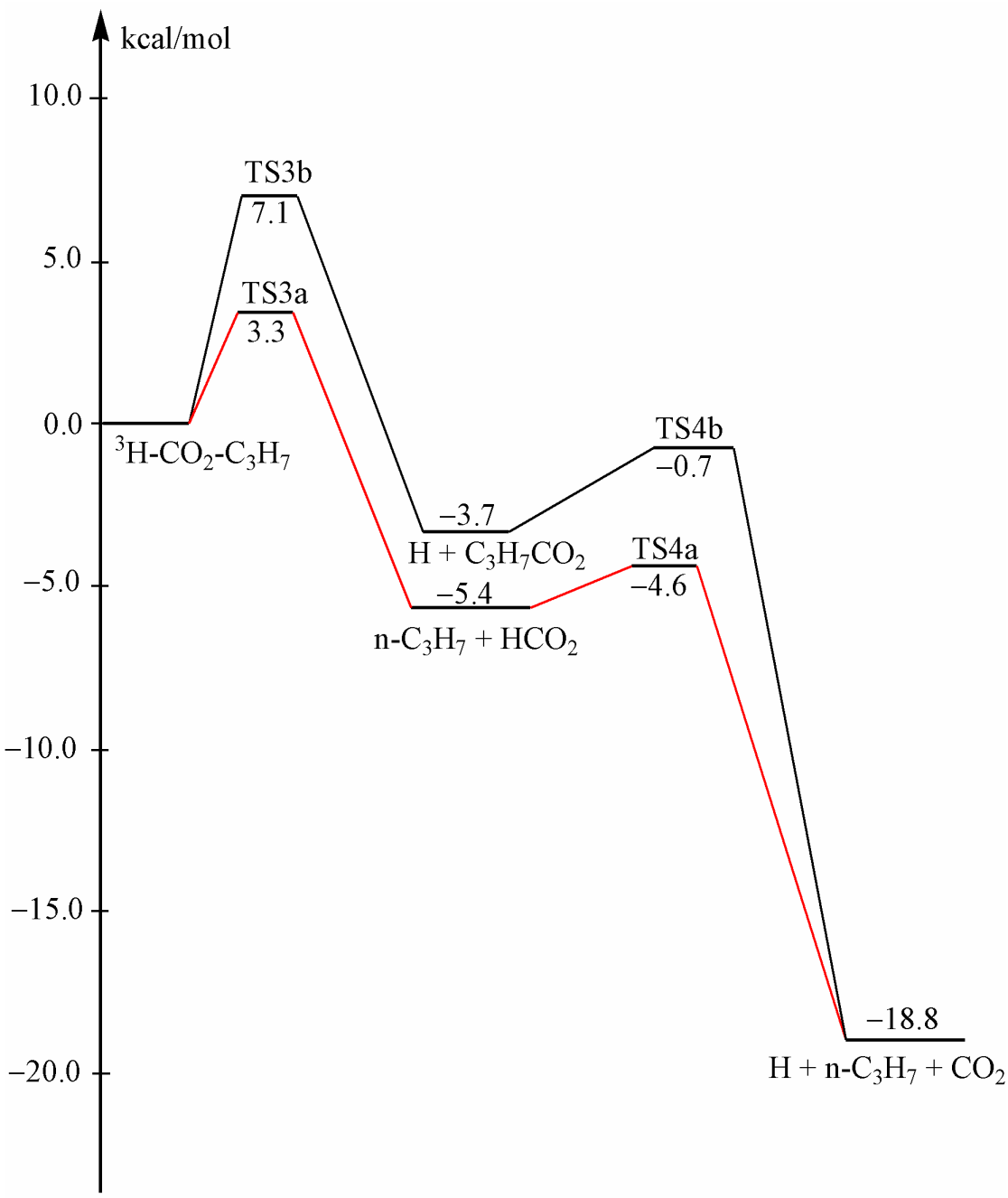


Figure S2: Triplet PES for decomposition of triplet n-propyl bis(oxy) computed at the CBS-QB3 level of theory.

Ozonolysis of b-caryophyllene initiated at the exocyclic double bond

Potential energy surface

The O_3 attack on the exocyclic double bond in β-caryophyllene proceeds primarily on one side of the double bond, with a low barrier of ~0.5 kcal/mol. Addition on the other side of the molecular plane shows a barrier of about 5 kcal/mol, and is hence not competitive at any relevant reaction conditions. The more favorable O_3-addition proceeds through two distinct channels, **TS3** and **TS4**, leading to the primary ozonides **POZ-3** and **POZ-4**, respectively (see Fig. S3); these ozonides correspond to the *syn* and *anti* conformers. The conformers, with relative energies 56 to 57 kcal/mol below the initial reactants, interconvert rapidly over a low barrier of *ca*. 2 kcal/mol. The POZs can either be thermalized by collisions with air molecules, or undergo a ring-opening reaction leading to Criegee intermediates **CI-3** or **CI-4** + HCHO, or to β-nocaryophyllone + H_2COO. The pathways to CI + HCHO are energetically favored by *ca*. 4 kcal/mol compared to those of the β-nocaryophyllone + H_2COO channel. Thermalized POZ will undergo the same ring opening reaction, on a timescale of a few seconds, leading to thermalized **CI-3**/**CI-4**.

Chemically activated Criegee intermediates react promptly via the so-called hydroperoxide or ester channels, in competition with collisional stabilization. The lowest exit channel for **CI-3** is the hydroperoxide channel, with a barrier of 20.3 kcal/mol above **CI-3**, ultimately leading to an $^{\bullet}OH$ radical and a vinoxy resonance stabilized radical. The barrier to formation of a dioxirane in the ester channel for **CI-3** has a barrier of 23.3 kcal/mol. As no hydrogen atoms are geometrically accessible in **CI-4** for a 1,4-H-shift, only the ester channel is viable in **CI-4**, with a rate-limiting barrier to dioxirane formation of 24.7 kcal/mol above **CI-4**.

Thermalized Criegee intermediates do not readily undergo unimolecular reactions; their atmospheric fate is usually determined by bimolecular reactions with specific co-reactants present, *i.e.*, H_2O-vapor, aldehydes, carboxylic acids, olefins, ozone, and so on.

Product distribution

The primary product branching ratios as obtained in RRKM/ME analyses are displayed in Fig. S4: 33.5% stabilized POZs, 46.5% **CI-3** plus HCHO, 4.6% **CI-4** plus HCHO, and 15.4% β-nocaryophyllone + H_2COO. HCHO and β-nocaryophyllone are stable species and will be thermalized. The stabilized POZs dissociate thermally to the same products, but at a longer timescale and without sufficient internal energy to undergo further unimolecular reactions. Incorporating these thermal reactions we then obtain yields of 15% β-nocaryophyllone, 51% HCHO, 34% thermalized CI, 15% chemically activated H_2COO, and 51% chemically activated CI (84% CI total). The nascent energy distribution of the chemically activated H_2COO^*, **CI-3*** and **CI-4*** intermediates depends on the distribution of the initial internal energy over the molecular degrees of freedom of the Criegee intermediate, the closed-shell co-product, and the degrees of freedom for their relative motion. As the O_3 addition on the exocyclic double bond has only a minor contribution in the total β-

caryophyllene ozonolysis, and in view of the uncertainties involved in such an energy redistribution analysis due to the error margins on the barrier heights, the (absolute) rigidities of the structures involved, and potential impact of dynamic effects, we opted to cease the product distribution analysis at this point.

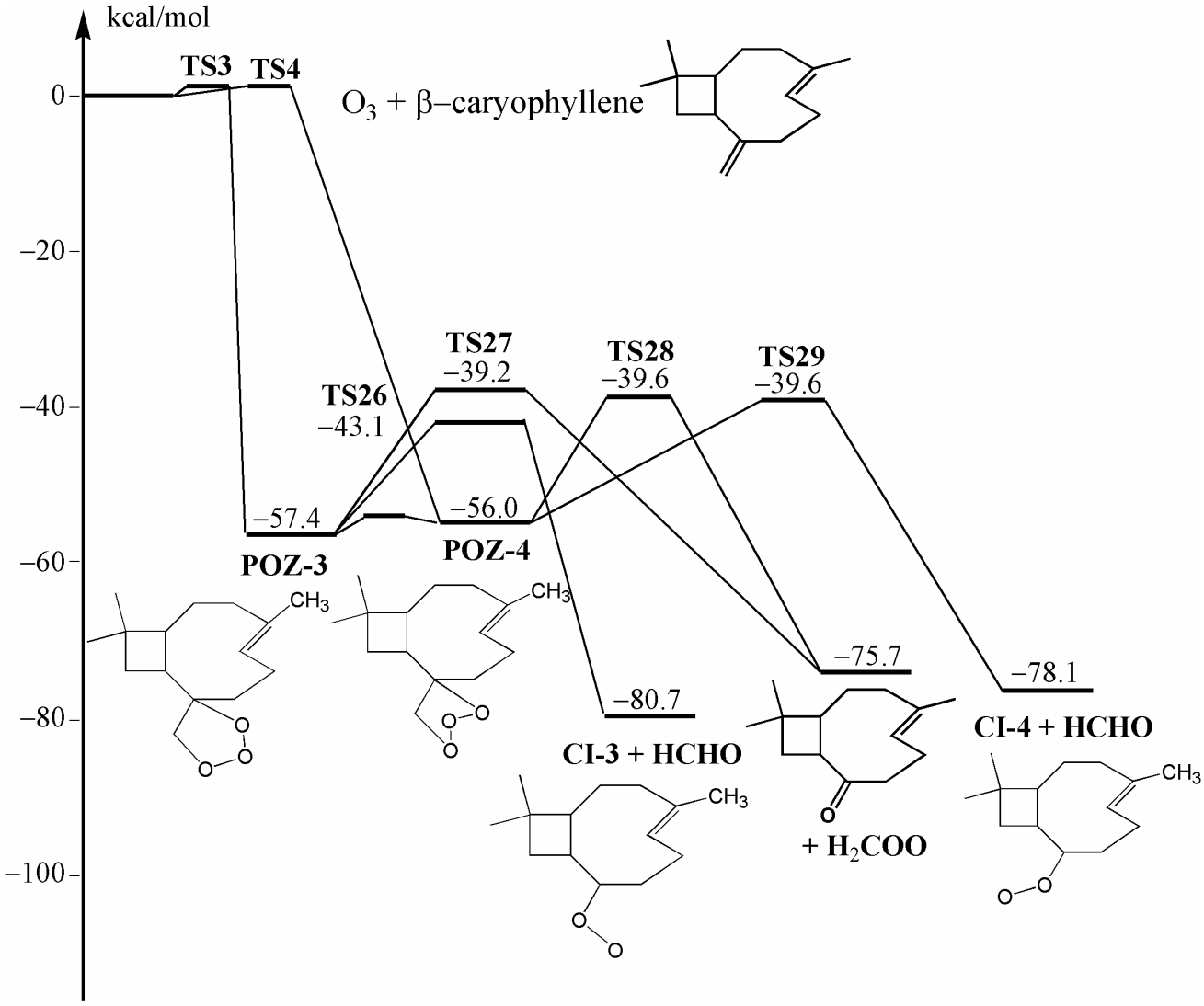


Figure S3: Schematic profile of the lowest-lying singlet potential energy surface for the ozonolysis of β-caryophyllene initiated at the exocyclic >C=C< bond.

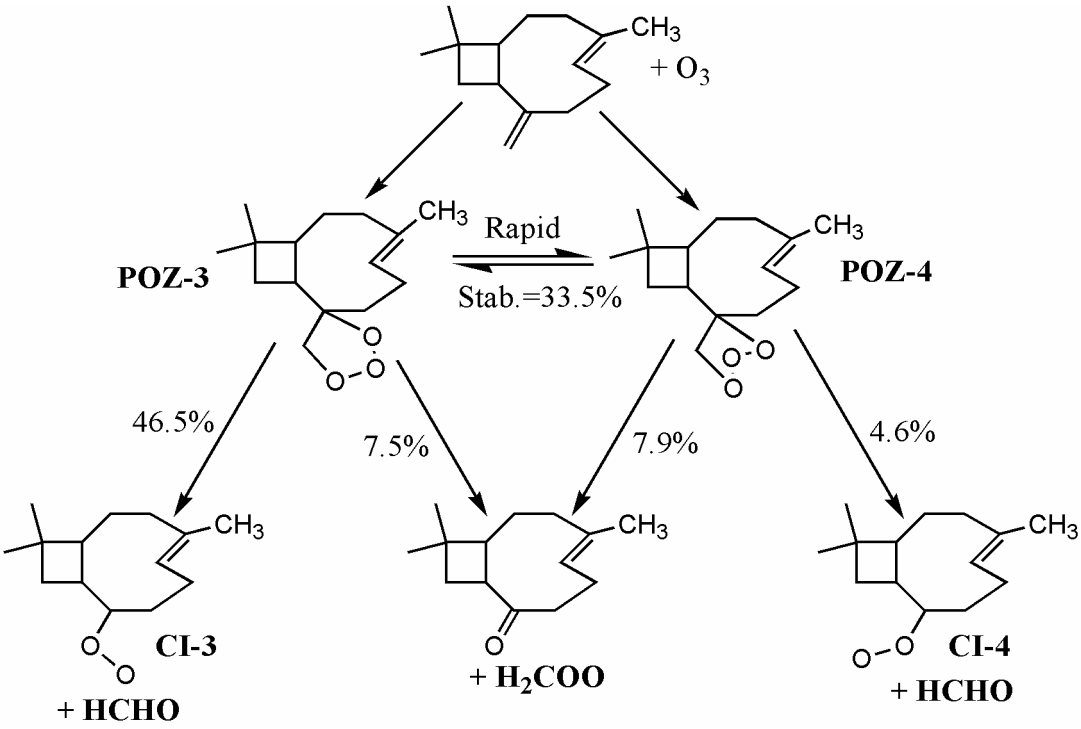
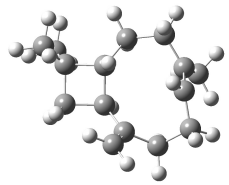
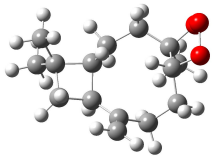
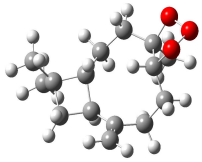
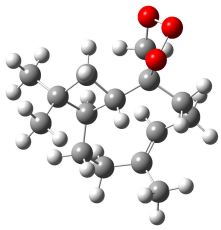
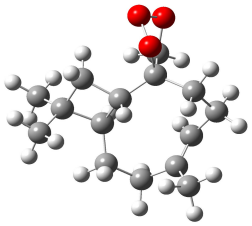
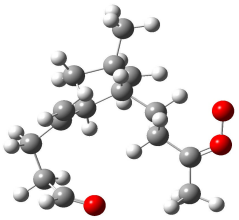
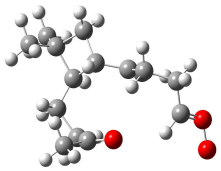
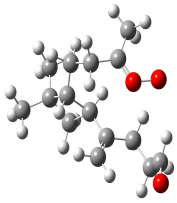
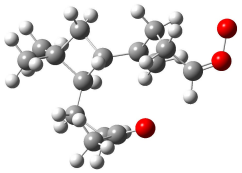
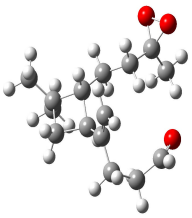
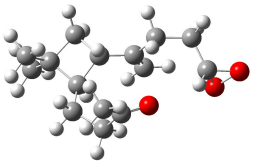
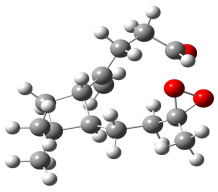
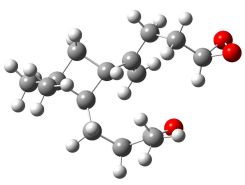
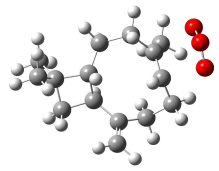
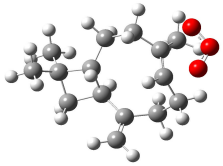
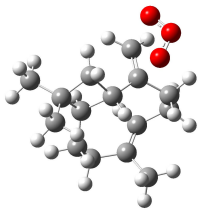
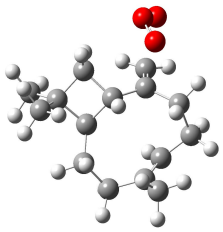
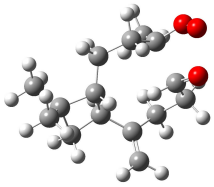
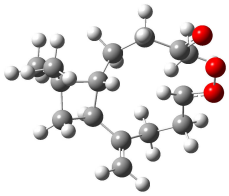
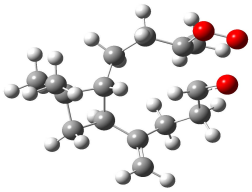
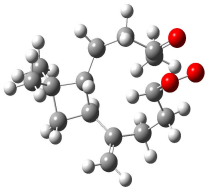
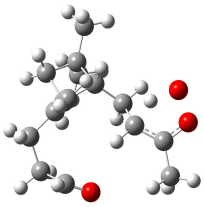
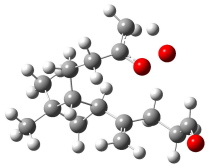
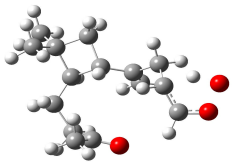
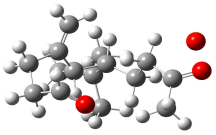
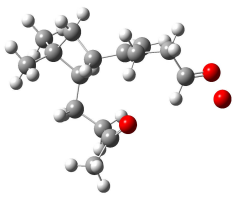
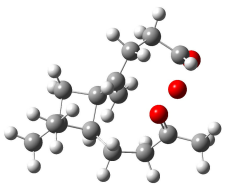
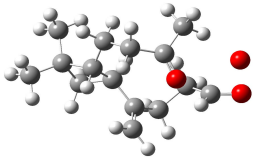
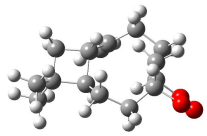
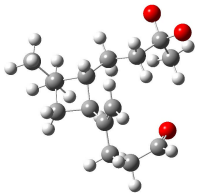
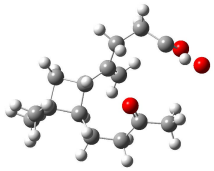
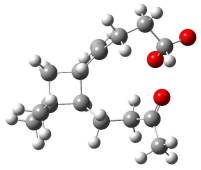


Figure S4: Schematic reaction mechanism and first generation product distribution from the chemically activated reactions following the ozonolysis of β-caryophyllene at the exocyclic >C=C< bond. 'Stab' indicates the yield of collisionally stabilized intermediates.

Ball and Stick models of B3LYP geometries of selected stationary points

 b-caryophyllene	 **POZ-1 (*syn*)**	 **POZ-2 (*anti*)**
 **POZ-3**	 **POZ-4**	 **CI-1a (*syn*)**
 **CI-2a (*anti*)**	 **CI-1b (*anti*)**	 **CI-2b (*syn*)**
 **Dioxirane-1a**	 **Dioxirane-2a**	 **Dioxirane-1b**
 **Dioxirane-2b**		

 **TS1**	 **TS2**	 **TS3**
 **TS4**	 **TS5**	 **TS6**
 **TS7**	 **TS8**	 **TS9**
 **TS10**	 **TS11**	 **TS12**
 **TS13**	 **TS14**	 **TS15**

 **TS16**	 **TS17**	 **TS18**
 **TS19**		

Cartesian coordinates, energetics and rovibrational data

b**-caryophyllene**: B3LYP/6-311G(d,p)

```
------------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -586.140759656
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.491052      0.813851       0.578064
     C      -0.977309     -0.361284      -0.372040
     C      -1.964368      1.305912       0.629723
     C      -2.458953     -0.054986       0.067256
     C      -2.987768     -0.962502       1.185156
     C      -3.471807      0.018206      -1.074365
     C       0.588591      1.810074       0.177983
     C       1.990277      1.640018       0.762808
     C       2.988373      0.935545      -0.202911
     C       0.347758      2.835410      -0.643670
     C       2.283531     -0.210845      -0.871918
     C       1.973041     -1.389365      -0.324561
     C       0.834822     -2.184072      -0.917250
     C      -0.502980     -1.814772      -0.229708
     C       2.552893     -1.910528       0.965585
     H      -0.217072      0.383513       1.546653
     H      -0.849323     -0.036309      -1.410690
     H      -2.154356      2.124351      -0.066113
     H      -2.340285      1.600240       1.613248
     H      -3.932933     -0.563665       1.567762
     H      -2.294825     -1.027074       2.028532
     H      -3.178527     -1.979536       0.830118
     H      -4.441382      0.384015      -0.718783
     H      -3.636033     -0.968043      -1.522989
     H      -3.129001      0.691835      -1.865141
     H       1.924112      1.049704       1.681739
     H       2.390317      2.619394       1.043781
     H       3.873051      0.621869       0.359358
     H       3.329384      1.652977      -0.954569
     H       1.128817      3.545154      -0.897699
     H      -0.619114      3.010423      -1.100030
     H       1.792886      0.042442      -1.808666
     H       0.998901     -3.262884      -0.808607
     H       0.752565     -1.977664      -1.989258
     H      -1.283412     -2.458181      -0.655758
     H      -0.448375     -2.080244       0.831754
     H       1.785976     -2.012374       1.742226
     H       3.344882     -1.272632       1.359712
     H       2.973454     -2.911279       0.812524
Rotational constants (GHz):    0.8435600    0.4928600    0.3696000
Vibrational harmonic frequencies (cm-1):
      44.3928                55.3890                83.4793
     118.2324               162.7221               174.0759
     204.7348               215.9773               232.8778
     243.2627               268.8709               285.9296
     299.2491               303.0388               329.7872
     352.0091               394.9096               408.8014
     432.7248               447.9046               485.5876
     507.0626               551.4403               560.7500
     587.1501               633.5021               721.2542
     742.8165               750.1914               814.0212
```

```
     823.9777                 843.7885                 872.7255
     895.9345                 903.9761                 917.0185
     920.2959                 943.0069                 952.8388
     964.7672                 978.5417                 991.8637
     999.5162                1009.7776                1015.5198
    1036.2536                1041.3174                1061.6741
    1078.4770                1100.3021                1133.4624
    1156.8279                1164.0170                1195.6661
    1200.6260                1207.7368                1226.2138
    1243.0890                1252.4238                1255.3129
    1263.2912                1280.3376                1306.8319
    1328.7680                1334.0801                1353.3997
    1361.5758                1376.6960                1388.9856
    1398.9760                1403.4819                1420.3273
    1421.6347                1447.3605                1477.0661
    1481.8027                1486.1785                1487.2196
    1492.2224                1494.9771                1496.0938
    1499.4788                1504.0401                1507.4602
    1509.9935                1692.4067                1733.3033
    3000.8110                3007.5066                3009.4402
    3015.0482                3018.3441                3021.4332
    3024.3108                3030.7699                3033.9740
    3040.1025                3046.6973                3049.5636
    3057.3415                3059.7695                3064.4713
    3075.0141                3076.4180                3078.6266
    3087.7334                3103.2781                3111.1700
    3131.5758                3132.1967                3207.4425
Zero-point correction (Hartree): 0.353640


β-caryophyllene: MPW1B95/6-31+G(d,p)
------------------------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -585.701402547
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.435587      0.786082       0.572033
     C      -0.980590     -0.318871      -0.397678
     C      -1.866858      1.354005       0.629451
     C      -2.424037      0.035116       0.067765
     C      -2.936610     -0.858571       1.189015
     C      -3.458071      0.142790      -1.035489
     C       0.680148      1.727997       0.182797
     C       2.056909      1.511328       0.780361
     C       3.016802      0.825554      -0.210760
     C       0.493013      2.738902      -0.668886
     C       2.274216     -0.281094      -0.892556
     C       1.860531     -1.409755      -0.311383
     C       0.741119     -2.182487      -0.939631
     C      -0.592006     -1.786921      -0.294266
     C       2.304925     -1.861864       1.046387
     H      -0.179688      0.314901       1.527637
     H      -0.838214      0.034234      -1.426465
     H      -2.001927      2.177394      -0.072504
     H      -2.230447      1.673885       1.608608
     H      -3.862881     -0.445269       1.595989
     H      -2.221071     -0.932402       2.011477
     H      -3.149577     -1.871122       0.838094
     H      -4.406857      0.527850      -0.651845
     H      -3.655351     -0.835136      -1.484487
     H      -3.117734      0.812910      -1.828048
     H       1.964221      0.884246       1.671201
```

```
     H       2.477765      2.466543       1.105222
     H       3.905751      0.472669       0.319624
     H       3.357203      1.554261      -0.948709
     H       1.306329      3.408382      -0.926405
     H      -0.457535      2.934026      -1.149182
     H       1.862233     -0.047769      -1.870666
     H       0.884833     -3.262502      -0.831722
     H       0.698087     -1.964112      -2.010298
     H      -1.390521     -2.373252      -0.764280
     H      -0.591015     -2.082368       0.759968
     H       1.502732     -1.758845       1.784867
     H       3.164022     -1.300809       1.412368
     H       2.576213     -2.920992       1.026586
Rotational constants (GHz):    0.8745300    0.5053800    0.3850900
Vibrational harmonic frequencies (cm-1):
      59.2397                  64.3701                 108.6975
     119.9403                 146.6194                 166.4571
     207.9209                 219.4659                 239.4263
     245.8877                 281.1602                 306.9692
     314.1783                 315.6785                 327.9290
     351.8707                 392.5700                 408.0980
     434.8154                 443.8206                 485.1381
     512.8489                 554.1117                 565.9412
     587.9450                 642.6484                 727.4438
     761.0562                 770.1417                 823.9302
     833.4705                 869.6626                 887.3557
     906.0681                 916.6752                 926.5340
     935.6302                 959.8575                 960.1959
     980.9933                1003.3518                1008.0020
    1020.2444                1023.3475                1029.3099
    1048.0271                1056.9513                1061.3350
    1101.2451                1132.2130                1143.7981
    1173.1803                1176.7641                1200.3214
    1216.0357                1230.4491                1235.0635
    1249.8923                1259.8669                1263.4419
    1274.1246                1304.3615                1324.3039
    1335.1332                1348.3733                1365.5376
    1373.6284                1382.7397                1398.4507
    1405.1090                1416.7277                1426.1328
    1431.3000                1452.1490                1473.5668
    1481.6780                1485.7284                1489.2175
    1493.3403                1495.3441                1501.3242
    1504.6239                1513.1651                1513.4060
    1518.8016                1731.3730                1775.2089
    3047.5273                3052.0107                3056.0174
    3056.8753                3062.9692                3065.0025
    3067.7176                3076.2567                3083.3243
    3095.6457                3096.9575                3115.9303
    3118.6828                3121.3873                3131.8782
    3138.1213                3141.7758                3144.4032
    3146.2147                3159.5106                3170.4399
    3185.4329                3186.9204                3270.8840
Zero-point correction (Hartree): 0.358589

O3: UB3LYP/6-311G(d,p)
------------------------
E(UB+HF-LYP/6-311G(d,p)) (Hartree): -225.473809652
Point group : C2V
Cartesian coordinates (Angs):
     O       0.000000      1.088099      -0.225319
     O       0.000000      0.000000       0.450637
```

```
     O       0.000000     -1.088099      -0.225319
Rotational constants (GHz):  103.7265200   13.3434700   11.8226000
Vibrational harmonic frequencies (cm-1):
     709.9044               1020.3796               1048.2558
Zero-point correction (Hartree): 0.006330


O3: UMPW1B95/6-31+G(d,p)
--------------------------
E(UmPW+HF-B95/6-31+G(d,p)) (Hartree): -225.345928869
Point group : C2V
Cartesian coordinates (Angs):
     O       0.000000      1.075328      -0.223535
     O       0.000000      0.000000       0.447070
     O       0.000000     -1.075328      -0.223535
Rotational constants (GHz):  105.3884400   13.6622900   12.0944000
Vibrational harmonic frequencies (cm-1):
     725.1136               1094.2254               1193.9475
Zero-point correction (Hartree): 0.006865
```

POZ-1

```
-----
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.711688887
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.689347      0.946944       0.457349
     C      -1.414705     -0.490135      -0.120975
     C      -3.089047      0.882388      -0.197137
     C      -2.973680     -0.669677      -0.253442
     C      -3.631453     -1.328367       0.965197
     C      -3.448057     -1.343392      -1.539008
     C      -0.746070      2.093906       0.207315
     C       0.519168      2.117153       1.057344
     C       1.825924      1.810971       0.300520
     C      -0.997024      3.070140      -0.667121
     C       1.849259      0.475472      -0.432116
     C       0.828848     -1.853999       0.102136
     C      -0.587721     -1.543843       0.631337
     C       2.315217     -0.747412       1.867778
     H      -1.803647      0.846138       1.544021
     H      -1.027946     -0.377353      -1.139345
     H      -3.090271      1.307905      -1.203150
     H      -3.923047      1.308293       0.366016
     H      -4.719308     -1.225990       0.900759
     H      -3.314255     -0.874276       1.907787
     H      -3.406054     -2.397744       1.017193
     H      -4.538029     -1.289850      -1.632628
     H      -3.168254     -2.402615      -1.556868
     H      -3.011710     -0.866750      -2.421421
     H       0.403095      1.422552       1.892896
     H       0.628194      3.109075       1.506021
     H       2.675566      1.870832       0.985200
     H       1.981186      2.584549      -0.457412
     H      -0.307838      3.897889      -0.802445
     H      -1.893484      3.088950      -1.274587
     H       0.981393      0.397245      -1.090972
     H       1.144414     -2.812522       0.526533
     H       0.785587     -2.000230      -0.982033
     H      -1.133488     -2.491914       0.570867
     H      -0.553224     -1.305837       1.700360
     H       1.465771     -0.382186       2.445426
```

```
     H       3.164302     -0.081027       2.020471
     H       2.586210     -1.731377       2.257812
     C       1.982867     -0.874040       0.383696
     O       3.189622     -1.451640      -0.189476
     O       3.232690     -0.900917      -1.518081
     O       3.028909      0.493755      -1.249662
Rotational constants (GHz):    0.6413000    0.3035500    0.2532200
Vibrational harmonic frequencies (cm-1):
      42.7129                 59.2519                 87.0877
      99.0175                150.6236                156.1678
     188.9906                209.4754                216.5239
     228.8946                235.0528                238.5675
     266.1297                287.7700                306.1364
     313.1316                340.4441                342.2071
     356.2961                396.3746                410.5649
     426.0338                449.9143                468.5208
     481.5341                523.4108                553.2881
     561.6918                598.0468                640.3627
     698.1976                712.4943                731.4631
     731.6512                759.9367                813.7295
     825.3014                849.3276                866.1305
     889.8470                897.8299                920.1388
     926.3434                927.8142                932.1230
     950.6162                959.5222                990.6024
    1001.6070               1005.1840               1018.6578
    1020.1427               1025.9995               1038.8616
    1061.5450               1094.6627               1103.6466
    1116.6555               1142.4826               1160.3788
    1165.6531               1184.2747               1199.2333
    1215.0309               1225.5537               1240.1774
    1251.7264               1263.0783               1274.0029
    1281.1335               1307.6558               1318.5256
    1344.8125               1351.5667               1368.6252
    1379.7429               1383.4154               1392.8275
    1398.2603               1407.4243               1408.9131
    1418.4104               1421.5293               1452.0264
    1478.3276               1483.5235               1485.6719
    1488.9253               1490.8304               1493.8150
    1498.5072               1507.1047               1508.3166
    1509.0885               1514.2257               1701.5421
    3002.0447               3009.6133               3015.4083
    3022.7100               3025.3077               3028.5830
    3038.2587               3044.3402               3046.1299
    3047.7663               3051.5333               3062.5670
    3066.8610               3070.0595               3075.0122
    3078.5287               3081.0699               3089.5809
    3089.8232               3096.2530               3114.2310
    3132.9056               3135.0560               3212.7466
Zero-point correction (Hartree): 0.367370
```

POZ-1

```
--------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.158513398
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.689671      0.961344       0.426259
     C      -1.403153     -0.468152      -0.111288
     C      -3.044211      0.888584      -0.284109
     C      -2.942693     -0.651366      -0.251516
     C      -3.596235     -1.231138       0.995034
     C      -3.406218     -1.399356      -1.485294
```

C	-0.718405	2.073946	0.204518
C	0.502726	2.055808	1.098236
C	1.814780	1.775281	0.368711
C	-0.900165	3.035903	-0.700652
C	1.816747	0.472872	-0.398737
C	0.803736	-1.837135	0.116569
C	-0.583038	-1.491788	0.666485
C	2.352639	-0.790307	1.833879
H	-1.852871	0.874573	1.507330
H	-1.013594	-0.371335	-1.131152
H	-2.976397	1.251052	-1.312337
H	-3.900465	1.357899	0.204030
H	-4.681223	-1.117937	0.934960
H	-3.262022	-0.735898	1.909143
H	-3.383236	-2.297869	1.098125
H	-4.494091	-1.359209	-1.584786
H	-3.118848	-2.453588	-1.435328
H	-2.968578	-0.974137	-2.390989
H	0.352979	1.318535	1.890524
H	0.598662	3.020475	1.602273
H	2.651371	1.800236	1.068848
H	1.988969	2.571096	-0.359709
H	-0.178591	3.835639	-0.827175
H	-1.772119	3.064564	-1.341326
H	0.927568	0.417795	-1.031983
H	1.112650	-2.799356	0.533361
H	0.736287	-1.978193	-0.966795
H	-1.146723	-2.430081	0.665750
H	-0.522037	-1.201077	1.721082
H	1.532485	-0.416246	2.444636
H	3.219941	-0.145964	1.968675
H	2.611378	-1.785817	2.197094
C	1.968226	-0.881389	0.371003
O	3.134200	-1.443801	-0.261423
O	3.115029	-0.869335	-1.555155
O	2.961785	0.497662	-1.240776

Rotational constants (GHz): 0.6524000 0.3113400 0.2607800

Vibrational harmonic frequencies (cm-1):

47.9234	62.7174	96.4050
103.0818	139.8231	144.1465
181.7641	195.5721	204.6486
224.6940	240.1884	246.5087
276.8529	301.0998	304.0613
320.6445	342.7071	348.1815
360.9325	394.5349	408.9353
429.9091	460.6789	475.7935
493.1462	527.5707	561.1842
563.0923	612.0641	647.2770
719.0438	734.2038	739.4227
749.6693	823.2752	839.9427
848.6725	866.8641	888.7897
906.8047	916.0068	931.7073
936.2507	945.0791	958.3829
977.0793	992.7604	1012.1074
1019.4367	1026.8941	1033.2822
1042.5911	1054.5044	1071.7917
1083.7651	1120.5030	1130.5321
1145.4742	1165.5681	1173.0113
1182.6414	1195.9521	1218.6528
1233.4645	1234.9867	1254.5467
1265.3817	1267.8390	1285.0789

1306.8722	1325.9072	1330.6126
1340.5839	1350.0876	1370.5655
1387.1061	1390.1216	1405.9221
1409.1508	1414.0036	1425.0237
1427.1220	1432.4018	1465.6993
1477.6331	1483.3884	1487.7398
1491.1447	1494.8117	1496.0965
1501.7287	1507.2587	1512.8968
1515.5571	1519.2257	1743.5164
3048.0772	3057.0228	3058.8733
3065.2551	3069.4447	3071.8240
3084.7121	3092.8317	3095.9085
3099.0434	3100.7130	3111.4718
3125.1019	3129.5708	3135.0572
3144.6121	3147.5065	3149.2705
3152.5290	3153.0012	3179.3586
3188.6048	3198.3555	3276.0088

Zero-point correction (Hartree): 0.372832

POZ-2

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.710771569
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.682086	0.938787	0.491937
C	-1.461615	-0.479761	-0.152411
C	-3.101818	0.935061	-0.121660
C	-3.027751	-0.615125	-0.247418
C	-3.666944	-1.310204	0.960818
C	-3.554917	-1.220281	-1.546377
C	-0.718767	2.073039	0.256598
C	0.556928	2.053177	1.090992
C	1.846446	1.725360	0.310520
C	-0.959159	3.071689	-0.595507
C	1.823215	0.436390	-0.510389
C	0.743240	-1.900710	-0.070870
C	-0.643335	-1.588662	0.526885
C	2.248179	-0.874518	1.730624
H	-1.766672	0.797125	1.576515
H	-1.099622	-0.333423	-1.175906
H	-3.122530	1.403461	-1.108141
H	-3.907447	1.356601	0.484353
H	-4.753360	-1.180098	0.931938
H	-3.313051	-0.903752	1.912102
H	-3.466189	-2.385771	0.961474
H	-4.645481	-1.137464	-1.605091
H	-3.301781	-2.283844	-1.618777
H	-3.132723	-0.714883	-2.419704
H	0.429731	1.353910	1.920639
H	0.696535	3.036775	1.549695
H	2.700835	1.717064	0.992321
H	2.029774	2.529965	-0.407041
H	-0.253918	3.887286	-0.721338
H	-1.861263	3.122574	-1.192716
H	0.956774	0.439726	-1.173447
H	1.051325	-2.891540	0.279542
H	0.663958	-1.973988	-1.160180
H	-1.216014	-2.518371	0.440992
H	-0.563905	-1.401680	1.603205
H	1.469838	-0.387696	2.318611
H	3.184384	-0.335411	1.877618

```
     H       2.377623     -1.889105       2.113727
     C       1.911237     -0.953026       0.241756
     O       3.039550     -1.577724      -0.428917
     O       3.881432     -0.463885      -0.733140
     O       2.949777      0.409764      -1.409614
Rotational constants (GHz):    0.6737700    0.2973100    0.2466800
Vibrational harmonic frequencies (cm-1):
      40.0914                 62.5914                 89.5300
      92.7304                149.4088                161.9971
     189.6502                208.7208                224.5272
     227.5486                238.7982                255.4927
     273.6146                288.5563                300.1517
     311.0577                328.2192                343.8228
     350.2267                394.4042                417.3315
     439.2599                456.0711                467.5624
     514.4656                516.7333                540.9494
     563.8148                600.0739                647.0574
     689.3673                727.2836                730.5076
     738.7988                756.1884                817.2301
     832.6482                850.1144                865.4823
     892.0710                900.2231                920.9358
     925.6208                933.4947                935.8620
     952.5092                961.7317                988.2019
     990.4943                999.6019               1011.1961
    1019.8354               1028.5719               1032.4632
    1058.0156               1088.9543               1092.5303
    1111.2995               1136.7878               1152.2571
    1164.3242               1180.0519               1200.2886
    1214.3973               1227.7890               1240.4927
    1254.6087               1260.2945               1274.4636
    1280.4587               1305.9431               1317.9080
    1332.0102               1349.7670               1359.2230
    1374.2441               1384.0936               1393.3818
    1398.6545               1403.4364               1408.3037
    1412.9465               1421.9670               1450.1008
    1480.4343               1484.0943               1486.4816
    1489.5971               1493.1380               1496.6723
    1499.6754               1507.8278               1508.7599
    1509.9912               1512.3993               1700.4302
    3004.8570               3009.5177               3017.6056
    3022.9449               3024.4816               3028.5845
    3038.4065               3046.2797               3046.5486
    3051.1655               3052.7656               3066.6874
    3067.6113               3073.7982               3079.1278
    3080.9541               3085.7286               3089.8881
    3095.3438               3096.5066               3117.1565
    3132.6810               3132.8606               3212.2751
Zero-point correction (Hartree): 0.367439
```

POZ-2

```
---------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.157482794
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.693042      0.954049       0.461101
     C      -1.451620     -0.458351      -0.138830
     C      -3.067239      0.938469      -0.215039
     C      -2.997811     -0.603014      -0.250901
     C      -3.635266     -1.222613       0.984692
     C      -3.505142     -1.286813      -1.504590
     C      -0.702275      2.052663       0.253655
```

```
      C       0.532132      1.982736      1.125910
      C       1.826081      1.686434      0.367545
      C      -0.876926      3.042164     -0.622988
      C       1.789169      0.435388     -0.489089
      C       0.715623     -1.883203     -0.047145
      C      -0.637813     -1.533482      0.573973
      C       2.287734     -0.894303      1.690123
      H      -1.830114      0.830093      1.542061
      H      -1.082030     -0.327497     -1.162441
      H      -3.021571      1.343972     -1.228177
      H      -3.899659      1.402513      0.317273
      H      -4.718610     -1.084687      0.954523
      H      -3.270339     -0.773299      1.910704
      H      -3.443064     -2.296930      1.037529
      H      -4.593830     -1.219367     -1.576536
      H      -3.240047     -2.348046     -1.507027
      H      -3.079064     -0.831512     -2.401149
      H       0.369344      1.236339      1.906768
      H       0.661578      2.934169      1.647687
      H       2.668669      1.640147      1.060662
      H       2.025284      2.514981     -0.315746
      H      -0.139093      3.828486     -0.738924
      H      -1.757756      3.108773     -1.248508
      H       0.908898      0.460597     -1.134502
      H       1.019311     -2.872355      0.306654
      H       0.606158     -1.964883     -1.132462
      H      -1.225717     -2.456195      0.557634
      H      -0.526020     -1.285630      1.634921
      H       1.564734     -0.362520      2.306295
      H       3.255957     -0.404417      1.790072
      H       2.378225     -1.911858      2.071705
      C       1.891622     -0.953566      0.225682
      O       2.981978     -1.558296     -0.491399
      O       3.812344     -0.452829     -0.752356
      O       2.895353      0.423596     -1.391697
Rotational constants (GHz):    0.6877100    0.3040800    0.2531400
Vibrational harmonic frequencies (cm-1):
      51.0886                  75.0916                  95.2452
      99.0175                 148.1856                 166.4656
     187.9677                 208.8193                 230.7629
     236.8145                 246.9443                 270.7269
     280.6995                 300.1594                 302.4295
     327.1267                 338.0486                 348.6549
     365.2394                 391.3873                 410.5987
     446.5513                 461.4506                 477.6451
     516.0595                 529.5876                 548.2910
     564.1241                 614.3087                 654.5245
     715.3914                 734.8267                 749.2548
     764.0460                 820.9986                 831.1139
     851.2186                 873.0320                 885.3990
     913.3987                 918.6509                 933.9178
     948.2785                 957.2891                 958.7041
     978.1033                 987.1827                1009.8159
    1017.4741                1026.1770                1031.9767
    1035.4799                1052.5695                1060.6102
    1072.8282                1114.4287                1120.3815
    1143.3031                1160.5038                1166.1154
    1178.8182                1190.0563                1219.2430
    1229.5590                1234.8006                1256.1323
    1261.0743                1266.5304                1285.7774
    1305.4850                1323.1792                1329.0637
```

1336.1614	1348.3054	1364.4703
1384.2221	1395.9874	1405.1396
1408.5178	1413.5429	1421.2792
1424.4270	1433.4595	1459.1414
1483.4775	1485.4291	1487.6808
1490.9735	1496.1722	1501.3225
1503.8462	1511.1275	1513.8168
1519.2458	1529.1008	1742.4861
3048.7027	3058.1866	3061.7959
3065.1581	3070.2348	3074.3721
3085.0692	3091.6959	3094.9545
3100.2376	3104.7801	3125.3186
3126.8778	3132.6513	3134.8351
3145.2295	3146.4617	3150.0335
3150.6480	3152.1285	3180.5356
3188.0880	3198.1881	3275.1238

Zero-point correction (Hartree): 0.373225

POZ-3

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.702006790
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.001914	-0.569175	-0.613977
C	-1.279829	-0.542823	0.317551
C	-0.065222	-2.120616	-0.576685
C	-1.516578	-2.061872	-0.034465
C	-2.536067	-2.300888	-1.155200
C	-1.827727	-2.960636	1.160899
C	1.400610	0.012039	-0.279787
C	1.692655	1.487324	-0.656456
C	1.333060	2.599216	0.360274
C	-0.034344	2.362874	0.930628
C	-1.197257	2.537274	0.296976
C	-2.403896	1.780275	0.786396
C	-2.473113	0.399070	0.092332
C	-1.358590	3.290187	-0.998060
H	-0.271601	-0.200030	-1.608346
H	-0.972485	-0.482381	1.367479
H	0.637134	-2.537234	0.148210
H	0.090783	-2.636200	-1.525499
H	-2.484997	-3.345121	-1.479047
H	-2.340072	-1.677426	-2.031696
H	-3.561573	-2.107435	-0.827733
H	-1.826942	-4.016155	0.869212
H	-2.814290	-2.735193	1.581006
H	-1.087806	-2.835984	1.957141
H	1.175128	1.686539	-1.599176
H	2.764825	1.536350	-0.867392
H	1.405898	3.561047	-0.155756
H	2.076409	2.634105	1.161338
H	-0.061358	1.814969	1.871249
H	-3.333511	2.325543	0.587627
H	-2.342407	1.632025	1.869406
H	-3.369664	-0.112548	0.462108
H	-2.633770	0.538967	-0.981886
H	-1.693825	2.632698	-1.808174
H	-0.439327	3.778403	-1.322062
H	-2.128062	4.062774	-0.887987
C	1.944927	-0.363246	1.139711
H	1.198739	-0.838465	1.775937

```
     H       2.371149      0.506289       1.643902
     O       2.954889     -1.342193       0.909258
     O       3.474269     -0.923431      -0.373121
     O       2.268509     -0.794323      -1.138722
Rotational constants (GHz):    0.4729000    0.4306000    0.2679900
Vibrational harmonic frequencies (cm-1):
      49.6717                 67.0118                 74.1908
      84.8075                124.7504                158.5074
     159.3900                202.4858                205.7186
     217.5783                228.6730                255.2328
     265.2988                277.2205                303.2539
     314.0231                328.9515                360.1061
     375.8858                393.0966                403.0911
     419.7996                447.9317                489.8540
     511.8749                523.4431                554.1080
     572.5026                599.8054                650.1467
     705.1307                722.3207                741.0813
     780.9365                805.7038                811.4873
     836.6624                866.0575                888.9024
     901.7586                914.1101                922.5283
     926.7511                949.7008                951.1028
     967.3616                974.6090                987.8263
     992.9721               1002.5335               1011.0733
    1013.7220               1036.5232               1054.7914
    1064.1386               1075.0483               1092.0813
    1112.8777               1141.7526               1156.3128
    1169.0863               1188.0676               1208.1634
    1221.8029               1229.3562               1242.3346
    1254.1500               1261.2750               1270.5341
    1281.5765               1302.0214               1308.6501
    1325.8645               1346.3073               1357.3322
    1364.5427               1366.9006               1380.8913
    1387.6060               1400.9896               1403.4642
    1419.7388               1420.7570               1478.1413
    1480.5648               1485.6759               1488.0582
    1489.3792               1493.0406               1496.8645
    1497.8500               1507.2688               1509.5447
    1511.2264               1516.0502               1733.0645
    3009.0026               3009.6654               3013.9729
    3019.4458               3021.7624               3024.5324
    3035.2980               3038.8877               3041.2771
    3045.6849               3054.1225               3058.7759
    3059.9078               3063.0955               3064.8780
    3067.9705               3077.5561               3080.9029
    3084.2171               3090.0293               3105.8019
    3109.7070               3115.1873               3127.0921
Zero-point correction (Hartree): 0.367339
```

POZ-3

```
--------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.150854279
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.153593     -0.519655      -0.616665
     C      -1.360645     -0.217054       0.329111
     C      -0.555141     -2.005096      -0.561719
     C      -1.943941     -1.615299      -0.035683
     C      -2.957797     -1.573824      -1.171369
     C      -2.484840     -2.418431       1.130222
     C       1.335855     -0.295683      -0.288969
     C       1.981800      1.043665      -0.678996
```

C	1.928794	2.184067	0.345939
C	0.562645	2.270436	0.943032
C	-0.532995	2.670428	0.292429
C	-1.874118	2.269578	0.818434
C	-2.305666	0.963327	0.142655
C	-0.511228	3.305255	-1.064343
H	-0.348325	-0.092309	-1.606234
H	-1.025156	-0.241346	1.373416
H	0.037121	-2.540105	0.185537
H	-0.507010	-2.569081	-1.493696
H	-3.164438	-2.590080	-1.515217
H	-2.585962	-1.007195	-2.028582
H	-3.905866	-1.129370	-0.860005
H	-2.747662	-3.433101	0.820111
H	-3.385152	-1.955324	1.544692
H	-1.746263	-2.494926	1.931860
H	1.506942	1.368791	-1.608270
H	3.024896	0.818992	-0.916430
H	2.212115	3.111253	-0.158929
H	2.677345	2.031803	1.125645
H	0.422673	1.801023	1.915443
H	-2.630003	3.040023	0.639522
H	-1.817963	2.109071	1.898763
H	-3.279715	0.670898	0.550060
H	-2.470386	1.135800	-0.925628
H	-0.810846	2.591271	-1.839238
H	0.472813	3.686916	-1.333526
H	-1.220728	4.135112	-1.110496
C	1.747268	-0.767102	1.131184
H	0.899748	-1.062986	1.749389
H	2.341096	-0.011708	1.647659
O	2.512803	-1.936078	0.915391
O	3.109245	-1.655498	-0.343863
O	1.976995	-1.301061	-1.106205

Rotational constants (GHz): 0.4894800 0.4437100 0.2789500

Vibrational harmonic frequencies (cm-1):

59.9188	86.2945	98.5839
107.0408	139.0108	160.0403
196.5364	210.5302	221.9273
225.9476	240.8515	264.5720
275.3542	294.9888	314.3186
323.7801	344.5892	362.1297
389.9687	398.2016	404.8229
425.1336	451.8529	495.1736
529.0615	529.5431	562.4366
576.2107	611.0772	668.2410
735.1360	754.9382	789.2798
815.9425	818.9513	829.0557
856.5836	877.6325	899.1428
920.2465	935.5102	948.3664
959.8226	971.1308	981.4224
991.3966	993.2143	1008.5560
1017.1307	1021.1627	1027.1136
1048.6905	1059.8186	1061.4474
1091.0267	1101.0053	1127.8073
1135.3618	1147.3983	1158.8363
1185.3383	1204.8519	1227.5005
1233.2622	1239.8112	1249.4773
1256.0399	1265.0745	1280.8505
1303.1005	1315.1124	1325.3270
1336.3461	1351.4258	1360.2579

1369.0025	1374.8527	1385.1131
1393.4256	1407.1935	1414.0091
1424.1632	1431.3088	1474.7900
1483.6150	1488.4531	1490.4975
1493.1182	1497.0061	1498.7106
1504.8299	1514.1547	1516.0398
1519.7590	1527.6257	1773.5012
3053.5772	3055.0518	3056.3720
3058.2272	3066.4689	3070.1286
3079.3880	3083.4413	3090.7235
3096.5485	3104.7916	3110.8099
3120.5739	3124.0578	3126.8879
3132.7058	3141.3334	3143.1517
3145.3118	3148.5536	3157.0273
3167.8204	3172.8291	3175.7012

Zero-point correction (Hartree): 0.373273

POZ-4

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.699665973
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.208311	0.497530	-0.607661
C	0.945711	0.982284	0.361280
C	-0.738226	1.957699	-0.641535
C	0.589605	2.471235	-0.025372
C	1.496324	3.089980	-1.096837
C	0.451844	3.425776	1.159976
C	-1.293096	-0.578077	-0.306045
C	-0.984360	-2.036159	-0.745010
C	-0.223697	-2.945318	0.252667
C	0.922464	-2.205600	0.876917
C	2.082393	-1.893352	0.293103
C	2.873499	-0.737893	0.849410
C	2.418447	0.580375	0.179710
C	2.570951	-2.479086	-1.006146
H	0.226008	0.239187	-1.578209
H	0.656485	0.819845	1.405749
H	-1.591834	2.109548	0.020047
H	-1.007138	2.345050	-1.625863
H	1.060863	4.033238	-1.441476
H	1.603871	2.441819	-1.970894
H	2.497497	3.309492	-0.714849
H	0.048580	4.392625	0.840376
H	1.421933	3.612592	1.634273
H	-0.221100	3.021671	1.922198
H	-0.421856	-1.985383	-1.681826
H	-1.947001	-2.495362	-0.981164
H	0.105281	-3.836749	-0.288892
H	-0.909784	-3.303390	1.025912
H	0.703818	-1.716549	1.824541
H	3.949394	-0.866454	0.685080
H	2.719416	-0.661260	1.930593
H	3.031139	1.390286	0.593477
H	2.657092	0.545256	-0.888621
H	2.620922	-1.721435	-1.796610
H	1.943216	-3.295187	-1.365505
H	3.588376	-2.867204	-0.883182
C	-1.914723	-0.479952	1.120189
H	-1.599908	0.431415	1.633990
H	-1.716324	-1.350719	1.741284

```
     O      -3.320025     -0.465040       0.900719
     O      -3.403605      0.383029      -0.253604
     O      -2.445356     -0.229111      -1.150652
Rotational constants (GHz):    0.4712000    0.4347000    0.2688900
Vibrational harmonic frequencies (cm-1):
      47.7155                  60.5682                  74.7303
      84.9456                 116.5585                 159.6127
     168.9789                 192.1509                 203.7933
     215.6777                 230.7148                 254.8414
     267.5379                 270.2415                 294.1488
     316.8960                 320.5279                 356.8145
     383.1637                 397.9468                 406.3408
     413.6265                 438.6656                 479.1037
     495.9757                 527.4507                 553.1757
     576.6917                 600.0341                 651.5640
     709.5067                 722.5586                 745.0610
     775.3470                 795.5586                 816.2481
     840.2891                 869.5872                 878.7002
     896.4129                 907.5026                 918.2261
     925.2252                 950.5971                 961.6762
     966.3355                 978.0010                 986.1029
    1000.8119                1007.7154                1012.6559
    1016.4744                1037.9656                1051.3995
    1063.0813                1074.6204                1090.7106
    1116.7364                1138.7587                1157.5523
    1175.2404                1185.0536                1206.5553
    1225.1170                1232.0802                1250.4388
    1255.3706                1264.0949                1270.2536
    1279.1909                1284.2847                1311.9474
    1328.8186                1345.1177                1355.4395
    1364.3717                1367.5309                1381.3082
    1389.5435                1402.6692                1404.7427
    1421.7577                1424.6283                1479.5504
    1483.0706                1484.9444                1488.0339
    1489.8096                1494.4000                1495.5100
    1498.6029                1504.8967                1508.7743
    1510.4312                1515.7640                1735.9353
    3007.8776                3009.2335                3013.3392
    3017.5667                3020.1570                3023.0167
    3034.3774                3038.0008                3043.3286
    3046.0293                3054.1551                3055.4285
    3062.1785                3063.4287                3063.8300
    3066.9467                3076.2178                3079.3244
    3088.0576                3088.9199                3110.4363
    3113.3764                3116.2036                3147.7040
Zero-point correction (Hartree): 0.367300
```

POZ-4

```
---------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.148305986
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.129017     -0.505002      -0.606472
     C      -1.322936     -0.252704       0.372063
     C      -0.510239     -1.996593      -0.607846
     C      -1.889232     -1.649868      -0.026670
     C      -2.939828     -1.594845      -1.127626
     C      -2.376296     -2.503178       1.127677
     C       1.364966     -0.247080      -0.315360
     C       1.944269      1.105922      -0.771379
     C       1.896949      2.255075       0.243669
```

C	0.553806	2.313116	0.894621
C	-0.580112	2.668819	0.286205
C	-1.880571	2.230598	0.879408
C	-2.302478	0.906986	0.232610
C	-0.638343	3.286097	-1.077364
H	-0.356010	-0.051921	-1.577398
H	-0.970159	-0.300759	1.410164
H	0.096484	-2.569145	0.095390
H	-0.484340	-2.509554	-1.570071
H	-3.137158	-2.604901	-1.494533
H	-2.606036	-0.996939	-1.979280
H	-3.886091	-1.179091	-0.774064
H	-2.626399	-3.513083	0.792444
H	-3.273344	-2.073459	1.583187
H	-1.612712	-2.588135	1.904779
H	1.409000	1.402683	-1.677099
H	2.979377	0.920607	-1.063285
H	2.137012	3.184279	-0.279618
H	2.681146	2.127321	0.992919
H	0.463411	1.861465	1.880669
H	-2.669272	2.974411	0.731440
H	-1.766931	2.082094	1.956902
H	-3.248419	0.590090	0.685874
H	-2.522603	1.070985	-0.826889
H	-0.955403	2.555914	-1.829723
H	0.322118	3.689590	-1.395932
H	-1.370729	4.096872	-1.098842
C	1.796509	-0.663232	1.108088
H	1.013415	-1.236452	1.610555
H	2.114401	0.166956	1.733277
O	2.933807	-1.471490	0.900672
O	2.505370	-2.225536	-0.214285
O	2.103893	-1.206035	-1.121464

Rotational constants (GHz): 0.4841800 0.4507000 0.2799500

Vibrational harmonic frequencies (cm-1):

46.9159	71.5923	93.7625
98.8517	134.2435	159.8339
193.9550	201.2864	218.9526
228.1516	232.4709	264.9939
280.6813	292.3575	308.9339
324.1894	347.7413	357.9116
394.0404	402.9265	409.7088
423.3774	450.1078	483.8848
502.2340	537.6902	556.7285
574.8674	612.2282	667.2272
727.6353	765.5278	789.3026
809.3054	819.7912	828.3426
858.1830	880.6212	894.9523
918.2925	926.9981	936.9314
958.8372	971.8390	977.9929
989.6331	1000.4793	1007.9502
1018.3863	1023.2736	1038.5567
1049.8465	1057.7585	1058.9404
1081.9858	1099.8665	1127.6486
1137.4888	1145.4330	1158.6628
1185.3058	1204.3048	1229.3224
1233.7234	1236.9095	1254.7301
1258.4474	1261.1331	1277.5118
1296.1795	1305.3761	1326.8233
1335.4724	1357.6334	1361.5787
1366.1513	1374.3781	1393.0389

1397.7474	1408.6994	1413.8333
1423.8401	1435.3232	1476.4020
1484.8423	1488.2743	1489.2451
1491.9331	1497.0049	1499.9364
1511.8810	1512.0772	1515.3717
1518.4492	1532.1459	1775.7136
3050.0730	3054.9812	3055.9954
3057.6373	3065.7479	3069.5402
3078.2159	3087.5196	3092.4019
3093.1512	3105.0298	3108.3108
3120.8864	3123.8707	3126.9234
3133.2259	3140.2914	3144.1529
3148.5161	3148.9572	3164.6357
3165.4432	3175.0516	3198.3329

Zero-point correction (Hartree): 0.373100

CI-1a

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.753966943
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.518477	0.415702	-0.077246
C	-0.317300	1.341308	0.261877
C	-2.407490	1.695059	-0.215309
C	-1.112116	2.553814	-0.352494
C	-0.775675	2.839138	-1.820104
C	-1.069691	3.843387	0.463493
C	-1.987910	-0.682852	0.843296
C	-2.927840	-1.703438	0.227149
C	-2.240574	-2.639503	-0.801187
C	-1.643900	-0.773146	2.129779
C	-1.128235	-3.444556	-0.175815
C	1.655565	-0.259364	0.460651
C	1.067623	0.979081	-0.264770
C	3.211862	-1.794041	-0.977358
H	-1.357218	-0.003187	-1.076597
H	-0.257615	1.497173	1.343813
H	-2.938691	1.904381	0.716600
H	-3.117072	1.728515	-1.046208
H	-1.485632	3.563147	-2.232571
H	-0.826351	1.940249	-2.441000
H	0.228053	3.261488	-1.923811
H	-1.773119	4.583614	0.067054
H	-0.069880	4.289366	0.441035
H	-1.331152	3.659210	1.509513
H	-3.750732	-1.192881	-0.285826
H	-3.379875	-2.308851	1.018619
H	-1.828714	-2.082557	-1.644995
H	-2.990133	-3.340960	-1.188644
H	-2.036531	-1.561511	2.763652
H	-0.966573	-0.071472	2.600928
H	-1.445546	-4.133622	0.638426
H	1.808266	0.006025	1.512554
H	0.983593	-1.113661	0.375453
H	1.762313	1.809545	-0.118330
H	1.013375	0.774979	-1.339659
H	2.863364	-2.713936	-0.497345
H	4.265603	-1.880717	-1.240940
H	2.613402	-1.682621	-1.888425
C	2.985198	-0.632009	-0.076020
O	4.012638	0.052657	0.218777

```
     O       3.861806      1.149184       1.046854
     O       0.034383     -3.372241      -0.493001
Rotational constants (GHz):    0.3894000    0.3398100    0.2128900
Vibrational harmonic frequencies (cm-1):
      15.7656                  31.3529                  43.3190
      49.3355                  61.5925                  73.2592
      76.6501                 106.9057                 119.1595
     135.3457                 159.4296                 173.1435
     201.0960                 212.4870                 234.9456
     241.6571                 271.8048                 278.1704
     295.6209                 319.6232                 339.4930
     347.8885                 376.3049                 377.6482
     390.2928                 457.8409                 484.6173
     497.5492                 504.7623                 558.4607
     584.0231                 617.3378                 648.9459
     721.6203                 740.9614                 778.7494
     794.0281                 814.1398                 863.7356
     877.7835                 883.2604                 893.9584
     916.7295                 923.8671                 932.2066
     950.3115                 956.2583                 978.6905
     994.7559                1001.2429                1010.5403
    1019.5832                1033.5043                1042.8345
    1045.3028                1056.9705                1078.3142
    1113.8096                1124.6120                1179.1059
    1187.6236                1204.9246                1209.3298
    1220.6056                1224.5191                1253.1074
    1260.6122                1268.3860                1284.9177
    1301.3001                1326.6453                1337.0977
    1340.8102                1354.9749                1373.7353
    1380.7754                1401.0667                1413.4110
    1416.6669                1419.8355                1422.3363
    1451.4948                1454.0431                1461.2203
    1467.4689                1470.7379                1484.5686
    1486.0840                1489.3582                1495.6203
    1501.1394                1507.6953                1507.9555
    1553.6898                1701.1865                1802.2248
    2868.2509                3010.8806                3016.8273
    3017.3917                3021.2570                3023.1422
    3024.7747                3026.8106                3034.4201
    3038.6957                3044.0711                3062.3723
    3071.1366                3072.6095                3079.4724
    3080.0465                3083.5414                3087.8456
    3092.7571                3098.5785                3124.0683
    3135.4919                3136.5307                3215.8306
Zero-point correction (Hartree): 0.362039
```

CI-2a

```
---------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.742362370
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.989561     -0.732129       0.556775
     C       1.826391     -0.166414      -0.633758
     C       2.099867     -1.814644       0.748204
     C       3.081305     -0.958141      -0.106173
     C       4.020132     -0.130554       0.778569
     C       3.880341     -1.708393      -1.170184
     C      -0.440002     -1.193742       0.352877
     C      -1.366521     -0.907648       1.516403
     C      -2.860534     -1.202815       1.307483
     C      -0.828194     -1.838379      -0.749686
```

C	-3.473430	-0.357798	0.245216
C	0.577456	2.032288	-1.207892
C	1.928267	1.336008	-0.894625
C	0.504229	3.593930	0.870698
H	1.021495	-0.030288	1.396456
H	1.487295	-0.650195	-1.554973
H	1.826039	-2.745666	0.247417
H	2.403227	-2.039844	1.773856
H	4.748424	-0.787610	1.264146
H	3.484198	0.402528	1.569146
H	4.579281	0.607550	0.195246
H	4.619179	-2.373388	-0.710462
H	4.422217	-1.014536	-1.822220
H	3.227342	-2.319462	-1.799937
H	-1.259108	0.148114	1.785730
H	-1.020008	-1.474865	2.389876
H	-3.379397	-0.988199	2.252679
H	-3.049380	-2.255598	1.082345
H	-1.839066	-2.194791	-0.896852
H	-0.140504	-2.038930	-1.563569
H	-3.223049	0.689546	0.088834
H	0.774120	2.910896	-1.833663
H	-0.087650	1.369007	-1.763270
H	2.596882	1.483517	-1.749538
H	2.412187	1.837839	-0.051701
H	1.187590	3.114016	1.578907
H	-0.253707	4.129411	1.441652
H	1.093341	4.292175	0.272032
C	-0.171651	2.530882	0.018148
O	-1.270180	2.111423	0.320026
O	-4.927050	-0.105050	-1.476553
O	-4.332049	-0.877115	-0.516531

Rotational constants (GHz): 0.5645800 0.2487900 0.2040000

Vibrational harmonic frequencies (cm-1):

18.8147	29.3899	33.8864
51.2236	56.2775	68.6513
77.3610	99.7308	108.6326
119.8182	150.0736	187.1273
214.7955	216.1077	230.5191
247.6210	264.2120	286.8694
290.6515	308.0789	333.2896
356.2965	372.0329	405.7607
438.7427	456.9028	484.3040
512.3410	526.1055	540.8158
567.7819	590.8618	609.1256
709.6354	735.4906	758.3107
792.4556	815.5631	868.7306
879.6398	885.7331	893.9366
906.6397	924.9533	933.9855
939.7079	951.9739	971.7422
986.2569	992.1734	993.4338
1015.9131	1025.1652	1045.5463
1046.8511	1051.1524	1108.4986
1115.6015	1124.5597	1162.1747
1179.0208	1202.4364	1209.0608
1222.5237	1227.4177	1239.8840
1253.3504	1258.6967	1274.4059
1282.0287	1312.1266	1325.4166
1346.7080	1356.7322	1373.7542
1378.9843	1385.2535	1398.8292
1401.0563	1412.5566	1419.4109

1454.7590	1467.1766	1469.7386
1471.6993	1477.8558	1483.6041
1487.3381	1488.0618	1496.5004
1500.2077	1508.8415	1511.0071
1552.0572	1702.9618	1775.0346
2992.3478	3010.2550	3012.3802
3017.9146	3019.3061	3027.8763
3030.5411	3036.1492	3040.6418
3043.9188	3052.2147	3066.5352
3069.6096	3079.0082	3079.6776
3080.6704	3083.6024	3095.4366
3097.0674	3102.3459	3138.1505
3149.3138	3159.7668	3225.9551

Zero-point correction (Hartree): 0.362017

CI-1b

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.753484593
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.795085	-0.726178	-0.451661
C	-1.801603	-0.141158	0.584520
C	-1.876947	-1.792198	-0.825926
C	-2.967903	-0.926977	-0.126175
C	-3.761393	-0.098011	-1.142459
C	-3.918329	-1.671173	0.809702
C	0.573429	-1.232551	-0.043549
C	1.598309	-1.196403	-1.159229
C	2.984311	-1.777175	-0.848442
C	0.831499	-1.713073	1.174785
C	3.797548	-0.944307	0.125573
C	-0.655509	2.068897	1.330111
C	-1.933002	1.367466	0.791501
C	0.083893	3.361455	-0.838033
H	-0.678298	-0.026566	-1.287221
H	-1.626351	-0.606569	1.559050
H	-1.695226	-2.731567	-0.299348
H	-2.022121	-2.002770	-1.888306
H	-4.412947	-0.754565	-1.727218
H	-3.111064	0.426146	-1.848671
H	-4.397581	0.645881	-0.652454
H	-4.586737	-2.331398	0.246916
H	-4.544646	-0.973470	1.376568
H	-3.367743	-2.287360	1.526064
H	1.723120	-0.152054	-1.473179
H	1.178115	-1.720494	-2.027662
H	3.560230	-1.787750	-1.784211
H	2.940312	-2.806598	-0.483795
H	1.801607	-2.105610	1.449606
H	0.078346	-1.732431	1.954478
H	3.766100	0.149039	-0.058150
H	-0.952587	3.011820	1.805562
H	-0.161073	1.454177	2.084296
H	-2.737057	1.549157	1.512616
H	-2.245467	1.856439	-0.136027
H	0.173739	2.840981	-1.797705
H	0.899989	4.092261	-0.846113
H	-0.887382	3.845037	-0.747284
C	0.332562	2.408455	0.264147
O	1.459684	1.835095	0.339049
O	2.384712	2.108571	-0.657129

```
     O       4.449859     -1.415434       1.027203
Rotational constants (GHz):    0.5372700    0.2926800    0.2214800
Vibrational harmonic frequencies (cm-1):
      27.9819                  35.9656                  44.7375
      52.4764                  70.3033                  84.9733
      96.7602                 111.2317                 141.5473
     161.0482                 172.5486                 193.8448
     208.8839                 222.4943                 245.4140
     257.1919                 265.6761                 285.4989
     298.7123                 319.9860                 348.6069
     358.1891                 361.7035                 387.6181
     403.4496                 449.8785                 481.5733
     507.7494                 519.4745                 541.8454
     566.2985                 602.6706                 618.5889
     717.5629                 738.4314                 770.9846
     781.2610                 811.5586                 864.6990
     879.7175                 882.5016                 894.6054
     903.5603                 910.4071                 927.5460
     943.0773                 952.1547                 982.9803
     992.2933                1008.4348                1014.5761
    1029.3471                1034.6054                1044.0164
    1048.8451                1065.3322                1089.6658
    1107.4878                1118.7379                1167.9547
    1186.0512                1207.5957                1211.1860
    1220.5617                1228.6520                1243.9513
    1256.6479                1264.8548                1279.8627
    1295.6202                1311.6009                1340.6489
    1349.0652                1362.7977                1377.5607
    1394.7685                1399.3260                1403.3956
    1412.2907                1422.1567                1430.4795
    1435.3691                1451.4656                1467.6599
    1471.8880                1475.7308                1479.0587
    1485.4221                1485.9689                1495.4912
    1499.5116                1507.6178                1510.0901
    1548.2920                1702.0388                1795.9801
    2922.0764                2996.4032                3008.3831
    3010.1096                3015.0686                3015.2987
    3018.8635                3026.7719                3027.9797
    3030.7198                3040.2017                3045.7117
    3066.3226                3067.6024                3068.8872
    3078.3793                3080.8944                3081.1292
    3083.0806                3099.5044                3102.8413
    3143.8151                3144.3098                3225.4114
Zero-point correction (Hartree): 0.362087
```

CI-2b

```
-------------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.749461400
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.702590     -0.763814      -0.241332
     C      -1.901360     -0.202783       0.578231
     C      -1.610755     -1.966285      -0.667582
     C      -2.868383     -1.175750      -0.198382
     C      -3.596740     -0.533362      -1.383849
     C      -3.856880     -1.946180       0.675303
     C       0.609840     -1.132825       0.406830
     C       1.705559     -1.567453      -0.547210
     C       2.514713     -0.380766      -1.153578
     C       0.820399     -1.140610       1.724469
     C       3.332144      0.307565      -0.133507
```

C	-1.089972	2.196832	1.164173
C	-2.220876	1.293311	0.614256
C	-0.574249	3.401779	-1.084227
H	-0.509081	-0.131140	-1.116288
H	-1.825243	-0.563046	1.608464
H	-1.418057	-2.842924	-0.045209
H	-1.585435	-2.264898	-1.718272
H	-4.086715	-1.308332	-1.981407
H	-2.914441	0.005339	-2.048041
H	-4.369791	0.168177	-1.054943
H	-4.367742	-2.724961	0.099111
H	-4.625382	-1.280690	1.083928
H	-3.350677	-2.430107	1.515225
H	1.276389	-2.129922	-1.382765
H	2.420759	-2.221217	-0.047723
H	1.856654	0.347372	-1.630911
H	3.212305	-0.800061	-1.887292
H	1.767452	-1.472269	2.136454
H	0.071241	-0.822112	2.439182
H	3.091430	1.278532	0.283795
H	-1.541947	3.113682	1.563774
H	-0.551645	1.712331	1.980036
H	-3.106577	1.431628	1.243672
H	-2.510751	1.643654	-0.380026
H	-0.945432	2.691138	-1.829615
H	0.247508	3.963923	-1.526557
H	-1.401603	4.071191	-0.836587
C	-0.064213	2.649876	0.135581
O	1.123428	2.448139	0.281680
O	4.765473	-1.449544	-0.100068
O	4.384468	-0.207657	0.343006

Rotational constants (GHz): 0.5587600 0.2682300 0.2094500

Vibrational harmonic frequencies (cm-1):

25.6306	34.8241	46.9395
51.8306	63.8459	72.2652
93.8878	110.0268	117.4151
120.9375	141.7608	182.6549
197.3492	240.5583	247.9084
269.9152	290.1904	302.4903
315.5535	328.1817	354.0405
372.3591	381.8694	412.6166
452.7220	469.6459	496.6726
530.9864	539.9179	565.5160
585.7227	636.0116	688.4655
723.3725	733.4730	759.7464
789.3170	828.4207	859.6070
868.2146	881.7736	883.4503
891.0154	893.1941	928.4041
936.7260	954.9744	968.8742
976.8277	993.8458	1001.0305
1010.1859	1028.7466	1031.4204
1044.6030	1053.8245	1055.1609
1110.0656	1122.9713	1170.4739
1175.6314	1193.5051	1209.6398
1226.1736	1235.8450	1240.4496
1252.4816	1258.7736	1264.8459
1280.2529	1312.5615	1337.6924
1340.9842	1349.7133	1356.9847
1375.6292	1380.9994	1386.5227
1403.7902	1407.9046	1421.6286
1448.6746	1452.2678	1467.9065

```
    1472.5743                1484.2129                1485.3511
    1489.9009                1495.6882                1502.7532
    1509.1725                1511.8640                1513.2634
    1552.2280                1701.5818                1779.1081
    3006.6983                3010.3414                3012.2548
    3018.1384                3028.1921                3030.5573
    3035.5877                3038.1052                3040.2827
    3044.9896                3068.1732                3072.4600
    3079.4748                3080.9954                3083.1662
    3094.4541                3097.5727                3098.3206
    3104.0118                3113.0166                3137.6820
    3138.2582                3207.1939                3214.9890
Zero-point correction (Hartree): 0.363080
```

ROOH-1a

```
------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.771218297
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.131191     -1.079697      -0.305071
     C      -1.457763      0.232520       0.467300
     C      -2.669084     -1.362875      -0.389311
     C      -2.956220      0.119891      -0.004055
     C      -3.297985      0.963635      -1.236598
     C      -4.000367      0.332955       1.090619
     C      -0.271471     -2.174927       0.281664
     C       0.426572     -3.066820      -0.727779
     C       1.760733     -2.462250      -1.232180
     C      -0.140979     -2.395652       1.591615
     C       2.847731     -2.568395      -0.189556
     C       0.815774      1.339482       0.474573
     C      -0.656453      1.495924       0.153368
     C       3.281931      1.832636       0.581662
     H      -0.752079     -0.823285      -1.300294
     H      -1.420879      0.045965       1.545704
     H      -2.980912     -2.060222       0.391506
     H      -3.061011     -1.707186      -1.349966
     H      -4.290104      0.690321      -1.610563
     H      -2.585978      0.811380      -2.052054
     H      -3.312792      2.032466      -1.003072
     H      -5.003484      0.070888       0.736799
     H      -4.025834      1.380120       1.411533
     H      -3.784590     -0.281865       1.969312
     H      -0.227613     -3.232863      -1.589349
     H       0.622508     -4.051126      -0.289461
     H       1.650696     -1.416356      -1.525434
     H       2.100225     -3.032893      -2.107088
     H       0.443353     -3.228273       1.969260
     H      -0.607450     -1.761832       2.336590
     H       3.034430     -3.606751       0.171195
     H       0.491123      4.651018       0.035086
     H       1.102368      0.402641       0.939064
     H      -1.089836      2.331926       0.713890
     H      -0.776996      1.761661      -0.899431
     H       3.376938      0.788138       0.871896
     H       3.655079      2.475713       1.384951
     H       3.914400      2.002063      -0.294544
     C       1.850277      2.156783       0.254669
     O       1.861582      3.420347      -0.310626
     O       0.536565      3.927272      -0.605038
     O       3.491778     -1.650232       0.250538
```

Rotational constants (GHz): 0.3776900 0.3462700 0.2031700
Vibrational harmonic frequencies (cm-1):

13.6676	16.6910	31.2794
53.8765	54.4987	64.6557
80.8568	89.2703	101.1596
139.6153	151.7138	172.2774
175.0278	208.4783	210.7184
217.3859	237.8238	252.3294
275.6531	286.3559	319.4015
340.2975	360.4069	366.2737
390.2024	400.1229	463.4069
480.6714	500.5147	519.1162
558.7026	572.7731	624.3581
662.6797	719.6082	745.1764
777.7225	787.7889	823.4594
864.5706	884.8381	890.2279
895.8645	899.1136	920.2738
937.0973	953.2325	958.4338
987.6276	993.0996	1006.0516
1013.2400	1022.7651	1033.9706
1049.2040	1070.8329	1074.9238
1087.6072	1113.8311	1120.1500
1161.5075	1187.4593	1193.5082
1209.5850	1219.9619	1222.7656
1224.5189	1255.8794	1266.3197
1276.4863	1307.9954	1318.9488
1338.4796	1351.9582	1362.5945
1378.2387	1397.3485	1402.7377
1410.9686	1420.0818	1421.7654
1423.0594	1451.9490	1466.2329
1474.1894	1476.9695	1486.1708
1487.9600	1495.2226	1496.2382
1497.1532	1506.9883	1509.4303
1700.7714	1737.5827	1813.6844
2844.3157	3008.4287	3008.8248
3016.1509	3018.4662	3023.1358
3027.1844	3028.3699	3034.7162
3039.9739	3062.5853	3065.4328
3068.3726	3077.3101	3077.9744
3078.9877	3088.6690	3094.5216
3098.1464	3133.7991	3149.4272
3170.4780	3210.9453	3768.9181

Zero-point correction (Hartree): 0.361251

ROOH-1b

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.779468834
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.084167	0.792296	0.264585
C	-1.821563	-0.374776	-0.447433
C	-2.439881	1.569116	0.304786
C	-3.191583	0.227967	0.044613
C	-3.712871	-0.383055	1.350255
C	-4.303491	0.271045	-1.001542
C	0.112861	1.478144	-0.342970
C	0.812067	2.465121	0.582891
C	2.318483	2.662700	0.316563
C	0.523560	1.267684	-1.594563
C	3.032553	1.343413	0.428933
C	-0.113940	-2.321584	-0.670074

C	-1.478486	-1.834597	-0.145562
C	1.147239	-1.917097	1.518212
H	-0.818780	0.479630	1.279486
H	-1.773805	-0.225658	-1.531601
H	-2.525616	2.255480	-0.541710
H	-2.687387	2.105822	1.224320
H	-4.552212	0.208834	1.729132
H	-2.948677	-0.405514	2.132002
H	-4.070416	-1.406450	1.201660
H	-5.160132	0.851479	-0.642266
H	-4.663733	-0.736390	-1.237077
H	-3.955549	0.729155	-1.931855
H	0.684970	2.123124	1.616339
H	0.311749	3.439070	0.534123
H	2.726238	3.334878	1.082648
H	2.526961	3.104316	-0.658915
H	1.387226	1.766957	-2.015389
H	0.018882	0.571093	-2.251127
H	2.800176	0.765027	1.346197
H	-0.148154	-3.408582	-0.806442
H	0.074182	-1.906355	-1.664842
H	-2.249105	-2.457338	-0.615415
H	-1.552802	-2.034203	0.926655
H	2.089787	-1.802105	2.030501
H	3.712163	-0.971181	-0.218672
H	0.242840	-1.993964	2.103079
C	1.097039	-2.029407	0.190643
O	2.181636	-1.980638	-0.650777
O	3.429018	-1.864660	0.069357
O	3.782381	0.884178	-0.404436

Rotational constants (GHz): 0.5904900 0.2940300 0.2262300

Vibrational harmonic frequencies (cm-1):

37.0078	51.6710	53.4462
70.4517	76.2694	94.4876
120.6321	121.3916	138.4911
153.0828	186.0120	218.8146
225.8127	238.1231	262.0711
273.4776	282.7768	295.3123
301.0921	356.6044	358.6211
376.0459	397.4605	425.2308
458.2497	482.7579	491.7390
515.5330	538.0885	573.1239
583.9733	626.5941	670.9339
706.8141	745.6192	747.5533
785.5024	794.8398	833.9699
837.1420	867.6131	875.0024
886.3237	909.5372	915.8268
925.8514	927.9006	950.1270
957.4139	971.8885	993.4966
1006.4773	1013.1242	1028.9564
1032.4619	1054.5020	1058.3463
1091.9271	1112.7937	1126.5815
1171.3350	1188.6890	1204.3081
1209.4806	1220.5483	1226.0685
1234.2521	1248.0036	1262.7485
1270.3487	1283.9295	1318.6449
1336.6800	1346.8482	1379.6608
1386.3015	1396.2525	1403.2942
1411.3620	1415.2884	1420.2834
1438.3889	1451.0245	1476.7800
1480.2068	1484.3904	1485.6624

1487.7408	1492.4242	1495.8770
1499.0355	1508.8237	1510.2497
1703.8032	1706.2832	1788.8892
2916.8950	3008.9625	3013.8955
3015.0407	3018.3460	3023.0589
3024.3562	3028.8529	3036.5334
3038.8121	3045.5299	3056.8951
3067.0991	3072.1726	3078.3896
3079.1372	3086.7310	3091.1296
3104.0699	3157.1956	3182.8894
3229.6176	3273.3318	3530.8236

Zero-point correction (Hartree): 0.363907

ROOH-2b

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.780379366
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.515168	0.440073	0.436081
C	0.852726	1.181445	0.449682
C	-1.225332	1.829191	0.366430
C	0.123251	2.479023	-0.066331
C	0.190118	2.673060	-1.585222
C	0.505924	3.772185	0.650890
C	-0.949662	-0.498309	1.530274
C	-2.323886	-1.125099	1.330554
C	-2.334207	-2.140211	0.211876
C	-0.227254	-0.766013	2.619881
C	-2.975205	-2.185492	-0.955821
C	2.623876	-0.655180	0.276371
C	2.026866	0.610113	-0.341293
C	4.484568	-2.437572	0.085044
H	-0.641001	-0.071929	-0.524748
H	1.163665	1.364107	1.484809
H	-1.543959	2.162462	1.357785
H	-2.065552	1.920294	-0.325687
H	-0.485585	3.480110	-1.887174
H	-0.106718	1.773477	-2.131025
H	1.197876	2.943918	-1.913558
H	-0.157099	4.594756	0.361130
H	1.530513	4.071929	0.404434
H	0.441350	3.657388	1.736816
H	-3.059909	-0.344901	1.144329
H	-2.612007	-1.631778	2.258029
H	-1.698446	-3.005823	0.379417
H	-4.351880	0.438571	-1.536682
H	-0.599711	-1.431302	3.391989
H	0.750271	-0.330062	2.788200
H	-2.853828	-3.031287	-1.626287
H	3.030991	-0.456952	1.276298
H	1.846830	-1.414339	0.435770
H	2.814951	1.367384	-0.426052
H	1.722856	0.384680	-1.366565
H	5.135281	-2.035404	0.869044
H	5.097136	-2.943496	-0.660295
H	3.807886	-3.150318	0.564964
C	3.716079	-1.300580	-0.566494
O	3.964316	-0.933549	-1.693154
O	-4.133184	-0.158488	-0.808326
O	-3.856140	-1.354375	-1.586828

Rotational constants (GHz): 0.4388600 0.2432700 0.1987800

Vibrational harmonic frequencies (cm-1):

15.0227	22.6970	38.0961
43.7594	52.5950	69.4779
75.5149	79.5104	86.7815
90.4249	106.7490	135.3391
168.4700	206.5717	208.9252
223.9243	237.6968	244.6673
274.3356	281.8633	326.2540
343.5139	367.9014	377.5514
393.5049	453.8760	466.7511
482.3500	502.3965	527.0341
564.9807	609.0948	657.1890
715.7069	734.3790	750.9846
757.8528	768.1696	808.9238
847.3710	859.8237	885.2790
900.3474	907.6749	916.0589
933.7416	944.7217	946.8519
951.1691	954.1335	977.2302
991.9783	998.1952	1020.3446
1031.4916	1049.8161	1078.1581
1103.4492	1112.0270	1133.5241
1167.9640	1182.2299	1191.7970
1209.5982	1211.7590	1221.4880
1261.4540	1269.7712	1273.4106
1300.9875	1306.2006	1309.0829
1331.0879	1333.5695	1361.7217
1382.5737	1390.8723	1393.8098
1401.7596	1408.4173	1418.7141
1435.1984	1444.3181	1453.7181
1466.9041	1478.0089	1483.3126
1486.4079	1486.9492	1491.5725
1496.4231	1506.4630	1509.2400
1696.9413	1732.8854	1793.4235
3007.7753	3008.4817	3015.0603
3018.4499	3022.9060	3027.7760
3027.8705	3028.3451	3035.7716
3040.0405	3065.7872	3075.5355
3077.7339	3079.8482	3085.2713
3087.9606	3092.5370	3120.9215
3131.3354	3137.2564	3141.1434
3173.5681	3209.2369	3791.7181

Zero-point correction (Hartree): 0.361332

Dioxirane-1a

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.779804836
Electronic state : 1-A
Cartesian coordinates (Angs):

C	1.596445	0.118822	-0.070219
C	0.851429	-1.180699	0.347824
C	2.905974	-0.726132	-0.203345
C	2.040687	-2.023280	-0.247328
C	1.808423	-2.502665	-1.684897
C	2.522254	-3.180321	0.625307
C	1.632775	1.356880	0.790544
C	2.087131	2.629219	0.097306
C	1.064286	3.173572	-0.932556
C	1.316040	1.370005	2.086957
C	-0.253701	3.524553	-0.285558
C	-1.600136	-0.509954	0.581344
C	-0.576579	-1.397658	-0.146988

C	-3.319230	-0.074595	-1.311980
H	1.261273	0.396387	-1.075475
H	0.875664	-1.294691	1.436667
H	3.506232	-0.666456	0.707870
H	3.547387	-0.527915	-1.066042
H	2.731035	-2.930542	-2.090031
H	1.503392	-1.691520	-2.351780
H	1.037157	-3.277470	-1.727253
H	3.451268	-3.609223	0.234350
H	1.777465	-3.982670	0.661692
H	2.711075	-2.850970	1.651063
H	3.030663	2.450389	-0.430436
H	2.289793	3.400694	0.846404
H	0.873178	2.458798	-1.734746
H	1.474682	4.086939	-1.381757
H	1.391608	2.277676	2.676526
H	0.972157	0.486219	2.610011
H	-0.193611	4.301412	0.509431
H	-1.633550	-0.773765	1.641200
H	-1.311990	0.542298	0.508353
H	-0.858434	-2.447508	-0.004559
H	-0.617360	-1.206337	-1.224562
H	-3.070561	0.989388	-1.332277
H	-4.378365	-0.213624	-1.526489
H	-2.731157	-0.575196	-2.085661
C	-3.007604	-0.650289	0.044687
O	-3.661850	-1.848696	0.369923
O	-4.030083	-0.537777	0.997730
O	-1.314087	3.023089	-0.567538

Rotational constants (GHz): 0.4028800 0.3279000 0.2136600

Vibrational harmonic frequencies (cm-1):

19.5152	36.0817	41.0596
48.1892	57.2389	73.6740
81.4968	88.2957	114.3582
145.8565	169.2469	190.5020
211.2766	216.2776	226.4787
247.4697	275.9983	280.4805
322.1744	346.7354	372.6364
377.6988	382.2749	388.2758
443.2145	472.7030	477.6448
494.8335	502.7979	551.5007
578.1073	649.2855	717.5257
730.8356	746.9365	774.9094
791.4034	822.9878	842.3221
868.2249	877.3188	888.7014
894.6437	920.3160	933.2085
950.3968	955.2988	984.3641
995.8118	1002.6155	1017.0546
1026.3227	1039.9812	1043.2887
1050.8083	1078.7763	1092.7549
1111.3041	1126.1811	1177.6043
1180.6810	1201.9273	1209.6340
1222.7828	1226.1050	1249.1237
1260.9411	1264.6399	1274.5666
1293.6210	1312.1727	1324.4447
1341.8651	1355.6992	1367.8915
1389.0484	1399.5817	1405.0665
1414.0897	1421.0927	1421.7232
1425.8531	1454.1112	1468.8718
1475.5474	1485.2120	1486.5694
1488.3167	1490.8659	1495.8333

1498.1364	1500.7487	1508.8071
1509.2874	1702.3756	1805.5870
2865.0828	3010.4129	3014.3983
3016.5773	3019.5338	3023.8564
3027.0689	3033.8059	3039.1796
3041.5863	3051.8168	3054.9853
3062.5534	3069.1506	3078.5422
3080.6786	3085.9464	3092.4945
3100.8621	3101.4366	3105.5316
3137.3576	3138.2715	3217.1338

Zero-point correction (Hartree): 0.362562

Dioxirane-2a

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.776816832
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.905595	-0.700523	0.533216
C	1.851347	-0.194292	-0.599436
C	1.953990	-1.820025	0.833963
C	3.029479	-1.027161	0.032392
C	3.942119	-0.220911	0.962775
C	3.865598	-1.837931	-0.956131
C	-0.521808	-1.114709	0.231671
C	-1.507965	-0.815954	1.343028
C	-2.992383	-1.100785	1.082645
C	-0.856848	-1.738871	-0.899405
C	-3.625357	-0.209671	0.043879
C	0.726140	2.040190	-1.262890
C	2.029598	1.299336	-0.871608
C	0.573886	3.516728	0.874871
H	0.901481	0.018110	1.359585
H	1.561159	-0.678656	-1.536631
H	1.678585	-2.753939	0.339516
H	2.173406	-2.026446	1.884683
H	4.600127	-0.898017	1.516420
H	3.377624	0.358395	1.699063
H	4.577750	0.473774	0.404508
H	4.542127	-2.520642	-0.430770
H	4.479796	-1.184721	-1.585662
H	3.231025	-2.438260	-1.614303
H	-1.400827	0.240477	1.615368
H	-1.197087	-1.378535	2.233662
H	-3.540776	-0.925247	2.015958
H	-3.173308	-2.141030	0.799991
H	-1.869019	-2.056756	-1.111377
H	-0.123467	-1.953892	-1.669028
H	-3.341980	0.842217	0.064607
H	0.991968	2.921538	-1.860237
H	0.080079	1.407266	-1.873576
H	2.747863	1.410788	-1.691179
H	2.486948	1.793257	-0.009397
H	1.129685	2.947277	1.626855
H	-0.190000	4.100388	1.387796
H	1.285954	4.177770	0.375397
C	-0.100088	2.556670	-0.094339
O	-1.260439	2.239342	0.063826
O	-4.964953	-0.463072	-0.261095
O	-3.855724	-0.717229	-1.236361

Rotational constants (GHz): 0.5858000 0.2572600 0.2077100
Vibrational harmonic frequencies (cm-1):

```
      34.0742                39.4839                46.9785
      51.5294                64.9223                84.6170
      91.5410               102.0251               114.3131
     116.5890               151.5669               201.0924
     219.9374               233.9337               255.9269
     265.1770               282.5118               287.7278
     304.8929               306.4892               356.8071
     375.0562               408.8492               439.6208
     447.1817               470.0777               497.3392
     520.6050               529.0862               565.3493
     585.5751               609.9220               719.7869
     734.7615               757.7187               788.8773
     800.0926               833.9830               864.4824
     870.2121               882.6787               891.2795
     897.3090               932.3634               940.0232
     953.1819               970.1589               976.4443
     989.1565               994.3839              1018.2382
    1029.3695              1044.3647              1050.2986
    1055.8355              1092.5438              1111.5485
    1124.9316              1164.2167              1165.2521
    1184.4367              1208.7462              1217.1433
    1223.9941              1229.8923              1240.5320
    1253.7217              1272.6247              1276.7953
    1282.6549              1299.3463              1313.1572
    1349.6926              1356.0525              1360.2495
    1379.1254              1386.0837              1400.1106
    1403.0096              1412.1159              1421.6198
    1455.5869              1460.6068              1467.7938
    1471.0277              1480.5683              1482.6936
    1483.5531              1486.4773              1488.1245
    1496.7760              1501.0893              1509.2152
    1510.6368              1704.1094              1777.8184
    3000.3130              3009.7557              3011.7582
    3016.9964              3024.2385              3028.3029
    3028.9088              3034.9898              3037.3942
    3040.7794              3044.8041              3066.1398
    3069.1128              3077.4226              3080.1549
    3082.2369              3083.7749              3094.3843
    3097.3052              3100.9483              3126.0087
    3136.9926              3145.0935              3226.4214
Zero-point correction (Hartree): 0.363654
```

Dioxirane-1b

```
------------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.777375576
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.951150     -1.220580      0.551244
     C       1.587170     -0.160374     -0.409441
     C       2.283645     -2.016939      0.449741
     C       3.006578     -0.727514     -0.050152
     C       3.699560      0.017282      1.096560
     C       3.964187     -0.900177     -1.227007
     C      -0.380007     -1.860996      0.218053
     C      -1.484641     -1.565871      1.215340
     C      -2.890302     -2.072172      0.868091
     C      -0.553351     -2.616955     -0.868543
     C      -3.517706     -1.347885     -0.303798
     C      -0.164774      1.641997     -0.753727
     C       1.241841      1.312778     -0.212848
     C      -0.166242      4.216661     -0.392183
```

```
      H       0.883231     -0.777481      1.550084
      H       1.360477     -0.450721     -1.441927
      H       2.238200     -2.781691     -0.328640
      H       2.654225     -2.475221      1.370193
      H       4.580634     -0.540941      1.428247
      H       3.046718      0.144911      1.963987
      H       4.036463      1.010168      0.782614
      H       4.858117     -1.458228     -0.928518
      H       4.295848      0.070011     -1.613449
      H       3.489827     -1.443748     -2.049234
      H      -1.526203     -0.480641      1.381664
      H      -1.186254     -1.983724      2.185206
      H      -3.543448     -1.878631      1.729981
      H      -2.915256     -3.147037      0.676621
      H      -1.505661     -3.059924     -1.130066
      H       0.265153     -2.816293     -1.552095
      H      -3.411335     -0.239527     -0.272836
      H      -0.130469      1.770772     -1.841054
      H      -0.847934      0.816053     -0.553152
      H       1.990250      1.942032     -0.708468
      H       1.288102      1.554720      0.854742
      H      -0.719809      4.982059      0.150513
      H      -0.196618      4.438734     -1.462363
      H       0.878685      4.231960     -0.072392
      C      -0.782345      2.869094     -0.126137
      O      -1.288247      2.675087      1.169567
      O      -2.180982      2.854024     -0.021402
      O      -4.112213     -1.883824     -1.204515
Rotational constants (GHz):    0.3950600    0.3196000    0.2012000
Vibrational harmonic frequencies (cm-1):
      27.3752                34.2171                38.1746
      42.2164                62.1142                77.8782
      85.3740               109.8469               134.8979
     153.1084               181.7388               189.0693
     212.9585               227.4352               236.8324
     252.2835               258.8354               277.7571
     299.0178               354.8922               362.9528
     366.3005               389.3683               401.8393
     428.7420               448.1689               492.7452
     509.4969               516.8692               552.2442
     581.4683               617.2271               709.7408
     719.0282               744.4321               771.5729
     781.2373               825.8281               849.4161
     863.8468               880.8302               882.8547
     894.0724               918.3214               931.3696
     948.4857               955.7089               986.0675
     993.6115              1015.5730              1023.4559
    1030.2551              1047.4144              1054.1126
    1060.7484              1076.8450              1091.2311
    1114.1421              1131.1314              1167.8671
    1190.3058              1206.4528              1211.6873
    1220.9571              1226.7121              1249.1871
    1250.0069              1270.6052              1279.0568
    1294.4172              1308.5985              1331.3116
    1343.7761              1365.4266              1386.3127
    1393.8181              1401.0303              1407.2330
    1417.2669              1422.2581              1423.1294
    1423.8669              1450.9957              1472.3876
    1474.2929              1480.9385              1485.8643
    1487.0536              1488.4636              1495.2100
    1499.9931              1500.5322              1507.5746
```

1509.8436	1703.4248	1811.5205
2861.3787	2998.5027	3008.1436
3010.8423	3013.4364	3016.6800
3021.8617	3023.1400	3033.5859
3036.4982	3041.6818	3045.7630
3055.9454	3066.2467	3078.0174
3078.5788	3090.7693	3092.0319
3098.9926	3102.6648	3111.4733
3139.1487	3141.7261	3222.9919

Zero-point correction (Hartree): 0.362626

Dioxirane-2b

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.777164820
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.817727	-0.768291	-0.159995
C	-1.973077	0.068800	0.465858
C	-1.862644	-1.883625	-0.497956
C	-3.016809	-0.866923	-0.254750
C	-3.558297	-0.311606	-1.577052
C	-4.166811	-1.357108	0.623428
C	0.382183	-1.215875	0.638806
C	1.414881	-2.007462	-0.143585
C	2.384125	-1.150906	-0.990364
C	0.534592	-0.995397	1.944801
C	3.346561	-0.354124	-0.151519
C	-0.983679	2.430256	0.939298
C	-2.079342	1.580211	0.256889
C	0.347136	3.016908	-1.219687
H	-0.478382	-0.301109	-1.092492
H	-2.025341	-0.137414	1.539466
H	-1.846221	-2.677088	0.252828
H	-1.810939	-2.334774	-1.491780
H	-4.120932	-1.089612	-2.102522
H	-2.759558	0.020287	-2.246699
H	-4.234629	0.533588	-1.416692
H	-4.746356	-2.134518	0.114200
H	-4.854671	-0.540086	0.867888
H	-3.797298	-1.777222	1.563063
H	0.903573	-2.702142	-0.818828
H	2.006503	-2.620711	0.541904
H	1.830084	-0.459963	-1.635736
H	2.981089	-1.799178	-1.636671
H	1.397466	-1.376182	2.480469
H	-0.174433	-0.420489	2.527020
H	2.935454	0.431688	0.478966
H	-1.347982	3.463113	1.012976
H	-0.785945	2.080403	1.954232
H	-3.047809	1.902036	0.656315
H	-2.109312	1.815616	-0.811163
H	-0.045137	2.251673	-1.896611
H	1.366790	3.258224	-1.517205
H	-0.293758	3.896441	-1.326601
C	0.352220	2.501415	0.211463
O	1.388747	2.190719	0.757298
O	4.589533	-0.062547	-0.717171
O	4.426454	-1.053198	0.396107

Rotational constants (GHz): 0.5869600 0.2644700 0.2143200
Vibrational harmonic frequencies (cm-1):

16.6007	36.9692	44.9815

54.4159	61.2654	68.2275
83.0506	99.7417	106.1207
116.1092	128.8280	184.2601
191.7463	229.7580	246.4018
266.9059	281.1251	287.8118
307.2446	346.6090	369.1985
382.6873	411.3972	435.4538
458.9151	467.8199	494.8627
500.2301	530.1323	563.2374
581.3109	653.6587	724.5701
732.0936	754.3868	781.9434
794.2018	850.8376	861.0667
871.8904	876.8029	880.6675
893.9764	930.8665	938.1197
954.0710	965.8754	977.2848
992.4452	1006.2731	1014.7445
1029.8597	1033.0908	1045.4085
1051.7823	1082.2779	1111.0140
1120.3949	1155.4946	1168.9967
1186.1927	1207.1449	1215.3845
1226.2930	1237.6041	1247.4678
1252.3436	1257.3388	1264.2582
1279.3440	1301.3936	1313.0496
1339.2764	1353.1960	1359.2039
1366.1003	1378.2789	1385.0515
1402.8912	1408.0700	1423.1823
1454.6979	1465.2580	1466.9882
1469.1012	1481.9010	1483.5966
1484.7158	1487.4008	1494.1468
1499.1553	1499.6006	1508.6309
1511.4156	1706.5671	1783.2885
3007.5447	3009.8797	3010.5839
3018.6765	3025.2804	3026.8433
3031.1244	3034.4972	3037.5045
3043.1521	3062.7068	3068.6282
3070.3540	3079.0640	3081.7635
3083.5989	3086.3863	3091.0479
3095.4454	3097.1456	3139.0374
3141.0985	3144.8161	3219.0676

Zero-point correction (Hartree): 0.363396

Acid-2a

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.928936113
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.883075	-1.243041	-0.527103
C	-1.653585	-0.221005	0.374759
C	-2.069823	-2.229559	-0.320140
C	-2.972231	-1.040482	0.130731
C	-3.828853	-0.508542	-1.024324
C	-3.837217	-1.276968	1.366609
C	0.530127	-1.661211	-0.179711
C	1.549261	-1.409200	-1.273294
C	3.017633	-1.699240	-0.940489
C	0.838972	-2.213997	0.995592
C	3.624258	-0.811747	0.123295
C	-0.244834	1.900872	0.410900
C	-1.590931	1.267690	0.053048
C	1.214823	4.029454	0.299269
H	-0.899264	-0.876426	-1.558639

H	-1.345438	-0.382417	1.414557
H	-1.871637	-2.923909	0.499499
H	-2.394388	-2.800556	-1.193860
H	-4.626225	-1.221334	-1.257644
H	-3.247241	-0.356286	-1.937540
H	-4.300009	0.444893	-0.767625
H	-4.642250	-1.988898	1.154506
H	-4.302356	-0.345239	1.706630
H	-3.246084	-1.678164	2.195188
H	1.459632	-0.369180	-1.606173
H	1.269705	-2.014641	-2.145249
H	3.614970	-1.552214	-1.847253
H	3.165056	-2.730809	-0.620159
H	1.845966	-2.507832	1.263181
H	0.079876	-2.392102	1.749786
H	-0.063472	1.841643	1.492688
H	0.591593	1.351139	-0.037715
H	-2.383728	1.796592	0.593523
H	-1.793849	1.438762	-1.007894
H	1.435940	3.979338	1.370064
H	1.184259	5.070183	-0.020599
H	2.023397	3.507486	-0.222402
C	-0.115696	3.360500	-0.002977
O	-1.015316	3.958235	-0.549535
O	4.290456	-1.182289	1.054645
O	3.370216	0.506801	-0.099174
H	3.809720	0.986850	0.618655

Rotational constants (GHz): 0.4168700 0.2920100 0.1916100

Vibrational harmonic frequencies (cm-1):

21.8700	24.8410	35.0061
40.2975	49.4595	60.9442
83.0988	84.2136	96.1551
120.8516	153.5210	176.9233
205.4382	225.5686	236.3829
249.1000	255.3318	278.0068
287.7326	337.8842	353.7130
383.3188	396.5145	440.6781
454.4716	476.7998	497.9167
533.6364	555.1757	559.5654
597.0494	614.7821	627.6130
693.4046	717.0378	736.7019
756.4397	806.0497	814.3212
849.1451	862.8095	885.6408
897.3713	921.5752	937.1192
943.0685	953.8476	961.7810
980.5200	989.1036	992.0947
1017.0882	1029.4652	1048.4203
1062.0502	1076.4814	1114.4844
1134.2831	1151.9255	1167.0319
1179.9875	1194.6848	1211.8353
1217.0383	1223.2246	1243.3286
1256.7859	1265.0917	1275.5228
1302.4886	1310.3465	1329.7186
1338.6986	1370.7450	1373.4327
1384.1597	1391.3499	1400.3636
1404.5820	1413.4432	1421.2785
1453.2165	1454.4459	1470.7875
1475.4575	1478.7117	1480.2728
1485.9788	1486.6272	1492.9203
1497.3090	1508.7906	1509.6137
1703.0524	1794.4026	1828.5092

```
    3007.5693                3008.3677                3008.6410
    3014.3875                3020.0919                3027.6818
    3028.9545                3033.3529                3041.0420
    3041.3183                3041.7369                3043.6796
    3067.6069                3075.0101                3077.3072
    3079.6987                3084.6560                3087.2405
    3095.0280                3113.8794                3138.1775
    3140.8239                3219.4804                3756.5063
Zero-point correction (Hartree): 0.364264
```

Ester-1a

```
----------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.903183961
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.588075     -0.168838      -0.173230
     C       0.714524     -1.300709       0.436058
     C       2.709837     -1.228881      -0.430557
     C       1.656638     -2.363608      -0.246028
     C       1.145316     -2.882670      -1.594497
     C       2.079638     -3.529726       0.645125
     C       1.971724      1.068026       0.599247
     C       2.605535      2.176106      -0.221404
     C       1.586936      2.944157      -1.100697
     C       1.808503      1.207298       1.916197
     C       0.579476      3.694543      -0.262542
     C      -1.542333     -0.145394       0.804861
     C      -0.785484     -1.320537       0.155494
     H       1.156975      0.129740      -1.135377
     H       0.878331     -1.354382       1.517264
     H       3.447562     -1.221549       0.375420
     H       3.229896     -1.188891      -1.391041
     H       1.927508     -3.467078      -2.089534
     H       0.862321     -2.072865      -2.272359
     H       0.274144     -3.532941      -1.470493
     H       2.865584     -4.124826       0.167724
     H       1.235765     -4.198209       0.847381
     H       2.464870     -3.175612       1.605609
     H       3.375429      1.759262      -0.879824
     H       3.112174      2.883129       0.442981
     H       1.046812      2.275808      -1.773922
     H       2.131638      3.677109      -1.709310
     H       2.137916      2.102916       2.432445
     H       1.343562      0.445021       2.529079
     H       1.016044      4.476086       0.400959
     H      -1.381568     -0.124913       1.883755
     H      -1.189709      0.803034       0.388730
     H      -1.204103     -2.263822       0.527736
     H      -0.970240     -1.300253      -0.921372
     C      -3.035833     -0.226809       0.585270
     O      -3.869935     -0.348505       1.447520
     O      -0.608589      3.494885      -0.268864
     O      -3.341275     -0.154562      -0.732261
     C      -4.741532     -0.217540      -1.050660
     H      -5.277539      0.609549      -0.582449
     H      -4.798272     -0.144505      -2.134674
     H      -5.172837     -1.158866      -0.705716
Rotational constants (GHz):    0.3891800    0.3054000    0.2018300
Vibrational harmonic frequencies (cm-1):
      22.3314                  24.9822                  36.4466
      41.4371                  56.4318                  64.7094
```

```
      68.8355                84.0358                107.7033
     119.3896                128.5414               163.9731
     180.7943                210.0082               223.4207
     232.8932                261.7460               274.7582
     291.1069                301.5089               328.1021
     354.5776                378.2334               383.9927
     426.3492                460.2166               489.3284
     500.3303                524.7366               565.6396
     649.7647                653.0074               722.1999
     739.0614                752.3011               781.2554
     794.4886                838.5748               867.0124
     880.0194                880.3129               895.3948
     923.9368                931.1512               951.9541
     957.2156                987.9668              1001.5949
    1013.5717               1022.1310              1029.0702
    1044.2251               1046.2637              1055.1792
    1077.6260               1112.9721              1123.8964
    1173.4671               1175.7564              1182.0911
    1200.9220               1207.8334              1209.2688
    1222.1880               1226.2641              1249.6005
    1260.8707               1267.0698              1274.7978
    1299.0030               1313.2667              1333.4310
    1341.0606               1353.6817              1362.1495
    1383.9703               1402.1220              1411.6703
    1418.1202               1421.4278              1452.9347
    1471.7515               1473.3373              1477.1622
    1482.4698               1486.7051              1488.3787
    1492.3756               1495.9970              1500.4641
    1500.7633               1509.5791              1511.4493
    1703.0305               1806.6165              1813.2486
    2850.2746               3010.4132              3012.5381
    3016.1663               3017.8238              3021.9138
    3027.4845               3036.1026              3041.2405
    3046.3792               3052.6087              3061.2706
    3068.5834               3073.4737              3079.8418
    3080.9653               3087.9365              3093.8906
    3099.5432               3112.0200              3116.3304
    3137.7675               3151.8780              3216.9445
Zero-point correction (Hartree): 0.364298
```

Ester-1b

```
----------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.908724332
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.482984      0.628963      -0.068127
     C      -0.125588      1.309470       0.263874
     C      -2.131510      2.050068      -0.144657
     C      -0.707209      2.673023      -0.267834
     C      -0.351520      2.978715      -1.726761
     C      -0.427731      3.889051       0.612676
     C      -2.130912     -0.377102       0.847904
     C      -3.389203     -1.033384       0.309463
     C      -3.116515     -2.064314      -0.812998
     C      -1.677161     -0.677421       2.066408
     C      -2.299551     -3.234218      -0.317009
     C       1.536807     -0.619706       0.230508
     C       1.166064      0.751113      -0.329268
     C       5.095575     -1.334413      -0.536930
     H      -1.430028      0.209320      -1.079110
     H      -0.011689      1.399450       1.349104
```

```
      H      -2.613408      2.314676       0.799876
      H      -2.826793      2.243234      -0.965480
      H      -0.934397      3.834836      -2.081171
      H      -0.565580      2.137769      -2.392079
      H       0.707692      3.229647      -1.836787
      H      -0.999867      4.759573       0.274212
      H       0.633405      4.159145       0.585389
      H      -0.697061      3.695171       1.654778
      H      -4.065656     -0.269346      -0.088920
      H      -3.923011     -1.527014       1.127502
      H      -2.597988     -1.617814      -1.663481
      H      -4.078239     -2.455655      -1.169232
      H      -2.199572     -1.383564       2.703230
      H      -0.777184     -0.236810       2.476775
      H      -2.758392     -3.794607       0.529919
      H       1.676109     -0.578002       1.311695
      H       0.789844     -1.374155      -0.014196
      H       1.987767      1.443340      -0.117846
      H       1.083934      0.667106      -1.417418
      H       5.024511     -2.424235      -0.521999
      H       6.022029     -1.013276      -0.065764
      H       5.077514     -1.021963      -1.583364
      C       3.922079     -0.735316       0.198976
      O       3.997699     -0.023734       1.169916
      O       2.758918     -1.109912      -0.376840
      O      -1.232590     -3.569354      -0.764698
Rotational constants (GHz):    0.4062600    0.2770400    0.1892400
Vibrational harmonic frequencies (cm-1):
      20.4619                23.8013                26.2627
      37.6332                42.9890                56.4631
      69.3846                71.1763                89.7081
     105.7155               124.9922               163.4575
     185.6414               213.8349               233.1087
     246.1832               276.3048               288.0668
     303.6949               320.0974               332.5322
     364.4960               380.2754               382.6666
     448.6698               461.9133               494.5780
     501.8944               541.4499               571.7603
     611.1790               648.7690               656.9990
     723.5780               745.4115               781.1218
     788.6492               842.9926               859.4279
     874.5947               879.7669               892.5114
     926.3391               934.4240               955.8909
     959.2070               978.6629               992.9749
    1006.3099              1016.3562              1030.0772
    1043.9675              1048.0161              1056.1761
    1064.9658              1071.7959              1080.2230
    1115.8657              1155.7865              1182.7872
    1196.2699              1209.3910              1223.8968
    1226.2874              1240.7010              1255.4803
    1263.4701              1269.5182              1279.9775
    1314.8423              1325.9949              1340.4748
    1347.4269              1356.1598              1374.8809
    1394.7108              1403.7066              1413.1223
    1422.0829              1422.5739              1429.1113
    1449.3343              1468.7434              1473.1226
    1476.2438              1484.7087              1487.9348
    1488.9927              1489.9474              1495.9507
    1501.2573              1509.7986              1510.8709
    1701.4614              1804.6275              1814.0632
    2850.8566              3010.7223              3014.2873
```

3018.6030 3022.4365 3027.1489
3029.9050 3035.6108 3039.6135
3050.5056 3061.3706 3068.2333
3070.3635 3074.2435 3079.7092
3081.4391 3087.7164 3092.0367
3098.8590 3110.7124 3133.8992
3138.7054 3156.4421 3219.6826
Zero-point correction (Hartree): 0.363924

Rad-1a

E(UB+HF-LYP/6-311G(d,p)) (Hartree): -736.000973370
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-0.747825	-1.097382	0.008072
C	-1.330436	0.339424	0.039877
C	-2.182865	-1.633461	0.329024
C	-2.777858	-0.260299	-0.113143
C	-3.290713	-0.302783	-1.556099
C	-3.833594	0.343932	0.809970
C	0.387965	-1.521742	0.905691
C	1.135577	-2.771450	0.479619
C	2.081126	-2.534018	-0.726345
C	0.730743	-0.875277	2.022224
C	3.176253	-1.552793	-0.388608
C	0.634189	1.692289	-0.759857
C	-0.808266	1.388143	-0.965119
C	2.559414	3.026094	0.227592
H	-0.502173	-1.358530	-1.027191
H	-1.241099	0.762908	1.043077
H	-2.306084	-1.805694	1.400702
H	-2.520985	-2.518218	-0.216506
H	-4.211232	-0.892821	-1.608660
H	-2.570339	-0.758283	-2.241459
H	-3.517989	0.700596	-1.928397
H	-4.762789	-0.235305	0.777398
H	-4.072175	1.371284	0.515566
H	-3.487641	0.365485	1.847145
H	0.425785	-3.557944	0.200995
H	1.717688	-3.158263	1.321693
H	1.539851	-2.164258	-1.599355
H	2.552757	-3.487711	-0.995325
H	1.529786	-1.238683	2.660152
H	0.235995	0.032514	2.344967
H	3.849637	-1.869217	0.438950
H	1.386839	1.045308	-1.199342
H	-1.388270	2.306224	-0.833803
H	-0.961882	1.018808	-1.984458
H	3.146804	2.120176	0.067317
H	2.763893	3.441884	1.215031
H	2.872071	3.766420	-0.516949
C	1.066700	2.777741	0.085907
O	0.246176	3.490532	0.675777
O	3.343711	-0.490180	-0.935073

Rotational constants (GHz): 0.4867500 0.3822200 0.2562800
Vibrational harmonic frequencies (cm-1):

22.7947	35.6863	42.5816
52.1553	62.4680	65.5644
77.3876	95.9889	112.2643
142.9398	156.6395	183.5900
203.2882	228.3295	259.2314

```
     266.7218                275.3901                288.0836
     327.8896                353.4430                374.4637
     383.3642                428.9525                465.4696
     482.7361                498.1477                519.6956
     534.5854                563.2636                604.4393
     652.4568                710.7715                728.7349
     754.2979                792.1130                793.9575
     839.0639                869.5393                879.2996
     894.8229                919.7458                934.1054
     946.3325                954.6716                980.3170
     993.1388                998.0475               1008.4690
    1023.5183               1031.9335               1033.3270
    1043.1825               1068.3641               1085.0968
    1096.1226               1132.8973               1175.4256
    1192.3937               1205.8747               1209.2471
    1220.9417               1224.0724               1232.9064
    1259.6546               1265.8701               1272.5630
    1306.8371               1319.4023               1337.7085
    1350.8052               1356.3101               1392.4210
    1401.9935               1409.4675               1422.3496
    1422.5453               1442.9093               1455.0281
    1468.7162               1470.8961               1482.5907
    1485.2498               1485.9274               1487.8728
    1491.7596               1496.0948               1507.3741
    1509.0072               1597.0846               1701.4337
    1805.0991               2867.9086               3011.6079
    3016.5984               3017.4522               3021.6806
    3025.1698               3027.8992               3028.9349
    3040.4240               3057.4997               3062.6633
    3070.5639               3077.5149               3079.7511
    3082.7665               3084.8901               3093.6182
    3095.7536               3098.2711               3130.1858
    3135.6750               3171.9829               3216.0185
Zero-point correction (Hartree): 0.345490
```

Rad-1b

```
-----------------
E(UB+HF-LYP/6-311G(d,p)) (Hartree): -735.984242788
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.602898     -0.726441      -0.487009
     C      -1.594360     -0.169256       0.579289
     C      -1.638524     -1.860080      -0.779713
     C      -2.746251     -1.027920      -0.065702
     C      -3.611741     -0.264733      -1.074358
     C      -3.629114     -1.789576       0.921149
     C       0.809516     -1.130018      -0.115311
     C       1.828964     -0.915579      -1.214721
     C       3.282702     -1.273154      -0.887339
     C       1.113394     -1.670980       1.066998
     C       3.908939     -0.375940       0.162216
     C      -0.499056      2.098695       1.201106
     C      -1.781648      1.335173       0.771680
     C      -0.280540      3.753428      -0.717828
     H      -0.562844     -0.044201      -1.341944
     H      -1.351074     -0.609782       1.551095
     H      -1.387256     -2.768731      -0.228062
     H      -1.811751     -2.117827      -1.827756
     H      -4.248754     -0.965871      -1.622720
     H      -3.010494      0.274718      -1.811509
     H      -4.267200      0.458959      -0.579626
```

```
     H      -4.286257     -2.493078      0.398578
     H      -4.266154     -1.105962      1.493143
     H      -3.026580     -2.361611      1.632570
     H       1.782709      0.139810     -1.508494
     H       1.509969     -1.482681     -2.098955
     H       3.882186     -1.133390     -1.797748
     H       3.407817     -2.314716     -0.581422
     H       2.115649     -1.989007      1.322778
     H       0.363787     -1.819849      1.836106
     H       3.616112      0.692796      0.095264
     H      -0.785405      2.938381      1.843635
     H       0.167421      1.453000      1.774871
     H      -2.551007      1.485417      1.536984
     H      -2.179529      1.785612     -0.143882
     H       0.275789      4.152576     -1.556741
     H      -1.231192      4.200894     -0.452644
     C       0.293569      2.663540      0.028995
     O       1.405006      2.225083     -0.286871
     O       4.685787     -0.757385      1.003093
Rotational constants (GHz):    0.5837400    0.3140900    0.2375600
Vibrational harmonic frequencies (cm-1):
      19.6955                34.3906                41.9034
      44.6422                56.6798                72.9597
      89.7237               109.5721               135.0254
     154.3705               196.4194               214.1115
     220.6341               255.0824               262.7599
     281.8253               294.9618               301.2692
     351.5394               361.9976               369.5009
     387.7965               397.9031               447.7970
     480.5403               510.4173               516.3125
     522.8212               565.3731               612.5988
     620.4211               713.0669               728.4813
     752.5233               772.3551               789.2132
     817.8083               871.1099               877.8002
     887.8445               900.5302               909.5695
     922.9986               944.3858               951.6868
     983.5289               991.4615              1004.3095
    1020.6497              1027.5695              1043.8837
    1049.4339              1054.1797              1085.9958
    1105.1786              1120.6271              1163.7436
    1185.8234              1205.0995              1210.4962
    1219.4145              1227.4058              1235.9232
    1252.6651              1274.0782              1277.7116
    1285.3169              1313.5602              1343.0044
    1346.8084              1354.7716              1380.1034
    1396.0383              1403.5611              1413.4360
    1422.5622              1426.3376              1450.4622
    1463.4084              1468.3072              1476.1391
    1483.0713              1485.3509              1486.0217
    1495.8839              1498.3232              1507.1508
    1510.1984              1585.5611              1701.5066
    1804.2144              2907.8526              3000.3525
    3008.8387              3011.3145              3014.7949
    3018.5252              3029.8731              3031.7499
    3037.7017              3040.7491              3042.1067
    3058.0493              3066.9861              3076.5227
    3078.9379              3083.5218              3083.6620
    3096.1101              3103.9377              3140.9839
    3147.9636              3224.5483              3255.5887
Zero-point correction (Hartree): 0.345305
```

Rad-2b

E(UB+HF-LYP/6-311G(d,p)) (Hartree): -735.995873897
Electronic state : 2-A
Cartesian coordinates (Angs):

C	-0.399018	-0.725558	-0.186128
C	-1.689424	-0.260206	0.547511
C	-1.178250	-1.995380	-0.669807
C	-2.522681	-1.305946	-0.287719
C	-3.218900	-0.723944	-1.522849
C	-3.502335	-2.154963	0.520918
C	0.890955	-0.985983	0.548361
C	2.092875	-1.305683	-0.335376
C	3.015033	-0.140404	-0.473950
C	1.023124	-0.983986	1.875170
C	4.434175	-0.297792	-0.422332
C	-1.072570	2.196876	1.128463
C	-2.116652	1.209704	0.551439
C	-0.517112	3.382737	-1.121452
H	-0.192569	-0.078142	-1.047196
H	-1.655472	-0.612172	1.582984
H	-0.959214	-2.855963	-0.033943
H	-1.059184	-2.287723	-1.715780
H	-3.602626	-1.536144	-2.148165
H	-2.538901	-0.131549	-2.142142
H	-4.066716	-0.087675	-1.250914
H	-3.905566	-2.973498	-0.084808
H	-4.349598	-1.555458	0.871736
H	-3.017066	-2.595222	1.396511
H	1.742422	-1.610177	-1.332862
H	2.664685	-2.151010	0.054990
H	2.604914	0.858252	-0.586380
H	1.973782	-1.216277	2.342568
H	0.203748	-0.748073	2.543050
H	5.028104	0.627853	-0.542407
H	-1.599647	3.093933	1.477121
H	-0.546919	1.768006	1.982819
H	-3.033583	1.292814	1.144820
H	-2.390713	1.527604	-0.458100
H	-0.827984	2.643189	-1.866352
H	0.297365	3.970763	-1.543198
H	-1.380655	4.021396	-0.919948
C	-0.023355	2.676018	0.133127
O	1.162753	2.522696	0.330480
O	5.001774	-1.382404	-0.260062

Rotational constants (GHz): 0.5653900 0.3076400 0.2320800
Vibrational harmonic frequencies (cm-1):

6.9898	22.6855	32.0784
46.8777	53.4076	62.3208
86.3038	113.6982	122.6245
140.5783	172.2606	194.4037
210.1081	232.4167	247.1300
282.6910	290.2536	305.9498
325.6262	349.7217	369.2866
379.5548	410.0178	457.8312
466.9879	501.4217	531.4181
567.1264	587.3345	649.5677
655.8690	703.9605	729.4419
734.2164	770.8908	790.9944
863.3311	882.2427	886.2788
891.8120	912.3798	925.1400

945.2314	954.5349	972.3305
981.7425	992.0435	997.6040
1003.3525	1023.3650	1029.4998
1044.0084	1053.1524	1109.8581
1122.4000	1143.5288	1169.7898
1177.2227	1193.0125	1207.3072
1226.0321	1233.4694	1249.1164
1251.9659	1262.8274	1279.8768
1290.5162	1315.3838	1344.2694
1355.9961	1379.3804	1385.3752
1395.8853	1404.2344	1408.5033
1422.3822	1441.9372	1452.4136
1468.4815	1471.4828	1472.4825
1484.1167	1484.7176	1488.1136
1494.8458	1502.9223	1509.8494
1512.1825	1573.9897	1701.9478
1782.2652	2930.5900	2978.4745
3009.6873	3010.4990	3013.3221
3017.9059	3029.8995	3034.9144
3040.4702	3045.6442	3068.0560
3071.5587	3077.3495	3078.8472
3080.5673	3082.4350	3093.1927
3098.3817	3103.6928	3137.4731
3140.0386	3177.8942	3217.0780

Zero-point correction (Hartree): 0.345530

TS1: MPW1B95/6-31+G at T = 300 K**

Scan-277-freq

E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.053745292

Electronic state : 1-A

Cartesian coordinates (Angs):

C	-1.587586	0.829422	0.474024
C	-1.546295	-0.504389	-0.349916
C	-3.091319	0.905395	0.152583
C	-3.094999	-0.588463	-0.213304
C	-3.552254	-1.434385	0.967362
C	-3.842242	-0.986559	-1.470388
C	-0.719390	2.016099	0.133476
C	0.506086	2.277824	0.986279
C	1.810782	1.846478	0.292086
C	-0.989288	2.828305	-0.890765
C	1.621604	0.502498	-0.324055
C	1.460767	-0.662100	0.385104
C	0.719597	-1.790649	-0.261219
C	-0.772636	-1.737339	0.091003
C	1.668940	-0.741495	1.862674
H	-1.449881	0.587589	1.533971
H	-1.295684	-0.253479	-1.388165
H	-3.287225	1.528237	-0.720683
H	-3.751470	1.226952	0.960927
H	-4.622490	-1.288660	1.132314
H	-3.036548	-1.159513	1.890647
H	-3.384908	-2.500012	0.794160
H	-4.922745	-0.890369	-1.334243
H	-3.634369	-2.026981	-1.736793
H	-3.551672	-0.359230	-2.315926
H	0.410764	1.738684	1.931781
H	0.568467	3.340088	1.233862
H	2.636326	1.836634	1.007728

H	2.069654	2.566674	-0.485214
H	-0.353415	3.678723	-1.110362
H	-1.836729	2.680028	-1.547615
H	1.306061	0.487778	-1.362392
H	1.124753	-2.751897	0.063037
H	0.837447	-1.734140	-1.346897
H	-1.251731	-2.607376	-0.372348
H	-0.895176	-1.874031	1.170307
H	0.726418	-0.576638	2.395232
H	2.389609	-0.004820	2.213781
H	2.031297	-1.731642	2.142524
O	3.955899	-0.922985	-1.039811
O	3.827185	0.344309	-1.000847
O	3.669748	-1.480881	0.070746

Rotational constants (GHz): 0.6891300 0.2762700 0.2327200

Vibrational harmonic frequencies (cm-1):

-152.2787	43.8674	54.9791
70.9521	74.4454	95.8409
127.0494	156.5557	162.6101
172.3782	202.4156	216.4827
232.8688	240.5965	262.0498
279.4828	288.8518	312.1514
322.4894	327.4678	354.1637
398.9480	410.7992	428.2991
436.0660	448.2027	490.7176
512.1326	557.8095	570.1191
587.9402	639.9738	726.5876
758.3977	762.3729	768.6446
826.1386	839.2096	866.3958
885.7731	917.0325	920.1897
932.8648	935.0419	955.9604
959.1656	985.7891	1004.0249
1009.1169	1022.1239	1024.0725
1027.7113	1045.3589	1054.0362
1063.4102	1106.0392	1135.5302
1143.9644	1163.8717	1167.5421
1177.9800	1205.8660	1211.4496
1217.2467	1228.4721	1234.5266
1253.3775	1263.8128	1271.2528
1276.4539	1305.5289	1324.8387
1341.9168	1349.1947	1355.4569
1374.3355	1386.8670	1403.3944
1410.0530	1420.2715	1421.0736
1436.1906	1453.5275	1477.8846
1484.1976	1488.2656	1489.0624
1495.1538	1499.3638	1502.5238
1508.1542	1512.2368	1514.0827
1514.5088	1632.0467	1732.0626
3051.2839	3056.2407	3057.1158
3064.8651	3065.7958	3068.7314
3077.2038	3087.5488	3095.0262
3097.5482	3107.2152	3132.4771
3133.3222	3134.3306	3142.6337
3144.1748	3145.3550	3147.6187
3151.2786	3159.3327	3188.0389
3188.5763	3208.9558	3275.7993

Zero-point correction (Hartree): 0.368239

TS2: MPW1B95/6-31+G at T = 300 K**

Scan-280-B-OK

```
-------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.052135593
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.591399      0.824468       0.483166
     C      -1.561675     -0.502446      -0.353121
     C      -3.097113      0.908846       0.171973
     C      -3.109192     -0.582129      -0.205048
     C      -3.559052     -1.435968       0.972706
     C      -3.868115     -0.968071      -1.458905
     C      -0.723210      2.012286       0.145595
     C       0.506915      2.269971       0.993163
     C       1.808508      1.841973       0.287976
     C      -0.997484      2.831551      -0.871808
     C       1.603337      0.502870      -0.339856
     C       1.439423     -0.661511       0.356343
     C       0.701766     -1.784502      -0.297598
     C      -0.786517     -1.741591       0.068706
     C       1.661079     -0.761382       1.834240
     H      -1.447606      0.573802       1.540269
     H      -1.318136     -0.241996      -1.390641
     H      -3.295461      1.538605      -0.695732
     H      -3.751073      1.227513       0.986554
     H      -4.627455     -1.288851       1.148164
     H      -3.034303     -1.170131       1.893561
     H      -3.395701     -2.500517       0.789268
     H      -4.947195     -0.869516      -1.313257
     H      -3.665601     -2.006994      -1.734977
     H      -3.582234     -0.335206      -2.301914
     H       0.417672      1.724782       1.935728
     H       0.570070      3.330882       1.246916
     H       2.631344      1.832303       1.008080
     H       2.066440      2.570180      -0.481610
     H      -0.361715      3.682624      -1.089213
     H      -1.847836      2.688071      -1.525892
     H       1.294878      0.497200      -1.378811
     H       1.119155     -2.747086       0.009349
     H       0.817129     -1.711174      -1.381561
     H      -1.269811     -2.605799      -0.401177
     H      -0.902901     -1.890161       1.147385
     H       0.724806     -0.587884       2.375668
     H       2.387691     -0.033686       2.195527
     H       2.011080     -1.758108       2.104141
     O       4.247767     -0.583008      -0.396680
     O       3.780562      0.175274      -1.299862
     O       3.577063     -1.647897      -0.229834
Rotational constants (GHz):    0.6957700    0.2730900    0.2301700
Vibrational harmonic frequencies (cm-1):
     -90.4365                  40.7365                  55.3623
      69.1266                  76.6580                  85.4522
     130.9664                 136.3114                 158.7608
     173.0866                 202.2915                 217.1511
     234.2944                 241.0419                 263.7439
     280.8500                 292.7719                 312.9113
     324.7678                 330.0218                 354.2997
     400.7246                 411.5010                 419.5248
     429.9577                 453.1624                 494.5924
     513.3434                 559.0528                 572.2085
     588.0267                 640.3825                 726.4385
     758.7900                 762.8823                 769.6162
     825.6000                 840.3636                 866.6413
```

886.6700	916.7920	922.1565
933.5633	934.6443	956.0223
959.2206	986.5659	1003.0506
1010.7433	1021.7749	1024.4921
1028.7428	1046.8311	1054.6649
1062.2286	1102.0296	1133.8771
1142.8427	1165.4626	1171.9167
1187.1972	1205.2460	1212.1274
1228.6191	1233.6972	1240.4555
1252.5128	1261.9687	1271.2075
1274.4196	1305.0169	1324.6364
1340.3477	1346.0232	1355.0753
1373.5310	1387.4803	1403.0933
1409.0340	1419.2306	1420.8605
1432.7982	1453.8791	1479.5609
1485.4495	1489.0072	1489.5707
1494.4647	1500.0976	1502.9238
1510.3308	1513.1517	1514.6769
1517.5695	1648.9711	1732.0934
3051.0192	3055.9065	3056.5876
3063.4842	3065.6144	3065.9163
3079.8437	3082.2819	3091.1804
3097.0810	3103.9214	3132.0913
3132.2473	3135.6572	3141.0427
3144.1224	3145.2291	3147.7174
3150.9939	3159.2523	3179.0638
3188.6952	3223.9634	3276.1150

Zero-point correction (Hartree): 0.368296

TS3: MPW1B95/6-31+G at T = 300 K**

Scan-265-external-freq

E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.051682962

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.030812	0.467110	0.446377
C	-1.266052	0.749015	-0.385428
C	0.306856	1.984582	0.423980
C	-1.148443	2.252413	0.002912
C	-1.997933	2.633342	1.207256
C	-1.361431	3.235346	-1.131081
C	1.115003	-0.419552	-0.096964
C	1.368122	-1.796487	0.470054
C	0.758361	-2.904304	-0.412856
C	1.730454	-0.103641	-1.309214
C	-0.578480	-2.444728	-0.912267
C	-1.654420	-2.231060	-0.149615
C	-2.752523	-1.349548	-0.659259
C	-2.592047	0.064777	-0.087963
C	-1.755469	-2.665450	1.280784
H	-0.236351	0.127111	1.450585
H	-1.026303	0.636689	-1.450786
H	1.032940	2.248846	-0.347155
H	0.646223	2.424432	1.361408
H	-1.725803	3.634913	1.548538
H	-1.843061	1.948566	2.044718
H	-3.064583	2.639711	0.970126
H	-1.121866	4.254726	-0.817528
H	-2.401765	3.228488	-1.469140

```
      H      -0.728101      2.991227      -1.987258
      H       0.942050     -1.845832       1.473825
      H       2.447146     -1.946677       0.573617
      H       0.696727     -3.831697       0.162873
      H       1.418831     -3.108984      -1.257480
      H       2.278330     -0.864853      -1.848852
      H       1.417425      0.759244      -1.881347
      H      -0.612003     -2.077579      -1.935312
      H      -3.739546     -1.736047      -0.386475
      H      -2.709487     -1.301799      -1.750860
      H      -3.390996      0.695434      -0.493816
      H      -2.753261      0.042879       0.994465
      H      -1.656969     -1.815435       1.964247
      H      -0.991306     -3.393682       1.549952
      H      -2.733697     -3.112393       1.475847
      O       3.704939      0.389775       0.482306
      O       3.472311      0.857713      -0.713031
      O       2.652572      0.573989       1.222663
Rotational constants (GHz):    0.4816900    0.4086100    0.2634800
Vibrational harmonic frequencies (cm-1):
    -365.0873                  40.6900                  67.9735
      81.0837                 105.4710                 125.4522
     144.1657                 155.2975                 168.5797
     198.5941                 210.7819                 222.0809
     233.5545                 248.3559                 266.3520
     280.3231                 301.4355                 312.4507
     320.7259                 333.2912                 357.5416
     394.6786                 399.3398                 433.4917
     444.7951                 488.1440                 496.7542
     519.0541                 555.5252                 574.1543
     595.4180                 640.9335                 757.9829
     761.7556                 767.1211                 815.0796
     818.8122                 830.5011                 870.5916
     879.9129                 891.9277                 916.1608
     936.3456                 945.8073                 958.7200
     959.2533                 980.2663                 997.0599
    1003.5907                1012.1256                1019.8018
    1026.9712                1044.7285                1050.5129
    1063.7952                1091.3459                1101.9546
    1118.1671                1129.1931                1141.4483
    1169.3442                1172.3089                1187.2036
    1211.6889                1224.5794                1231.7795
    1246.4757                1255.9839                1260.9870
    1267.8473                1301.9763                1323.5727
    1332.3403                1341.4961                1349.4104
    1368.0915                1376.2154                1395.2090
    1404.4737                1414.9953                1420.3108
    1425.5839                1434.6087                1471.9971
    1477.0854                1487.7009                1487.9508
    1494.5369                1496.1920                1498.2294
    1502.1550                1510.8345                1511.9956
    1517.8283                1558.2860                1769.4723
    3045.8602                3055.9626                3056.8337
    3061.3705                3064.7853                3067.6209
    3073.9581                3087.5620                3100.5711
    3101.9750                3111.6446                3121.8255
    3124.8454                3127.4843                3134.0958
    3142.1330                3144.1144                3144.8590
    3146.5766                3168.8030                3172.5044
    3176.9808                3203.0213                3300.5850
Zero-point correction (Hartree): 0.367797
```

B3LYP-Optimization

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.619173890
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.159452	0.483816	0.354495
C	-1.168507	0.974331	-0.365115
C	0.664335	1.952843	0.306208
C	-0.771222	2.456265	-0.006983
C	-1.452076	3.009096	1.251545
C	-0.900398	3.454419	-1.156205
C	1.041807	-0.593037	-0.246677
C	1.019406	-2.005402	0.326190
C	0.143448	-2.992716	-0.501299
C	-1.123480	-2.294404	-0.915376
C	-2.149115	-1.968090	-0.123666
C	-3.058823	-0.839460	-0.541649
C	-2.568194	0.503978	0.054182
C	-2.367385	-2.527388	1.258872
H	-0.075461	0.202430	1.384143
H	-1.048375	0.835463	-1.445704
H	1.359027	2.128068	-0.516370
H	1.130574	2.321294	1.220956
H	-0.980178	3.954250	1.538204
H	-1.361482	2.328859	2.102730
H	-2.515994	3.206386	1.089980
H	-0.466222	4.423172	-0.886276
H	-1.950925	3.625041	-1.417088
H	-0.386735	3.096834	-2.053480
H	0.639496	-1.966457	1.349394
H	2.042745	-2.390784	0.382544
H	-0.039288	-3.889280	0.098691
H	0.696126	-3.316736	-1.387423
H	-1.089265	-1.826639	-1.896649
H	-4.090655	-1.011806	-0.213349
H	-3.076962	-0.759610	-1.633302
H	-3.281274	1.280872	-0.248937
H	-2.628930	0.457397	1.146678
H	-2.311269	-1.746220	2.025490
H	-1.646898	-3.303560	1.518612
H	-3.370765	-2.962409	1.333402
C	1.766833	-0.364643	-1.382076
H	1.727103	0.577886	-1.910150
H	2.290094	-1.171427	-1.880209
O	3.862616	0.300936	-0.581563
O	3.850726	-0.312056	0.544036
O	2.914037	0.062286	1.340456

Rotational constants (GHz): 0.4656500 0.3744300 0.2451000
Vibrational harmonic frequencies (cm-1):

-51.0660	42.0115	46.5123
59.0905	65.3792	104.4408
116.8535	141.4584	157.7893
165.4678	174.3365	219.9118
225.8419	240.6853	247.9763
275.9184	293.4783	303.8381
305.7798	334.7467	356.6572
394.9444	399.9236	411.9202
435.9453	451.5619	489.4656
509.8488	554.4080	568.5974

591.1458	640.8724	739.6245
743.1260	752.3089	757.2873
812.9304	824.7796	849.0222
873.2144	893.9195	900.5060
915.7669	934.9856	941.9802
952.7955	963.2130	979.3409
988.1483	997.8099	1006.8000
1016.7670	1035.1240	1041.1344
1060.7000	1079.4342	1098.5970
1106.6309	1116.7427	1135.2021
1158.3519	1165.0827	1194.4618
1200.4923	1209.6814	1226.8356
1244.4058	1252.2152	1255.2802
1258.2743	1282.3686	1308.3698
1332.3765	1337.9030	1355.0644
1362.4327	1371.0084	1384.4368
1397.9724	1403.1259	1418.5023
1419.8666	1435.5355	1477.4706
1482.4256	1485.9279	1488.2413
1492.1464	1494.6206	1495.7781
1498.9235	1507.3436	1508.8155
1510.8054	1592.5589	1730.4368
3004.5753	3007.0571	3011.6754
3016.7219	3018.4612	3021.7853
3027.9433	3037.5282	3042.7432
3051.2812	3053.2715	3062.5965
3064.3223	3064.8628	3065.7483
3076.9259	3078.9804	3086.7695
3087.9642	3112.0026	3112.3951
3127.1903	3155.5671	3242.4637

Zero-point correction (Hartree): 0.362719

TS4: MPW1B95/6-31+G at T = 300 K**

Scan-267-external-B

E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.051715434

Electronic state : 1-A

Cartesian coordinates (Angs):

C	0.209680	0.388577	0.418651
C	-0.925567	1.095677	-0.398607
C	0.989282	1.717780	0.375062
C	-0.296462	2.468107	-0.012835
C	-0.940452	3.107852	1.208936
C	-0.186563	3.473203	-1.142042
C	0.906989	-0.834959	-0.114997
C	0.645137	-2.198455	0.474767
C	-0.311083	-3.030872	-0.401311
C	1.606000	-0.763286	-1.309836
C	-1.407612	-2.139954	-0.901627
C	-2.337321	-1.561058	-0.136812
C	-3.057808	-0.351396	-0.646924
C	-2.403488	0.916322	-0.084520
C	-2.574067	-1.925350	1.297176
H	-0.138501	0.183367	1.434783
H	-0.749970	0.910752	-1.466353
H	1.728667	1.735652	-0.429169
H	1.487245	2.014683	1.299087
H	-0.339231	3.958150	1.539355
H	-1.008649	2.409239	2.046131
H	-1.946840	3.474466	0.993578

```
      H       0.384745      4.352294     -0.832463
      H      -1.175481      3.815879     -1.459833
      H       0.312914      3.037023     -2.010272
      H       0.213118     -2.070826      1.469291
      H       1.599713     -2.714017      0.603664
      H      -0.687905     -3.877074      0.179482
      H       0.237476     -3.453664     -1.244878
      H       1.916219     -1.669941     -1.810674
      H       1.603581      0.141059     -1.904632
      H      -1.315291     -1.788123     -1.926235
      H      -4.115948     -0.362586     -0.366818
      H      -3.008110     -0.326238     -1.739038
      H      -2.935521      1.787439     -0.483799
      H      -2.548790      0.952224      0.999728
      H      -2.182172     -1.158017      1.973228
      H      -2.106420     -2.871472      1.567721
      H      -3.645216     -2.004858      1.499903
      O       3.496445      0.065348      0.466254
      O       3.622703     -0.517300     -0.678083
      O       2.745900     -0.629114      1.251546
Rotational constants (GHz):    0.4806300    0.4114000    0.2642800
Vibrational harmonic frequencies (cm-1):
    -297.9492                  53.8704                  71.8342
      87.7190                  89.3176                 131.2637
     146.3265                 163.8146                 183.9004
     206.2358                 213.4689                 223.4448
     233.9195                 255.3440                 262.1550
     284.3228                 310.2893                 316.9249
     327.0511                 336.3571                 360.1139
     396.0777                 403.7172                 440.5406
     449.4328                 485.9761                 504.3051
     515.1661                 551.9190                 572.5771
     590.3196                 642.3074                 758.4579
     760.5956                 767.0456                 806.2849
     818.5017                 831.1297                 874.6992
     889.4323                 895.9708                 925.6017
     935.5127                 948.6253                 960.7727
     964.5698                 986.9867                1004.4418
    1011.9032                1015.0017                1022.1587
    1031.8828                1047.7174                1056.2727
    1065.1246                1097.6212                1127.2201
    1128.7242                1152.7642                1160.7401
    1164.9580                1175.1165                1195.1581
    1214.7360                1232.2419                1247.3640
    1248.5549                1256.9819                1262.7790
    1273.2574                1316.7375                1330.0975
    1340.9835                1344.4891                1357.2244
    1371.0871                1376.1211                1396.0476
    1403.5941                1413.9459                1428.6081
    1430.5964                1436.5822                1474.6217
    1479.0791                1489.6872                1491.3496
    1496.3137                1497.7291                1501.2931
    1506.7388                1511.2131                1517.2705
    1520.8284                1582.1972                1770.2390
    3047.2333                3053.4886                3057.6477
    3060.4685                3066.2158                3067.8144
    3084.8870                3095.2418                3096.7351
    3100.4464                3100.9661                3120.7931
    3122.7602                3130.4229                3135.6140
    3142.4486                3146.6692                3149.2386
    3152.6528                3159.8616                3169.8168
```

3179.4518 3205.2527 3302.4057
Zero-point correction (Hartree): 0.368745

B3LYP-Optimization

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.619250275
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.256628	0.408557	0.364931
C	-0.933806	1.147484	-0.383140
C	1.045913	1.746159	0.319631
C	-0.254195	2.523987	-0.023951
C	-0.835879	3.212531	1.216696
C	-0.156797	3.516024	-1.181689
C	0.912257	-0.832746	-0.210776
C	0.600237	-2.201110	0.377123
C	-0.442696	-3.004416	-0.453946
C	-1.538067	-2.071751	-0.895152
C	-2.489213	-1.536963	-0.123868
C	-3.147907	-0.254073	-0.568231
C	-2.405204	0.972947	0.017778
C	-2.836033	-2.023374	1.259936
H	-0.046711	0.193752	1.392269
H	-0.827759	0.978382	-1.460765
H	1.771653	1.780529	-0.495733
H	1.560114	2.020248	1.242650
H	-0.188721	4.043600	1.514727
H	-0.909042	2.533035	2.070103
H	-1.832597	3.621564	1.027116
H	0.455798	4.381878	-0.908096
H	-1.146462	3.889012	-1.467799
H	0.294218	3.053189	-2.064501
H	0.218245	-2.069116	1.392246
H	1.532911	-2.765076	0.460483
H	-0.810275	-3.838118	0.151337
H	0.046112	-3.444317	-1.327561
H	-1.398405	-1.633264	-1.880778
H	-4.197015	-0.210799	-0.252510
H	-3.137570	-0.187872	-1.660958
H	-2.943338	1.872246	-0.307378
H	-2.487750	0.958197	1.109704
H	-2.614249	-1.268728	2.023323
H	-2.307301	-2.937893	1.530628
H	-3.911193	-2.225485	1.327969
C	1.666890	-0.774911	-1.353717
H	1.810997	0.146214	-1.903171
H	1.988062	-1.682356	-1.846810
O	3.816924	-0.731858	-0.585669
O	3.640727	-0.097129	0.517807
O	2.845788	-0.693372	1.338332

Rotational constants (GHz): 0.4680700 0.3815900 0.2483800
Vibrational harmonic frequencies (cm-1):

-90.7349	44.0461	45.8379
61.7439	68.2501	101.6938
119.2086	150.3231	157.8306
168.4078	172.1460	217.5789
224.5104	241.6871	246.2537
273.8786	291.7374	303.0961
307.3698	333.8487	358.0295

396.1997	401.4191	421.1744
437.7191	452.5290	487.6543
505.5617	550.9517	564.7270
589.4812	638.1915	738.1652
742.2095	749.5330	760.6410
811.2150	822.9165	849.0728
872.2086	891.8072	902.4973
917.0324	931.7335	940.0772
952.4246	964.7680	978.4154
990.9526	998.3596	1006.2272
1016.6704	1032.5996	1040.7947
1060.7021	1076.6507	1094.5223
1098.1228	1112.3866	1134.7678
1158.1420	1162.8659	1191.6657
1199.5181	1207.1286	1226.3450
1242.5375	1251.7698	1254.2571
1258.6032	1278.6205	1309.3707
1328.2575	1334.7593	1354.6416
1361.2599	1373.6940	1386.3722
1398.1554	1403.8573	1420.5781
1421.9360	1432.0190	1477.4979
1482.5349	1486.3519	1487.1678
1491.7119	1495.2575	1496.4122
1497.8305	1505.1641	1507.5565
1511.2185	1581.0805	1729.5377
3004.1462	3008.9183	3011.9658
3017.1141	3019.9828	3023.2081
3035.1764	3042.6228	3045.5331
3052.0137	3056.0350	3057.6614
3062.5527	3067.0791	3067.4233
3077.9778	3079.1923	3089.3952
3091.3775	3104.6437	3112.5998
3124.0493	3156.3962	3242.1890

Zero-point correction (Hartree): 0.362628

TS5: B3LYP

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.680352037
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.460551	0.867211	0.516170
C	-1.378827	-0.492151	-0.304366
C	-2.973107	0.906400	0.175184
C	-2.945299	-0.605186	-0.178305
C	-3.423608	-1.461965	1.000947
C	-3.670759	-1.016548	-1.457955
C	-0.599486	2.082742	0.210845
C	0.699858	2.268627	0.995717
C	1.983760	1.882465	0.219409
C	-0.957451	3.007869	-0.683531
C	1.807803	0.633006	-0.647214
C	0.914049	-1.861050	-0.274096
C	-0.570640	-1.728036	0.124349
C	1.687914	-0.772546	1.948647
H	-1.346553	0.630916	1.579890
H	-1.149369	-0.247802	-1.347397
H	-3.182857	1.513329	-0.706591
H	-3.644359	1.220916	0.978140
H	-4.499870	-1.322763	1.143027
H	-2.933170	-1.189730	1.939667

```
      H      -3.250787     -2.528221      0.828469
      H      -4.756038     -0.926356     -1.341083
      H      -3.454109     -2.058239     -1.719626
      H      -3.371048     -0.390143     -2.302882
      H       0.640390      1.709346      1.930745
      H       0.786142      3.319616      1.284448
      H       2.839798      1.782073      0.893070
      H       2.233675      2.689964     -0.475343
      H      -0.335852      3.878832     -0.864555
      H      -1.864649      2.941024     -1.270480
      H       0.765535      0.475670     -0.944234
      H       1.236735     -2.885460     -0.039807
      H       1.049769     -1.739171     -1.348402
      H      -1.070595     -2.587777     -0.337732
      H      -0.678115     -1.883474      1.202103
      H       0.706405     -0.370129      2.180524
      H       2.453514     -0.118927      2.366474
      H       1.767979     -1.749356      2.437976
      C       1.885448     -0.948209      0.460141
      O       3.209837     -1.164144      0.257652
      O       3.511243     -1.318654     -1.019416
      O       2.661769      0.390308     -1.575993
Rotational constants (GHz):    0.6340700    0.3153100    0.2588400
Vibrational harmonic frequencies (cm-1):
    -461.0779                  49.4684                  62.1218
      79.5254                 115.3087                 134.5076
     158.8789                 183.2341                 189.7705
     220.9635                 228.8037                 231.4702
     246.9996                 262.3354                 272.4950
     295.9105                 302.7246                 314.2869
     341.9331                 363.5099                 366.2986
     407.9922                 408.6548                 428.7084
     460.9430                 492.6650                 498.4609
     518.2039                 554.4719                 572.6531
     594.8234                 629.0023                 666.8058
     721.1044                 731.2256                 751.1341
     807.3101                 827.7716                 836.0750
     863.6797                 899.5346                 919.6197
     926.4774                 941.4054                 951.1424
     954.8652                 982.8463                 987.4454
     992.3461                1004.4672                1008.8983
    1014.0086                1018.5398                1048.3177
    1054.0002                1085.7636                1105.9753
    1130.0442                1143.6223                1162.0979
    1170.0229                1192.2763                1207.4478
    1215.5314                1229.7954                1244.1847
    1255.2550                1268.7877                1278.8822
    1284.0709                1288.6537                1317.6903
    1334.1066                1345.6153                1349.1846
    1356.7133                1380.1815                1381.4243
    1398.8136                1404.9287                1412.6258
    1420.9604                1446.6260                1451.0777
    1474.3295                1478.5617                1485.6985
    1487.4514                1488.3153                1495.2722
    1499.1246                1499.3392                1508.1683
    1509.8403                1511.9754                1692.0224
    2998.8457                3009.8192                3014.6142
    3017.6351                3023.0874                3028.5310
    3032.5299                3035.3854                3037.1308
    3051.0060                3052.1806                3056.6361
    3067.3942                3069.6391                3079.6407
```

```
    3081.7179                3086.5380                3093.5867
    3106.0315                3111.8497                3112.3644
    3137.0335                3169.2817                3216.2616
Zero-point correction (Hartree): 0.364455

TS5: MPW1B95
--------------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.119785526
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.410105      0.865548       0.501724
     C      -1.364217     -0.467530      -0.332137
     C      -2.912035      0.929973       0.174668
     C      -2.907944     -0.570460      -0.160067
     C      -3.327851     -1.403962       1.042825
     C      -3.673845     -1.001783      -1.394881
     C      -0.543833      2.064967       0.192208
     C       0.737943      2.266597       0.980379
     C       2.008589      1.838205       0.225969
     C      -0.879504      2.961166      -0.738488
     C       1.785281      0.611482      -0.638300
     C       0.897643     -1.842194      -0.332670
     C      -0.579593     -1.721776       0.042092
     C       1.530050     -0.748175       1.915277
     H      -1.294611      0.619475       1.562980
     H      -1.163351     -0.199512      -1.376521
     H      -3.109401      1.525396      -0.716832
     H      -3.575047      1.269095       0.973074
     H      -4.395323     -1.268466       1.231187
     H      -2.793700     -1.113537       1.950758
     H      -3.153452     -2.469858       0.877387
     H      -4.752391     -0.919007      -1.237525
     H      -3.457317     -2.043691      -1.648091
     H      -3.410157     -0.385145      -2.256715
     H       0.662352      1.748261       1.936152
     H       0.832937      3.325853       1.226898
     H       2.853153      1.698545       0.905388
     H       2.297648      2.635450      -0.462818
     H      -0.248103      3.820571      -0.933417
     H      -1.773358      2.875549      -1.341638
     H       0.730820      0.463917      -0.899596
     H       1.228761     -2.869145      -0.133805
     H       1.060864     -1.669853      -1.396747
     H      -1.087108     -2.548514      -0.467344
     H      -0.709001     -1.924678       1.109260
     H       0.535659     -0.342088       2.065437
     H       2.265158     -0.086683       2.371003
     H       1.572018     -1.715202       2.423931
     C       1.819088     -0.948520       0.458787
     O       3.138633     -1.142306       0.318769
     O       3.481358     -1.358385      -0.922086
     O       2.605629      0.322195      -1.570025
Rotational constants (GHz):    0.6492300    0.3261300    0.2671500
Vibrational harmonic frequencies (cm-1):
    -490.3262                  46.8776                  74.9632
      89.0487                 122.3702                 154.1788
     155.7588                 190.0605                 206.2708
     221.2574                 235.4836                 251.6980
     268.2909                 290.5170                 294.0553
     302.0442                 310.3662                 322.7573
     345.9629                 374.4094                 376.9693
```

408.0535	408.8815	432.3472
465.0696	495.9598	508.6748
526.6412	560.2755	574.7549
599.4243	640.8986	682.3942
728.8499	752.8960	771.1447
817.5754	841.1563	857.0543
880.6397	918.7318	931.4390
936.5449	954.4968	958.1250
959.2376	986.6379	999.4281
1007.7334	1018.0898	1024.9170
1028.5837	1038.2413	1064.3828
1078.1732	1108.2277	1131.7558
1143.2447	1166.8093	1173.1606
1206.1760	1216.3115	1224.0511
1230.9995	1234.2778	1255.6902
1268.7093	1279.6328	1307.0366
1314.1564	1317.9807	1333.2202
1337.0838	1348.0176	1353.9557
1388.9991	1392.1740	1409.3855
1413.2016	1421.0773	1421.6239
1423.3917	1459.4561	1472.9207
1483.8922	1488.3443	1489.3945
1494.2763	1499.1753	1503.9329
1510.6199	1513.0784	1514.0961
1518.2655	1520.0383	1731.4130
3052.8243	3056.5829	3058.8669
3065.9279	3066.3504	3069.4460
3072.9529	3087.4103	3089.6925
3100.9279	3106.4051	3109.8764
3134.9270	3135.0115	3146.3603
3147.1326	3148.4451	3154.9915
3162.0274	3163.1674	3177.0642
3193.9283	3234.7734	3283.3091

Zero-point correction (Hartree): 0.370267

TS6: B3LYP

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.679929287
Electronic state : 1-A
Cartesian coordinates (Angs):

C	1.780841	0.982181	-0.469554
C	1.408785	-0.453207	0.030713
C	3.103474	0.864635	0.320462
C	2.942109	-0.687391	0.314333
C	3.701054	-1.327345	-0.853233
C	3.268136	-1.410907	1.618730
C	0.804751	2.104796	-0.270293
C	-0.436665	2.036826	-1.152794
C	-1.769743	1.836482	-0.412486
C	0.997302	3.110207	0.584753
C	-1.895976	0.598532	0.446990
C	-0.730050	-1.935864	-0.212525
C	0.587619	-1.428355	-0.832260
C	-2.525857	-0.866605	-1.821291
H	1.999265	0.916330	-1.543140
H	0.936038	-0.347704	1.012908
H	3.011681	1.261392	1.334422
H	4.002143	1.280451	-0.141254
H	4.779471	-1.243189	-0.685964

```
      H       3.477504     -0.848578     -1.810517
      H       3.467988     -2.391922     -0.950568
      H       4.344389     -1.391584      1.821163
      H       2.959981     -2.461217      1.575085
      H       2.758836     -0.947389      2.468419
      H      -0.306904      1.251017     -1.899734
      H      -0.524934      2.970632     -1.716671
      H      -2.593111      1.851857     -1.131741
      H      -1.928596      2.693112      0.252327
      H       0.275762      3.914567      0.690023
      H       1.882924      3.175717      1.205063
      H      -1.063539      0.312959      1.083579
      H      -0.938452     -2.929640     -0.626268
      H      -0.605200     -2.091870      0.863042
      H       1.202168     -2.314053     -1.021687
      H       0.406094     -1.000334     -1.823988
      H      -1.800510     -0.275080     -2.381289
      H      -3.482848     -0.344875     -1.794806
      H      -2.673892     -1.809884     -2.355957
      C      -2.080654     -1.195265     -0.387659
      O      -3.011157     -1.712250      0.339999
      O      -3.226531     -0.467641      1.844265
      O      -3.076940      0.604512      1.085016
Rotational constants (GHz):    0.6100400    0.3006500    0.2511100
Vibrational harmonic frequencies (cm-1):
    -474.8813                  42.2152                  60.4113
      81.6471                  88.7119                 131.4280
     152.5918                 179.2050                 201.1144
     214.5677                 226.0120                 231.7568
     247.9269                 251.8921                 268.2106
     274.1552                 288.9092                 318.7056
     327.6415                 348.7818                 354.6463
     390.3089                 406.6442                 438.9157
     468.0686                 476.2450                 500.3416
     522.7829                 543.4183                 555.1368
     572.2201                 615.2346                 628.9647
     711.8910                 728.7862                 746.9541
     801.8083                 823.3640                 835.7070
     869.1986                 893.2159                 902.2282
     925.9006                 928.1156                 950.9602
     957.5358                 985.2868                 993.5082
    1007.0614                1011.1397                1016.4593
    1028.7944                1044.6702                1061.1438
    1074.3397                1104.8662                1112.3327
    1119.0829                1128.6004                1157.3380
    1174.5082                1196.8649                1200.4045
    1217.8370                1226.2078                1230.2886
    1253.3389                1256.8997                1276.3518
    1281.7089                1294.8357                1307.6456
    1330.5688                1344.0147                1355.2651
    1378.8158                1384.7276                1388.4037
    1394.3622                1397.9146                1407.8093
    1412.9187                1421.6428                1449.3521
    1470.5377                1475.7759                1483.0262
    1483.6266                1487.0292                1491.4559
    1496.3323                1498.4012                1505.4403
    1509.1944                1510.2292                1703.6392
    3000.3928                3010.3533                3015.1114
    3020.3395                3023.2942                3027.3164
    3029.1263                3036.2383                3041.5664
    3044.1977                3051.0465                3067.7949
```

```
    3069.2752                3070.4392                3078.7514
    3080.4998                3086.6895                3088.5231
    3094.2132                3100.8229                3131.0180
    3132.2652                3147.6777                3212.1434
Zero-point correction (Hartree): 0.363791

TS6: MPW1B95
--------------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.115515481
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.763515      0.993910      -0.447383
     C       1.407691     -0.431056       0.041489
     C       3.054939      0.891268       0.366961
     C       2.928207     -0.648303       0.307431
     C       3.674163     -1.223173      -0.887717
     C       3.277651     -1.414823       1.567134
     C       0.755603      2.075814      -0.264344
     C      -0.437032      1.969489      -1.189796
     C      -1.778177      1.789723      -0.489516
     C       0.870308      3.053599       0.634066
     C      -1.878139      0.595718       0.413558
     C      -0.698571     -1.921135      -0.180517
     C       0.595797     -1.404287      -0.811537
     C      -2.495866     -0.900692      -1.791654
     H       2.004285      0.929671      -1.515612
     H       0.947685     -0.329126       1.031298
     H       2.911499      1.246814       1.390111
     H       3.956607      1.346990      -0.046096
     H       4.751182     -1.107848      -0.744916
     H       3.408284     -0.725703      -1.822965
     H       3.473253     -2.290090      -1.009628
     H       4.354453     -1.393236       1.754228

     H       2.978144     -2.463163       1.483909
     H       2.775586     -0.989767       2.438794
     H      -0.272681      1.146957      -1.887181
     H      -0.504685      2.871272      -1.803385
     H      -2.583638      1.750880      -1.225752
     H      -1.970823      2.670187       0.131284
     H       0.110365      3.819876       0.740795
     H       1.730154      3.128736       1.287320
     H      -1.028290      0.320130       1.031961
     H      -0.891318     -2.928153      -0.563931
     H      -0.568684     -2.043857       0.898109
     H       1.220621     -2.279884      -1.008740
     H       0.402098     -0.976419      -1.800587
     H      -1.777968     -0.303040      -2.351975
     H      -3.457177     -0.389441      -1.766455
     H      -2.631450     -1.845443      -2.322864
     C      -2.050631     -1.219461      -0.369715
     O      -2.964788     -1.716456       0.373630
     O      -3.156539     -0.429841       1.855826
     O      -3.037955      0.595561       1.056984
Rotational constants (GHz):    0.6243600    0.3068400    0.2576100
Vibrational harmonic frequencies (cm-1):
    -504.2340                 55.7892                  70.7270
      93.2754                100.9163                 130.3988
     154.7456                186.7401                 198.7686
     227.9023                233.9465                 252.5845
     259.1148                264.2677                 276.1693
```

```
     301.1689                307.1233                319.0880
     332.2248                354.5403                357.8554
     389.3198                405.2687                447.2089
     472.1484                480.0781                502.2408
     523.1207                544.7358                558.2953
     577.2581                618.1855                630.3649
     731.1537                731.6846                767.2923
     807.8642                829.5923                854.8624
     884.7089                901.7471                924.0467
     934.8563                949.6728                961.1470
     969.3523                998.0148               1011.4958
    1017.6173               1023.3853               1037.8093
    1053.9264               1067.2919               1077.9469
    1100.2081               1134.3487               1138.3817
    1148.7663               1176.1532               1178.9722
    1198.2533               1216.1314               1224.5787
    1234.3075               1244.5869               1254.9716
    1263.2945               1267.4518               1290.5935
    1306.9513               1310.9967               1325.1712
    1344.9666               1346.5458               1367.1571
    1390.5749               1399.6007               1407.5738
    1415.3613               1426.7015               1432.7501
    1439.6602               1453.8765               1463.3201
    1467.3010               1471.7884               1480.0587
    1486.7861               1491.8975               1494.5184
    1502.8459               1505.7593               1512.2330
    1522.9881               1527.3045               1746.5106
    3048.4639               3059.8750               3062.6816
    3065.6417               3070.1065               3073.4498
    3080.5792               3086.1877               3091.2669
    3094.1041               3104.9761               3122.4188
    3132.5285               3137.7706               3145.3826
    3146.6715               3147.0988               3150.5114
    3152.4871               3167.0388               3187.1978
    3197.1044               3206.3249               3275.2625
Zero-point correction (Hartree): 0.369697
```

TS7: B3LYP

```
------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.680376076
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.813360      0.962750      0.476044
     C      -1.433704     -0.469172     -0.025848
     C      -3.143797      0.829387     -0.299468
     C      -2.966139     -0.720859     -0.295335
     C      -3.707906     -1.368462      0.879213
     C      -3.296711     -1.447821     -1.596786
     C      -0.850137      2.094941      0.263297
     C       0.418328      2.019855      1.106738
     C       1.733370      1.867292      0.324379
     C      -1.082336      3.110640     -0.569047
     C       1.870955      0.702300     -0.669084
     C       0.715684     -1.929537      0.208663
     C      -0.600534     -1.431911      0.837172
     C       2.555763     -0.747232      1.617551
     H      -2.019502      0.897202      1.552451
     H      -0.962882     -0.360859     -1.007657
     H      -3.066277      1.228077     -1.313736
     H      -4.042499      1.234182      0.171669
```

```
      H      -4.788477     -1.297412      0.720593
      H      -3.483035     -0.884724      1.833718
      H      -3.462793     -2.430641      0.976622
      H      -4.374441     -1.435291     -1.791460
      H      -2.982757     -2.496773     -1.554819
      H      -2.796672     -0.981636     -2.450382
      H       0.313057      1.209520      1.832356
      H       0.499328      2.935497      1.702208
      H       2.581298      1.845113      1.013392
      H       1.877056      2.763058     -0.287831
      H      -0.371224      3.921831     -0.688427
      H      -1.988826      3.174960     -1.158901
      H       0.961332      0.454537     -1.234909
      H       0.998017     -2.861892      0.714928
      H       0.542488     -2.193259     -0.838387
      H      -1.196199     -2.328362      1.033974
      H      -0.410738     -0.998073      1.824066
      H       1.859391     -0.206709      2.254991
      H       3.477454     -0.180728      1.519299
      H       2.784354     -1.704168      2.101859
      C       1.962640     -1.051446      0.259691
      O       2.838334     -1.581754     -0.635449
      O       3.941045     -0.859832     -0.754268
      O       2.955602      0.713113     -1.363870
Rotational constants (GHz):    0.6411000    0.2970300    0.2434000
Vibrational harmonic frequencies (cm-1):
    -484.0093                  45.7128                  67.4906
      88.5316                  94.0825                 131.4936
     149.4471                 177.9503                 189.4260
     197.3997                 225.0374                 240.2833
     251.3591                 261.4814                 278.4160
     286.8629                 301.3138                 326.4155
     335.2665                 343.1457                 371.6788
     390.3143                 402.6367                 408.8430
     452.5031                 490.9169                 511.2543
     534.6611                 543.4161                 557.7527
     584.9751                 625.2679                 642.2591
     722.6533                 727.5485                 765.7445
     805.6044                 816.6273                 848.5442
     853.5498                 902.7245                 906.1626
     921.9616                 938.0470                 951.3311
     960.0494                 977.4495                 993.7739

     998.5141                1008.6165                1016.5071
    1028.1801                1035.6927                1055.3119
    1069.1281                1087.4211                1110.8076
    1125.9663                1133.5445                1162.0834
    1175.6107                1196.9007                1210.3380
    1226.4808                1237.3789                1245.8684
    1248.4052                1255.2864                1273.9096
    1286.9708                1303.4632                1304.8498
    1326.7367                1351.9126                1354.4432
    1372.7832                1388.0238                1391.3892
    1399.0541                1402.9821                1408.6539
    1421.2818                1426.5764                1448.7079
    1475.0335                1478.1728                1483.4522
    1484.2861                1485.8582                1488.4344
    1496.6513                1497.9298                1507.5433
    1509.2127                1510.8790                1704.8663
    2980.2676                2996.2192                3004.2390
    3009.7068                3019.3430                3026.7470
```

```
    3028.6617                3032.0971                3038.4167
    3041.8966                3046.0547                3056.6373
    3067.0693                3067.3993                3072.9017
    3077.2637                3081.4464                3084.6573
    3086.2084                3095.7828                3126.1560
    3132.7380                3172.8646                3211.6018
Zero-point correction (Hartree): 0.363978

TS7: MPW1B95
---------------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.116984139
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.805178      0.970540       0.455551
     C      -1.436389     -0.450053      -0.033603
     C      -3.103017      0.849685      -0.347003
     C      -2.954884     -0.687930      -0.291834
     C      -3.687069     -1.273699       0.906648
     C      -3.301367     -1.456873      -1.551031
     C      -0.813379      2.065080       0.257606
     C       0.417348      1.941019       1.129520
     C       1.735594      1.834918       0.374912
     C      -0.982875      3.065855      -0.605683
     C       1.866659      0.714292      -0.647667
     C       0.683880     -1.909974       0.193775
     C      -0.616580     -1.411066       0.823108
     C       2.541762     -0.761957       1.585659
     H      -2.034045      0.906297       1.526907
     H      -0.973295     -0.345586      -1.020508
     H      -2.971951      1.211020      -1.369731
     H      -4.008280      1.290241       0.074343
     H      -4.766103     -1.171558       0.769556
     H      -3.423104     -0.772078       1.840283
     H      -3.473961     -2.338627       1.027504
     H      -4.378966     -1.445537      -1.734132
     H      -2.992531     -2.502992      -1.470369
     H      -2.807116     -1.025766      -2.424117
     H       0.289808      1.079149       1.787649
     H       0.476560      2.808987       1.792293
     H       2.574988      1.785982       1.070351
     H       1.885034      2.751867      -0.201155
     H      -0.236409      3.842280      -0.729282
     H      -1.873307      3.145595      -1.216370
     H       0.952259      0.473564      -1.208389
     H       0.962786     -2.846897       0.689625
     H       0.505339     -2.162224      -0.854280
     H      -1.218934     -2.303041       1.015061
     H      -0.426189     -0.983233       1.812109
     H       1.845898     -0.247148       2.242714
     H       3.450127     -0.177252       1.479736
     H       2.795530     -1.722044       2.045971
     C       1.932174     -1.054167       0.245918
     O       2.780051     -1.563501      -0.663401
     O       3.895193     -0.888013      -0.746925
     O       2.947980      0.718388      -1.329802
Rotational constants (GHz):    0.6578100    0.3020300    0.2484500
Vibrational harmonic frequencies (cm-1):
    -516.8828                 54.0751                 80.3711
      99.8463                103.8949                141.9134
     153.3825                189.7464                197.4139
     221.1709                240.2399                249.7803
```

262.8211	270.5686	286.9673
301.5524	322.6239	335.4618
349.7154	356.3863	366.2097
393.3043	408.3428	411.7166
456.8537	501.2755	514.0768
539.7431	551.3350	561.5539
588.2961	630.1847	648.4040
731.9020	743.9109	784.1071
812.8582	832.7334	869.3119
874.3218	908.8287	924.0176
931.8550	956.1367	960.7859
971.9154	986.4445	1007.9992
1012.2636	1021.8189	1027.6778
1051.3525	1068.3940	1074.0446
1099.0034	1110.5050	1140.2793
1149.1876	1172.1384	1193.9087
1204.4186	1217.2923	1230.2696
1235.6157	1248.4503	1255.1502
1260.3099	1279.2829	1297.7494
1308.5546	1322.3433	1326.9240
1345.9950	1358.6813	1371.7727
1394.9236	1403.3655	1407.3523
1411.2272	1416.6911	1427.0430
1431.2842	1458.3349	1471.9644
1477.0914	1483.6041	1487.1604
1489.4525	1491.2954	1496.2177
1502.3120	1506.8223	1513.9272
1522.1285	1529.5458	1748.2577
3040.9650	3045.5200	3055.8891
3059.3859	3067.5579	3071.4371
3077.4959	3080.4324	3084.6261
3091.6293	3095.2763	3110.9154
3126.9500	3133.6660	3135.9544
3143.5873	3147.8665	3149.3198
3150.0662	3152.8768	3187.2674
3188.3777	3238.2889	3274.4145

Zero-point correction (Hartree): 0.370087

TS8: B3LYP

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.674602768
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.452799	0.893633	0.544668
C	-1.429155	-0.451006	-0.305557
C	-2.943756	1.042903	0.149372
C	-3.002890	-0.462234	-0.225250
C	-3.567297	-1.301072	0.928622
C	-3.716071	-0.811620	-1.529691
C	-0.506110	2.058356	0.316162
C	0.789630	2.093206	1.121370
C	2.043558	1.595850	0.361603
C	-0.778868	3.059402	-0.525161
C	1.754354	0.449400	-0.577689
C	0.736129	-2.028171	-0.318188
C	-0.714329	-1.743235	0.121277
C	1.718864	-1.010150	1.879741
H	-1.393651	0.617874	1.603407
H	-1.162135	-0.202953	-1.339742
H	-3.077001	1.671003	-0.732969
H	-3.622472	1.394731	0.930326

```
      H      -4.636104     -1.094896      1.043253
      H      -3.086267     -1.072864      1.883489
      H      -3.456960     -2.373588      0.745773
      H      -4.797128     -0.660605     -1.440078
      H      -3.551991     -1.860303     -1.800959
      H      -3.358110     -0.191840     -2.356886
      H       0.661479      1.519927      2.039846
      H       0.986419      3.122253      1.432886
      H       2.859567      1.368337      1.045007
      H       2.404841      2.400255     -0.292921
      H      -0.093257      3.892535     -0.643417
      H      -1.681419      3.098821     -1.121661
      H       0.784031      0.495989     -1.058152
      H       0.936415     -3.084106     -0.103867
      H       0.850509     -1.918353     -1.400292
      H      -1.307672     -2.563150     -0.302378
      H      -0.798884     -1.868019      1.205348
      H       0.781324     -0.533769      2.160064
      H       2.559557     -0.432807      2.263274
      H       1.749630     -1.990476      2.365758
      C       1.891504     -1.254751      0.372824
      O       3.075598     -1.634439      0.045498
      O       3.841215     -0.085095     -1.014157
      O       2.647272      0.154900     -1.532557
Rotational constants (GHz):    0.6530000    0.3073800    0.2553500
Vibrational harmonic frequencies (cm-1):
    -472.3322                  48.7579                  61.7628
      84.2773                 105.2756                 143.6066
     157.5004                 186.9597                 214.2251
     222.6418                 226.6802                 240.0078
     270.5148                 276.8493                 287.2121
     293.9661                 304.2343                 318.2289
     326.5303                 345.5073                 358.8529
     405.4270                 413.7265                 430.4661
     452.7533                 481.1366                 516.0346
     532.2314                 550.4361                 567.6218
     580.7315                 626.8404                 694.3922
     729.1771                 733.6321                 758.3999
     802.3231                 818.5823                 841.1510
     868.4000                 899.6375                 906.0238
     933.4911                 941.4951                 952.3987
     953.6854                 974.2381                 989.3357
     996.1329                1005.8364                1013.9850
    1021.6609                1029.1728                1047.1202
    1056.1470                1066.4433                1096.9754
    1116.5940                1129.9411                1163.7006
    1170.0095                1180.8813                1202.7090
    1210.4299                1224.4299                1231.1664
    1257.8299                1263.0176                1265.9856
    1282.7934                1287.3491                1316.9197
    1331.3022                1337.2707                1358.0765
    1367.0252                1383.1064                1386.8923
    1394.5226                1397.9054                1405.4964
    1421.5753                1449.3830                1458.5447
    1473.4861                1477.9660                1485.2449
    1486.0378                1488.0907                1494.1386
    1498.1339                1504.8881                1508.5626
    1510.0096                1514.0390                1693.8938
    3006.2015                3007.9727                3010.0727
    3010.6480                3022.9396                3027.4343
    3028.4875                3041.1228                3049.2139
```

```
    3052.1301                3054.2397                3068.1917
    3074.2858                3079.5579                3081.5117
    3090.1458                3096.5196                3100.3191
    3109.0922                3124.1816                3136.1626
    3150.3527                3190.6194                3216.6892
Zero-point correction (Hartree): 0.364776

TS8: MPW1B95
---------------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.112523170
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.389818      0.892720       0.518860
     C      -1.407433     -0.425297      -0.343241
     C      -2.866267      1.074571       0.132714

     C      -2.958888     -0.420477      -0.208548
     C      -3.463474     -1.223612       0.982771
     C      -3.723545     -0.797786      -1.461345
     C      -0.438080      2.042983       0.295669
     C       0.840449      2.090571       1.106272
     C       2.068217      1.534585       0.368166
     C      -0.689909      3.024719      -0.573537
     C       1.721108      0.410784      -0.558448
     C       0.722897     -2.022345      -0.369167
     C      -0.726700     -1.739792       0.025014
     C       1.520811     -0.987934       1.858802
     H      -1.335939      0.603512       1.574195
     H      -1.174821     -0.154820      -1.381282
     H      -2.976431      1.680765      -0.767383
     H      -3.534678      1.465697       0.902351
     H      -4.521874     -1.009777       1.148662
     H      -2.928428     -0.975268       1.902248
     H      -3.364262     -2.298761       0.817865
     H      -4.797808     -0.647281      -1.326888
     H      -3.567933     -1.850820      -1.713051
     H      -3.402801     -0.197125      -2.315261
     H       0.696768      1.564019       2.049116
     H       1.056240      3.127519       1.369364
     H       2.873218      1.265934       1.048844
     H       2.473654      2.311040      -0.292027
     H       0.004032      3.849049      -0.694606
     H      -1.578258      3.053756      -1.189746
     H       0.739912      0.464893      -1.015048
     H       0.917223     -3.080894      -0.172646
     H       0.880452     -1.883188      -1.441798
     H      -1.325586     -2.518604      -0.462032
     H      -0.853267     -1.919188       1.096738
     H       0.566735     -0.498287       2.035662
     H       2.328496     -0.418150       2.313640
     H       1.486453     -1.960622       2.355817
     C       1.819994     -1.258040       0.388988
     O       3.026069     -1.611609       0.153640
     O       3.779937     -0.109685      -1.000867
     O       2.589336      0.077882      -1.505341
Rotational constants (GHz):    0.6678100    0.3187700    0.2643900
Vibrational harmonic frequencies (cm-1):
    -496.9483                 52.8049                 75.1247
      91.6646                112.7501                150.4069
     157.7515                187.2151                217.2778
     226.0668                233.7159                239.6458
```

```
     273.2671                279.9183                294.1986
     297.3983                306.8901                320.6544
     323.6104                345.3944                377.6786
     399.7111                419.4246                433.9471
     456.9101                478.2688                519.5054
     542.0576                559.8229                565.3059
     584.8489                636.9574                708.0264
     737.8351                750.5452                772.3230
     810.1649                828.0656                857.0078
     883.2310                911.7011                922.0455
     942.2897                950.4096                957.9208
     962.9396                976.5661               1001.1578
    1008.7361               1014.5010               1023.4336
    1029.7655               1041.9496               1056.7771
    1075.6764               1108.3937               1123.0801
    1144.0179               1153.6042               1172.0619
    1182.6511               1205.6817               1217.1054
    1229.2697               1233.6373               1240.9150
    1264.1338               1269.3307               1287.6285
    1307.8126               1315.1381               1328.6373
    1330.9986               1343.0050               1361.4686
    1366.5707               1389.6661               1391.5130
    1410.0515               1414.6180               1423.8028
    1448.9405               1452.1903               1467.8080
    1477.3361               1484.3763               1486.6411
    1489.0862               1496.4206               1499.7776
    1504.8062               1508.0134               1511.5568
    1513.3863               1519.9797               1730.3471
    3042.9183               3051.8315               3058.5288
    3062.7513               3068.4965               3072.0583
    3079.7743               3089.8385               3097.9386
    3107.2711               3108.2575               3130.8901
    3135.5155               3146.2163               3148.2998
    3151.2265               3157.2189               3158.7969
    3169.2374               3176.9262               3192.5902
    3216.4733               3243.5154               3281.2682
Zero-point correction (Hartree): 0.369830
```

TS9: B3LYP

```
----------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.721398225
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.462917      0.601983     -0.089778
     C       1.105212     -0.890492      0.161048
     C       2.972492      0.192261     -0.093337
     C       2.550035     -1.292786     -0.316868
     C       2.634805     -1.688994     -1.795221
     C       3.258001     -2.331064      0.550733
     C       1.031265      1.710666      0.838649
     C       1.095602      3.113806      0.263221
     C      -0.027038      3.406066     -0.764352
     C       0.633115      1.513158      2.096886
     C      -1.399234      3.365838     -0.137099
     C      -1.429524     -0.832555      0.020953
     C      -0.130361     -1.477172     -0.515121
     C      -3.867882     -0.726274     -0.891794
     H       1.172460      0.862637     -1.113804
     H       1.041511     -1.082308      1.236763
     H       3.421507      0.344713      0.890979
     H       3.615265      0.645280     -0.852750
```

```
 H       3.682905     -1.775500      -2.099537
 H       2.162529     -0.953435      -2.452249
 H       2.155487     -2.655484      -1.977546
 H       4.309441     -2.435741       0.261749
 H       2.786464     -3.314344       0.449788
 H       3.227141     -2.052511       1.607894
 H       2.057976      3.270356      -0.236391
 H       1.039999      3.847491       1.073376
 H      -0.008694      2.703715      -1.600032
 H       0.122154      4.416347      -1.167509
 H       0.370815      2.345443       2.741864
 H       0.548005      0.524532       2.530545
 H      -1.551293      4.079633       0.703316
 H      -1.459518     -1.613561       1.150240
 H      -1.426771      0.246622      -0.109202
 H      -0.163589     -2.556946      -0.358403
 H      -0.076425     -1.304133      -1.596069
 H      -3.851706      0.343556      -0.667928
 H      -4.812601     -1.166426      -0.569847
 H      -3.775584     -0.825870      -1.978400
 C      -2.709616     -1.376697      -0.219120
 O      -2.997363     -2.489560       0.412154
 O      -1.916416     -2.847464       1.256379
 O      -2.294499      2.634458      -0.483489
Rotational constants (GHz):    0.3831200    0.3525100    0.2163100
Vibrational harmonic frequencies (cm-1):
    -1581.1157                  24.6850                  31.4525
      44.6208                   50.5580                  61.9934
      76.6950                   78.2933                 108.8645
     138.1396                  149.3638                 155.5621
     194.9362                  211.5491                 219.1782
     240.7309                  253.7947                 275.8399
     283.8753                  307.2393                 325.4019
     353.9186                  374.5241                 382.1766
     393.2506                  461.1919                 485.5370
     499.2407                  508.5066                 563.7963
     613.7590                  637.1592                 653.3741
     686.4698                  720.2929                 747.4097
     785.6826                  816.5186                 866.7172
     872.6900                  880.3917                 893.4699
     916.3240                  920.3648                 929.8035
     932.9459                  953.5097                 956.8357
     994.5640                 1001.1216                1007.2277
    1020.6305                 1030.3557                1037.1703
    1044.2536                 1048.6671                1067.0036
    1075.8059                 1116.8130                1122.2840
    1180.5212                 1192.2390                1206.8865
    1217.4387                 1221.6977                1224.1810
    1254.5437                 1262.6050                1270.4338
    1288.3809                 1312.8987                1327.1470
    1337.1853                 1346.3234                1354.0853
    1374.7265                 1401.3502                1403.4583
    1415.5366                 1419.8378                1420.8264
    1422.9037                 1455.6074                1468.8975
    1470.7466                 1484.7300                1487.1536
    1488.1996                 1490.1726                1492.8555
    1497.6831                 1507.2732                1510.2838
    1528.0858                 1703.4819                1804.4436
    1836.7233                 2865.2755                3010.5524
    3012.7869                 3013.9132                3019.1958
    3021.4942                 3026.4159                3029.0737
```

```
    3037.6573                3045.0999                3062.0866
    3069.8550                3078.1597                3080.9294
    3085.7396                3088.1146                3089.8750
    3093.0596                3097.9070                3127.0162
    3135.6888                3142.8508                3216.7962
Zero-point correction (Hartree): 0.357981
```

TS10

```
---------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.723158258
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.858909     -0.709006       0.469044
     C       1.832831     -0.061075      -0.563078
     C       1.979365     -1.750411       0.794644
     C       3.032443     -0.828336       0.110804
     C       3.807254     -0.002884       1.144340
     C       3.998557     -1.511022      -0.855365
     C      -0.497778     -1.247135       0.061043
     C      -1.533330     -1.214448       1.167383
     C      -2.893826     -1.859179       0.868518
     C      -0.736369     -1.754592      -1.150042
     C      -3.743869     -1.089457      -0.123926
     C       0.622344      2.127822      -1.253850
     C       1.912926      1.456023      -0.724557
     C      -0.399311      3.232596       0.889782
     H       0.733380     -0.037222       1.325053
     H       1.658265     -0.504447      -1.548299
     H       1.820930     -2.677373       0.239445
     H       2.144681     -1.991095       1.847782
     H       4.489614     -0.652957       1.700647
     H       3.146750      0.475438       1.873111
     H       4.409088      0.779347       0.671222
     H       4.692271     -2.166812      -0.318592
     H       4.597869     -0.775564      -1.403510
     H       3.462978     -2.121380      -1.587952
     H      -1.696261     -0.167994       1.456653
     H      -1.101526     -1.696572       2.053907
     H      -3.470091     -1.875667       1.804009
     H      -2.800408     -2.892546       0.526061
     H      -1.695754     -2.170417      -1.428065
     H       0.025549     -1.772583      -1.921291
     H      -3.792115      0.005279       0.051017
     H       0.877759      3.121928      -1.640180
     H       0.184965      1.559020      -2.077632
     H       2.719183      1.684906      -1.430124
     H       2.189361      1.930904       0.220940
     H      -0.574966      2.795366       1.873807
     H      -1.751715      3.262000       0.789699
     H       0.393003      3.974261       0.889280
     C      -0.418647      2.344331      -0.205805
     O      -1.569770      1.773966      -0.441329
     O      -2.526770      2.219231       0.504564
     O      -4.352436     -1.603843      -1.030809
Rotational constants (GHz):    0.5398500    0.2908300    0.2200200
Vibrational harmonic frequencies (cm-1):
    -1605.4842                 26.5709                 38.3834
      47.7723                  50.1352                 62.7241
      79.4878                  85.9356                108.2502
     141.1413                 155.8024                192.5282
     209.1349                 221.6903                239.4182
```

257.6431	266.8394	289.9374
298.1673	343.6303	349.0984
361.7739	388.3794	407.3761
448.8102	487.2966	505.2430
518.8742	530.0129	557.4736
565.2490	616.2614	700.6881
719.8599	738.6470	744.1986
772.8191	797.8991	846.6099
870.7747	879.4571	881.3824
898.3417	914.8906	925.2668
932.0459	945.1001	948.7864
955.0164	987.8241	1002.2215
1014.3199	1022.8573	1031.4984
1043.5613	1051.1367	1059.6631
1088.1058	1105.5931	1119.6816
1163.2170	1184.3608	1207.5171
1209.6581	1220.3183	1227.3389
1241.6520	1255.1504	1266.2293
1279.6343	1310.3462	1318.5836
1336.7901	1344.5794	1349.5237
1377.2883	1392.0282	1394.8712
1404.4778	1413.3799	1423.0100
1429.0068	1451.4811	1466.6281
1467.2069	1475.7791	1485.2048
1487.1979	1492.6050	1492.9322
1499.6040	1509.6923	1509.9378
1528.7591	1703.3794	1801.0404
1834.3230	2915.0396	2998.8979
3009.7080	3010.1653	3017.7216
3020.6505	3024.4140	3027.4796
3031.4019	3039.3579	3045.1159
3067.7292	3070.4233	3078.8091
3081.6797	3084.0280	3085.0681
3086.1841	3092.6640	3099.7502
3143.9652	3175.9271	3226.6506

Zero-point correction (Hartree): 0.358212

TS11

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.715740876
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.734689	-0.778221	-0.162995
C	-1.953959	-0.101212	0.527862
C	-1.678116	-1.954815	-0.583245
C	-2.917496	-1.066604	-0.262273
C	-3.515935	-0.461774	-1.536920
C	-4.011544	-1.724387	0.576836
C	0.508478	-1.163069	0.599986
C	1.659998	-1.685308	-0.243077
C	2.438639	-0.548630	-0.959634
C	0.618196	-1.111687	1.928246
C	3.321274	0.286625	-0.248529
C	-1.069939	2.282592	1.075674
C	-2.181786	1.409725	0.446427
C	-0.192685	3.235204	-1.184064
H	-0.447377	-0.211955	-1.056699
H	-1.977739	-0.396728	1.581055
H	-1.584543	-2.797734	0.105480
H	-1.592404	-2.323615	-1.608278
H	-4.007730	-1.244458	-2.122939

```
      H      -2.754550     -0.006732     -2.176988
      H      -4.266128      0.301996     -1.310036
      H      -4.528796     -2.504558      0.008138
      H      -4.763176     -0.992022      0.891438
      H      -3.595275     -2.187297      1.475986
      H       1.278990     -2.365181     -1.012912
      H       2.350595     -2.252290      0.378796
      H       1.803440      0.017151     -1.639012
      H       3.558867     -1.322282     -1.169169
      H       1.523033     -1.441528      2.427137
      H      -0.171190     -0.735012      2.567462
      H       3.273572      1.363763     -0.120838
      H      -1.508259      3.249646      1.356321
      H      -0.669826      1.830602      1.984678
      H      -3.122349      1.633090      0.961989
      H      -2.338193      1.714684     -0.592130
      H      -0.436919      2.446119     -1.902379
      H       0.690917      3.762631     -1.542246
      H      -1.047990      3.914287     -1.146608
      C       0.109445      2.618654      0.173414
      O       1.254851      2.438682      0.529679
      O       4.532172     -1.570044     -0.313476
      O       4.454695     -0.228030      0.130735
Rotational constants (GHz):    0.5621900    0.2697700    0.2120700
Vibrational harmonic frequencies (cm-1):
    -1614.5901                  25.1170                  33.7641
      42.7742                   50.0868                  56.1162
      69.5860                   93.6147                 113.8404
     128.1222                  133.4150                 157.8726
     186.8243                  210.6314                 234.7804
     245.8580                  269.5658                 284.3919
     294.3429                  308.0581                 353.4425
     368.9929                  382.3791                 409.2714
     460.7915                  470.2160                 498.4290
     531.0725                  550.4100                 563.7988
     579.6952                  645.4135                 677.9373
     715.8304                  728.9659                 762.2372
     785.6320                  794.1283                 852.9678
     863.4607                  880.5959                 881.9101
     892.0158                  901.2451                 910.4834
     922.1436                  944.9367                 949.7094
     973.4181                  987.1521                 991.8576
     998.9326                 1010.2671                1027.0359
    1031.4278                 1044.0702                1052.3147
    1109.8861                 1120.1724                1153.9677
    1170.0822                 1183.4125                1202.7686
    1211.5736                 1229.0708                1239.0067
    1251.3891                 1258.4361                1262.6476
    1267.9227                 1280.5183                1312.2009
    1313.6876                 1342.2164                1350.0840
    1356.9395                 1380.6932                1385.0091
    1395.9556                 1400.4608                1410.1852
    1418.4076                 1450.8229                1465.9465
    1468.0150                 1481.7143                1486.1430
    1487.1387                 1496.5902                1496.8784
    1500.9541                 1508.3051                1510.8904
    1520.5589                 1701.3754                1779.1126
    1835.4034                 3006.8319                3009.2517
    3011.8150                 3018.4219                3027.9738
    3029.2099                 3034.6867                3040.6822
    3044.8659                 3066.4663                3069.1623
```

```
    3079.2317                3081.2553                3083.4179
    3093.6826                3096.1085                3100.8328
    3108.7285                3125.1399                3136.3772
    3137.0450                3188.3480                3212.7355
Zero-point correction (Hartree): 0.358429
```

TS12

```
----------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.715239291
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.532716     -0.080801       0.072563
     C       0.583773     -1.286436       0.317252
     C       2.715362     -1.092063      -0.071121
     C       1.680284     -2.237211      -0.296237
     C       1.485513     -2.537444      -1.786520
     C       1.929390     -3.529610       0.477919
     C       1.681217      1.056209       1.050135
     C       2.507896      2.239037       0.575241
     C       1.957030      2.927753      -0.702883
     C       1.152798      1.056302       2.275823
     C       0.502165      3.297234      -0.548581
     C      -1.784677     -0.348669       0.535214
     C      -0.820349     -1.247913      -0.284065
     C      -3.146533      0.616411      -1.450322
     H       1.303056      0.332066      -0.914628
     H       0.512814     -1.504779       1.387491
     H       3.251413     -1.208235       0.874228
     H       3.438108     -0.912973      -0.871369
     H       2.369448     -3.046362      -2.183595
     H       1.336064     -1.630143      -2.378131
     H       0.624491     -3.191471      -1.953994
     H       2.812532     -4.052594       0.095804
     H       1.077330     -4.212336       0.390125
     H       2.091322     -3.330687       1.541045
     H       3.533111      1.917356       0.357991
     H       2.576541      2.973781       1.382171
     H       2.058557      2.288817      -1.581662
     H       2.533591      3.843587      -0.879048
     H       1.302869      1.890199       2.953409
     H       0.557463      0.233999       2.652459
     H       0.287178      4.068709       0.222964
     H      -1.984489     -0.779989       1.512025
     H      -1.333704      0.636566       0.680738
     H      -1.236424     -2.261435      -0.311184
     H      -0.761852     -0.903936      -1.321313
     H      -3.704438      1.528196      -1.199520
     H      -3.740476      0.085314      -2.199653
     H      -2.172100      0.911098      -1.834068
     C      -3.081786     -0.176767      -0.193040
     O      -4.164919     -0.786183       0.133526
     O      -4.198359     -0.213507       1.513659
     O      -0.399372      2.798321      -1.178503
Rotational constants (GHz):    0.4156500    0.3086600    0.2200200
Vibrational harmonic frequencies (cm-1):
    -423.7448                  25.9753                  30.5048
      49.1747                  53.8188                  64.7779
      81.1066                  86.3051                 105.2121
     116.6808                 140.6173                 158.6794
     182.5735                 200.9829                 211.8951
     230.0806                 256.4493                 277.3870
```

289.4666	312.0684	348.6852
355.5387	375.2190	385.8794
400.9046	435.9718	463.3930
488.7811	501.9047	508.9630
545.2210	565.7459	638.6379
719.4597	739.7884	758.1637
782.7321	798.0799	807.8239
862.6016	871.7505	879.4076
894.8069	920.9409	933.4427
948.0933	955.5535	964.9949
988.6543	996.5505	1001.9649
1020.7241	1029.9633	1037.8948
1042.8767	1053.1952	1082.2739
1103.2674	1116.9829	1175.4101
1178.3464	1202.1038	1208.2763
1219.4358	1225.3914	1242.5364
1261.5926	1267.3987	1272.9150
1291.6071	1299.8983	1324.8587
1336.6252	1343.9326	1354.2383
1378.4068	1381.3494	1403.0690
1416.9002	1421.9916	1422.7039
1447.3660	1453.4969	1474.3880
1476.4854	1479.2353	1487.2711
1487.8682	1488.8349	1496.0218
1499.1719	1509.5555	1511.8475
1520.1365	1700.4804	1800.7979
2877.9318	3011.2825	3018.5039
3018.8014	3019.0695	3022.8140
3030.0193	3032.4800	3037.9372
3044.3522	3061.8000	3065.6221
3066.4211	3070.1795	3076.5504
3080.2879	3082.0117	3087.9057
3092.0324	3102.8284	3138.9741
3154.7922	3156.1923	3220.0796

Zero-point correction (Hartree): 0.360478

TS13

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.715713073
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.994997	-0.801252	0.465872
C	1.926777	-0.109836	-0.574181
C	2.106953	-1.880704	0.664021
C	3.144956	-0.918698	0.011095
C	3.949897	-0.159942	1.072315
C	4.082826	-1.537866	-1.023181
C	-0.398805	-1.263304	0.099469
C	-1.386017	-1.224530	1.247925
C	-2.841244	-1.539087	0.894876
C	-0.715105	-1.705576	-1.119888
C	-3.468517	-0.535354	0.000134
C	0.691117	2.104884	-1.144153
C	2.005237	1.412275	-0.677581
C	0.185783	3.878691	0.669147
H	0.932912	-0.179410	1.363932
H	1.709781	-0.510759	-1.569321
H	1.914517	-2.757211	0.041284
H	2.308784	-2.208665	1.686891
H	4.645762	-0.842867	1.569462
H	3.311176	0.275232	1.846051

```
      H       4.540311      0.648572      0.630201
      H       4.791926     -2.224556     -0.548674
      H       4.666289     -0.768269     -1.540655
      H       3.526643     -2.101418     -1.777712
      H      -1.342028     -0.224868      1.692237
      H      -1.048160     -1.916869      2.029215
      H      -3.451951     -1.526848      1.811231
      H      -2.983308     -2.536302      0.465967
      H      -1.702983     -2.067787     -1.374997
      H       0.009316     -1.726985     -1.925666
      H      -3.128541      0.496525     -0.020225
      H       0.946993      2.986798     -1.739570
      H       0.103273      1.429200     -1.767791
      H       2.797307      1.661249     -1.391803
      H       2.323931      1.838786      0.279396
      H       1.265579      3.989654      0.798497
      H      -0.323993      3.978876      1.626426
      H      -0.141700      4.688593      0.007652
      C      -0.174128      2.552772      0.024422
      O      -1.110976      1.895623      0.428288
      O      -5.269303      0.243843     -0.371378
      O      -4.407248     -0.893905     -0.788632
Rotational constants (GHz):    0.5703000    0.2450900    0.1938300
Vibrational harmonic frequencies (cm-1):
    -440.3431                  21.2519                  26.9366
      39.7470                  48.6815                  64.9002
      76.7339                  91.0380                 100.3429
     108.1081                 123.7695                 150.1400
     191.8027                 209.1931                 222.9182
     245.6949                 260.8787                 270.7566
     297.4059                 307.0877                 309.7372
     358.1365                 372.8173                 380.5538
     418.1474                 447.3503                 472.7746
     507.8079                 521.1138                 523.6699
     565.6153                 601.9793                 612.5286
     703.7387                 735.1191                 753.7941
     768.8453                 778.2423                 797.4439
     856.3747                 875.7640                 879.6115
     899.0334                 901.0264                 914.6604
     940.3913                 957.0048                 971.8565
     985.9153                 989.7333                 994.1775
    1017.9815                1027.4548                1046.1288
    1050.3049                1051.6251                1097.7858
    1111.7512                1124.1397                1164.7311
    1175.9989                1192.1971                1206.7595
    1218.0256                1224.9158                1235.1795
    1249.4213                1254.4095                1274.3501
    1282.0809                1312.6958                1339.1775
    1342.3089                1352.2617                1363.6748
    1380.6447                1384.1254                1395.9792
    1404.3547                1416.2437                1424.3927
    1431.7136                1460.4251                1463.5275
    1475.6202                1476.7267                1485.5004
    1487.1733                1488.4999                1495.8288
    1498.7484                1511.8846                1512.1404
    1527.5963                1700.2222                1780.5513
    2989.1998                3009.6704                3016.3293
    3017.3224                3021.5528                3027.6512
    3031.1582                3038.2223                3042.3664
    3044.8549                3051.4648                3059.0503
    3066.7626                3067.8479                3079.0306
```

```
    3080.1948                3085.3130                3087.4600
    3096.9650                3102.2460                3140.4068
    3146.9366                3166.7456                3218.7323
Zero-point correction (Hartree): 0.360536
```

TS14

```
-----------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.717863883
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.895830     -0.821083       0.364209
     C       1.782010      0.023314      -0.594388
     C       2.126026     -1.757103       0.591698
     C       3.061328     -0.636641       0.039731
     C       3.689659      0.182101       1.173004
     C       4.132409     -1.081737      -0.953852
     C      -0.414303     -1.427073      -0.088750
     C      -1.384968     -1.687745       1.043901
     C      -2.774898     -2.206433       0.654902
     C      -0.677426     -1.720836      -1.365937
     C      -3.599262     -1.175608      -0.086898
     C       0.223741      2.002891      -1.121369
     C       1.617418      1.541792      -0.629535
     C      -1.853687      3.377563      -0.465858
     H       0.711373     -0.244813       1.274450
     H       1.683027     -0.361167      -1.615156
     H       2.090469     -2.622792      -0.074290
     H       2.311279     -2.099507       1.612747
     H       4.438794     -0.419904       1.696781
     H       2.950881      0.501918       1.912440
     H       4.193062      1.076218       0.791453
     H       4.900102     -1.686819      -0.459869
     H       4.634250     -0.220493      -1.408825
     H       3.700976     -1.683731      -1.758856
     H      -1.499803     -0.744666       1.593504
     H      -0.918628     -2.391079       1.745719
     H      -3.325595     -2.426712       1.579867
     H      -2.744450     -3.128607       0.069583
     H      -1.611468     -2.169420      -1.678938
     H       0.040917     -1.531017      -2.155727
     H      -3.539485     -0.150277       0.337943
     H       0.289782      2.771136      -1.898168
     H      -0.308061      1.164158      -1.599653
     H       2.370174      1.967188      -1.301202
     H       1.809832      1.964907       0.358279
     H      -2.414141      3.687620       0.410630
     H      -2.531589      2.867093      -1.155207
     H      -1.436654      4.239177      -1.003664
     C      -0.726290      2.477607      -0.072778
     O      -0.453821      2.203685       1.154785
     O      -1.809363      1.592066       1.372640
     O      -4.284386     -1.408809      -1.052716
Rotational constants (GHz):    0.5097100    0.3000400    0.2250900
Vibrational harmonic frequencies (cm-1):
    -424.2300                  10.4812                  33.9582
      47.8183                  49.8171                  60.9997
      72.5301                  91.9227                 108.2123
     136.0909                 149.5402                 193.1525
     215.5643                 221.0177                 236.7133
     248.5543                 263.8123                 271.6212
     293.6564                 302.3976                 325.0260
```

351.5684	364.6795	385.7585
392.4505	426.1799	453.3016
491.5050	512.5421	516.0701
567.0337	579.2307	617.5179
717.3543	732.6352	751.8677
769.6873	775.6782	790.1163
867.3155	881.5850	883.6909
887.6209	907.3324	921.7256
945.1159	952.9675	957.8450
991.9063	1004.4572	1019.4413
1023.9287	1030.5824	1043.8337
1051.8661	1054.0539	1090.7401
1115.3293	1126.8754	1173.9159
1191.2596	1206.8170	1210.6371
1215.8146	1221.0494	1232.3711
1251.9035	1255.3118	1275.3061
1287.0510	1315.2649	1341.5799
1348.9346	1381.7407	1389.2630
1401.9468	1403.4385	1407.2197
1417.9851	1420.8989	1425.3935
1426.5555	1436.2265	1452.0322
1463.8410	1469.5736	1482.1042
1484.7964	1487.9567	1492.0480
1498.6795	1508.3411	1511.4682
1529.5746	1696.7905	1804.4952
2889.3244	2978.2127	2999.4317
3007.9518	3009.2299	3010.0341
3018.5470	3025.9077	3030.4934
3033.4775	3041.3249	3057.6404
3058.6707	3067.0408	3076.7361
3079.5132	3080.0886	3083.3689
3088.6836	3092.3758	3096.2455
3145.1099	3176.2371	3221.4885

Zero-point correction (Hartree): 0.360345

TS15

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.709846257
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.977061	-0.845959	-0.134890
C	-1.913709	0.322565	0.303116
C	-2.251826	-1.711899	-0.405844
C	-3.122232	-0.421843	-0.385491
C	-3.436352	0.063025	-1.805891
C	-4.401598	-0.489201	0.445970
C	0.065077	-1.458965	0.770846
C	1.118543	-2.294457	0.068041
C	2.133100	-1.451231	-0.748876
C	0.055367	-1.337294	2.098346
C	3.096106	-0.733356	0.138377
C	-0.593303	2.547668	0.729522
C	-1.630678	1.768440	-0.113780
C	1.512753	2.571231	-0.799220
H	-0.517699	-0.587056	-1.095167
H	-2.069827	0.291014	1.385995
H	-2.466247	-2.366754	0.441605
H	-2.269319	-2.302583	-1.325083
H	-4.146957	-0.620320	-2.281283
H	-2.545822	0.100653	-2.439606
H	-3.888580	1.059349	-1.804249

```
      H      -5.137626     -1.154699      -0.017533
      H      -4.864356      0.499454       0.540254
      H      -4.200204     -0.863187       1.453771
      H       0.632601     -2.980190      -0.635670
      H       1.647428     -2.920158       0.793077
      H       1.588641     -0.718997      -1.350447
      H       2.710934     -2.047504      -1.457723

      H       0.794561     -1.836040       2.715832
      H      -0.671745     -0.728586       2.621190
      H       2.730020     -0.359495       1.099094
      H      -0.690706      3.611554       0.481610
      H      -0.804640      2.427766       1.794497
      H      -2.574217      2.321516      -0.041877
      H      -1.347219      1.805402      -1.170759
      H       0.823302      2.524637      -1.645625
      H       2.401366      1.968023      -0.995358
      H       1.823843      3.617897      -0.699395
      C       0.859463      2.153519       0.504535
      O       1.484393      1.560502       1.360156
      O       4.148461     -0.004059      -1.367225
      O       4.362219     -0.660837      -0.037396
Rotational constants (GHz):    0.6138600    0.2682800    0.2273100
Vibrational harmonic frequencies (cm-1):
    -640.9104                   33.8901                   38.1976
      53.9313                   63.0129                   67.3053
      82.0232                  103.1062                  113.0678
     138.2024                  146.2296                  160.1204
     190.9964                  197.1663                  234.6729
     247.3949                  261.1511                  280.1286
     282.0374                  316.5546                  338.6591
     360.8538                  385.5561                  398.8501
     407.7854                  456.0518                  466.1820
     491.7989                  508.9900                  532.0778
     565.9054                  598.8155                  643.1346
     715.0599                  725.6960                  737.7768
     763.4360                  804.5814                  827.1865
     855.0908                  861.9954                  879.2299
     896.8110                  909.4148                  926.2901
     938.6326                  954.8675                  970.7125
     978.0071                  992.7272                 1000.6145
    1017.4290                 1030.4846                 1040.8720
    1049.8654                 1054.3849                 1083.1237
    1110.2214                 1119.3893                 1164.1431
    1168.3586                 1188.3172                 1207.6880
    1226.6405                 1229.5619                 1238.4027
    1253.2860                 1260.3466                 1265.2387
    1279.5521                 1314.3274                 1328.8826
    1336.7819                 1344.0916                 1364.2574
    1365.5887                 1386.2006                 1394.8160
    1402.8150                 1411.6691                 1421.6335
    1450.4070                 1454.7046                 1467.9019
    1481.2676                 1482.8012                 1487.6880
    1490.0498                 1492.9116                 1493.4217
    1497.2866                 1508.7459                 1511.2343
    1550.9474                 1707.6541                 1774.7991
    3010.5374                 3012.3805                 3017.4258
    3018.8825                 3021.0436                 3022.6351
    3025.9745                 3037.4039                 3042.8928
    3054.1949                 3055.6261                 3067.7658
    3068.5212                 3079.3453                 3081.0894
```

```
    3082.6474                3085.0233                3089.8294
    3092.9674                3096.9131                3104.4852
    3117.7845                3140.8677                3219.1680
Zero-point correction (Hartree): 0.360993
```

TS16

```
-------------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.699828096
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.441244      0.875574       0.522227
     C      -1.402916     -0.485333      -0.304384
     C      -2.953000      0.963991       0.185511
     C      -2.973264     -0.542388      -0.189161
     C      -3.490244     -1.399665       0.973064
     C      -3.703063     -0.908839      -1.480048
     C      -0.548740      2.069743       0.216599
     C       0.752029      2.231117       1.003258
     C       2.015021      1.738629       0.247849
     C      -0.873132      2.994005      -0.691747
     C       1.762708      0.410633      -0.451547
     C       0.848024     -1.925600      -0.238057
     C      -0.641814     -1.748490       0.132278
     C       1.680933     -0.797694       1.894964
     H      -1.329248      0.632778       1.584331
     H      -1.157538     -0.247225      -1.345810
     H      -3.148900      1.590855      -0.685417
     H      -3.611213      1.286263       0.996237
     H      -4.562382     -1.225906       1.108590
     H      -2.998256     -1.158161       1.919201
     H      -3.351104     -2.468221       0.785847
     H      -4.785740     -0.785997      -1.368738
     H      -3.517129     -1.952374      -1.757188
     H      -3.377759     -0.278473      -2.312627
     H       0.663498      1.716706       1.962195
     H       0.893823      3.288789       1.239793
     H       2.877076      1.688479       0.918719
     H       2.260946      2.460678      -0.535692
     H      -0.228872      3.848496      -0.872291
     H      -1.776076      2.945098      -1.287032
     H       0.798392      0.477892      -0.953115
     H       1.165691     -2.919000       0.093913
     H       0.972894     -1.904286      -1.325135
     H      -1.166234     -2.593065      -0.331043
     H      -0.766191     -1.893563       1.209634
     H       0.676640     -0.511492       2.199684
     H       2.397493     -0.084225       2.299770
     H       1.897556     -1.776267       2.329943
     C       1.814981     -0.899944       0.374361
     O       3.192998     -1.298349       0.213960
     O       3.671549     -0.787990      -1.057169
     O       2.647323      0.137313      -1.537387
Rotational constants (GHz):    0.6648500    0.3125800    0.2600500
Vibrational harmonic frequencies (cm-1):
    -203.4540                 53.3989                  57.4285
      87.2479                125.0292                 153.2545
     163.8954                198.0283                 220.8406
     233.2285                251.1545                 256.2254
     275.3994                276.4806                 289.3540
     306.6957                328.1180                 336.9331
     368.3047                378.0900                 405.1211
```

422.4768	435.0830	454.5010
492.9811	520.6466	532.3403
576.1710	615.5932	648.6171
702.3410	727.4815	738.8015
753.2283	806.8826	816.9710
820.2180	853.0678	865.3612
877.9839	898.3019	924.1479
924.7050	929.0510	943.4747
948.3435	953.9542	984.4455
996.9135	999.1452	1010.9543
1013.2527	1023.7390	1033.0904
1052.0548	1080.3460	1099.1350
1106.1757	1141.9236	1150.5308
1159.2398	1186.5889	1202.9790
1210.1036	1227.9592	1233.1579
1247.3625	1258.5056	1276.9042
1282.2135	1306.8470	1317.0010
1327.6527	1341.0128	1353.5101
1358.6916	1380.0922	1381.2003
1396.4184	1404.5124	1410.7251
1420.6291	1425.5810	1449.3102
1476.9865	1485.8985	1487.1854
1488.8444	1495.0977	1499.3480
1500.4952	1508.0863	1510.0371
1511.3678	1516.1944	1691.8473
3009.1357	3013.0184	3013.7593
3022.4120	3028.0262	3036.1557
3042.2378	3050.9503	3051.8607
3055.5878	3058.0536	3067.3627
3076.0012	3077.1199	3080.1490
3080.8819	3088.0069	3092.1201
3106.0179	3113.8794	3122.7270
3136.6957	3154.2057	3215.9912

Zero-point correction (Hartree): 0.367151

TS17a: B3LYP/6-311G**

TS-rp-Dio-1a-B3LYP

E(UB+HF-LYP/6-311G(d,p)) (Hartree): -811.734898946

Electronic state : 1-A

Cartesian coordinates (Angs):

C	1.524176	-0.040182	0.005028
C	0.645601	-1.265887	0.378101
C	2.730830	-1.015117	-0.187974
C	1.727004	-2.205340	-0.280095
C	1.428861	-2.577862	-1.736468
C	2.084597	-3.452389	0.525196
C	1.708330	1.143373	0.919296
C	2.440741	2.333502	0.324317
C	1.699756	2.996944	-0.866222
C	1.285950	1.176940	2.184986
C	0.289782	3.389152	-0.496106
C	-1.703345	-0.342452	0.664495
C	-0.804478	-1.310879	-0.107232
C	-3.324631	0.304755	-1.261016
H	1.203908	0.319607	-0.978317
H	0.672961	-1.435020	1.459573
H	3.342732	-1.066893	0.716125
H	3.381031	-0.848301	-1.050532
H	2.297777	-3.075111	-2.178994

```
      H       1.203951     -1.702387      -2.351632
      H       0.580871     -3.265146      -1.809592
      H       2.954518     -3.961248       0.096337
      H       1.254353     -4.166753       0.533099
      H       2.321535     -3.201177       1.563022
      H       3.430081      2.024743      -0.032348
      H       2.610194      3.079376       1.106257
      H       1.655238      2.338564      -1.735285
      H       2.246646      3.903171      -1.153913
      H       1.461672      2.042557       2.814927
      H       0.754821      0.350921       2.641161
      H       0.207208      4.142209       0.318766
      H      -1.756740     -0.624994       1.717656
      H      -1.343801      0.686557       0.603676
      H      -1.198199     -2.326570       0.004548
      H      -0.831540     -1.076873      -1.175434
      H      -2.887619      1.304328      -1.257582
      H      -4.382480      0.354385      -1.515348
      H      -2.805921     -0.323564      -1.986605
      C      -3.191110     -0.317790       0.151027
      O      -3.768346     -1.538302       0.246714
      O      -3.982447      0.311518       1.053688
      O      -0.702406      2.930159      -1.007097
Rotational constants (GHz):    0.4107700    0.3282900    0.2201800
Vibrational harmonic frequencies (cm-1):
    -517.2389                  19.7153                  36.0768
      41.1000                  46.0961                  60.3697
      79.4789                  82.6571                 113.6094
     118.6447                 142.5392                 171.3879
     206.1594                 208.5237                 220.8622
     236.4661                 243.5285                 277.2686
     280.4605                 313.2449                 336.9777
     344.6526                 367.9858                 378.0460
     391.2446                 421.9835                 456.1719
     463.4943                 491.2851                 503.8764
     545.1781                 564.1145                 642.8082
     707.3626                 728.6146                 749.9948
     777.5925                 797.4488                 846.5670
     868.1941                 871.3895                 891.1509
     896.8497                 926.6685                 930.1274
     935.1156                 952.4788                 956.3536
     989.4020                1003.0513                1012.8158
    1024.7624                1029.4522                1038.0551
    1044.1068                1052.7705                1074.2709
    1079.9754                1089.1191                1114.5919
    1147.6131                1178.7111                1190.2255
    1205.4692                1211.6582                1220.6379
    1224.9883                1255.8309                1263.2163
    1266.9191                1286.2445                1302.5662
    1327.0186                1338.2531                1348.5280
    1355.7370                1379.8098                1382.5720
    1404.2924                1415.1634                1420.9849
    1423.5384                1453.1791                1472.3229
    1473.0313                1476.4669                1484.5392
    1485.9034                1487.0297                1488.1578
    1495.4500                1500.3034                1508.9382
    1510.5403                1700.3582                1804.6152
    2870.7963                3011.2602                3018.9473
    3020.2367                3026.5849                3028.7775
    3029.1396                3036.9743                3040.7428
    3047.7616                3061.8252                3063.5853
```

```
    3068.7192                3071.2022                3080.5486
    3081.0411                3088.3137                3093.3585
    3101.9138                3118.2483                3131.9791
    3138.1590                3147.4785                3218.8079
Zero-point correction (Hartree): 0.359225
```

TS17b: B3LYP/6-311G**

```
TS-rp-Dio-1b-B3LYP
------------------
E(UB+HF-LYP/6-311G(d,p)) (Hartree): -811.732283041
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.997958     -1.163015       0.549106
     C       1.592813     -0.105828      -0.439579
     C       2.351010     -1.922838       0.445590
     C       3.033113     -0.620573      -0.079335
     C       3.707424      0.165311       1.050656
     C       3.988492     -0.782465      -1.259216
     C      -0.322553     -1.838548       0.244773
     C      -1.426802     -1.525972       1.237410
     C      -2.831278     -2.043087       0.902268
     C      -0.488541     -2.630901      -0.816739
     C      -3.460659     -1.344093      -0.284285
     C      -0.214625      1.615729      -0.813038
     C       1.201275      1.361223      -0.270532
     C      -0.375943      4.129443      -0.166971
     H       0.931006     -0.701810       1.539501
     H       1.369829     -0.427544      -1.463374
     H       2.321169     -2.699204      -0.321988
     H       2.742693     -2.356643       1.369142
     H       4.608132     -0.358168       1.386100
     H       3.055650      0.286234       1.919746
     H       4.010229      1.163056       0.717927
     H       4.900822     -1.307439      -0.956427
     H       4.287939      0.190876      -1.663436
     H       3.526993     -1.354364      -2.069363
     H      -1.471193     -0.437905       1.382599
     H      -1.125552     -1.923519       2.215017
     H      -3.483883     -1.832874       1.760533
     H      -2.854450     -3.121639       0.732321
     H      -1.435585     -3.095073      -1.060007
     H       0.330054     -2.839480      -1.497457
     H      -3.361491     -0.234410      -0.274195
     H      -0.206156      1.917287      -1.863729
     H      -0.825891      0.717682      -0.735954
     H       1.921781      2.008070      -0.783157
     H       1.244819      1.620486       0.791958
     H      -0.969966      4.837111       0.409410
     H      -0.377603      4.416928      -1.219697
     H       0.646804      4.113277       0.212130
     C      -1.002798      2.722170      -0.021133
     O      -1.174864      2.355132       1.272307
     O      -2.311308      2.710646      -0.370957
     O      -4.048762     -1.900812      -1.176532
Rotational constants (GHz):    0.4169800    0.3186700    0.2072100
Vibrational harmonic frequencies (cm-1):
    -503.6722                  18.1973                  34.0877
      37.2037                  40.2048                  63.6670
      78.5237                  84.4809                 119.1224
     139.2773                 157.1467                 186.9050
```

```
     202.8252                218.1725                233.8287
     240.0575                252.1443                258.7079
     269.9354                298.1505                337.7701
     350.9615                356.0506                363.7435
     402.2089                413.9304                432.5089
     467.4015                506.0689                511.6796
     548.6340                572.5508                615.6424
     700.3034                707.0917                744.7087
     770.6627                780.6653                851.4532
     869.3342                881.1176                886.5890
     905.5522                921.9323                925.1047
     930.2545                952.3713                958.8254
     988.3865               1010.9263               1019.1477
    1024.0445               1029.0102               1041.8429
    1050.0559               1055.4885               1078.6056
    1087.6495               1096.7299               1108.3542
    1139.1350               1174.3113               1194.7296
    1205.2189               1212.3151               1222.4269
    1227.9911               1248.7122               1257.8823
    1274.8956               1288.5289               1295.4921
    1320.6890               1342.7839               1352.9882
    1376.2715               1386.2460               1396.1230
    1401.9806               1416.7707               1422.1763
    1422.7174               1449.8557               1470.2246
    1472.8775               1474.9633               1481.8148
    1485.4967               1487.1271               1490.0244
    1494.8530               1499.0940               1506.8926
    1508.6848               1703.4879               1810.3725
    2857.1927               2998.5822               3008.7726
    3011.5985               3016.5834               3020.6767
    3022.8888               3022.9625               3037.2473
    3045.6471               3048.4198               3054.5949
    3065.6701               3067.1805               3078.1337
    3079.2456               3091.3659               3091.8316
    3099.3845               3127.1824               3131.2440
    3141.4925               3148.2841               3223.0359
Zero-point correction (Hartree): 0.359024
```

TS18: B3LYP/6-311G**

```
TS-13Hs-CI2a
------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.696741106
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.124165     -0.760040      -0.330525
     C      -1.957338      0.277193       0.473143
     C      -2.337802     -1.739035      -0.237961
     C      -3.259497     -0.528420       0.104343
     C      -3.985137     -0.002212      -1.139291
     C      -4.249541     -0.737674       1.248137
     C       0.231150     -1.233770       0.137813
     C       1.083358     -1.813402      -0.974023
     C       2.527105     -2.214120      -0.603711
     C       0.626894     -1.175047       1.411699
     C       3.360666     -1.004573      -0.371688
     C      -0.539464      2.433765       0.562003
     C      -1.855460      1.765594       0.142774
     C       1.965925      2.809575       0.052928
     H      -1.024874     -0.400282      -1.356985
     H      -1.782712      0.140897       1.546223
```

```
      H      -2.232948     -2.421395      0.609488
      H      -2.587602     -2.316381     -1.132065
      H      -4.758600     -0.711899     -1.450222
      H      -3.308153      0.139604     -1.985593
      H      -4.475360      0.955751     -0.940706
      H      -5.034227     -1.447675      0.965382
      H      -4.739785      0.202792      1.523208
      H      -3.749999     -1.128918      2.139199
      H       1.123909     -1.079487     -1.786213
      H       0.576606     -2.694334     -1.385961
      H       2.969508     -2.716314     -1.473323
      H       2.563436     -2.907256      0.242244
      H       1.589588     -1.538020      1.746669
      H      -0.008992     -0.758927      2.183495
      H       3.949225      0.211073     -0.588812
      H      -0.679677      3.519725      0.653117
      H      -0.217827      2.108050      1.559309
      H      -2.678701      2.284941      0.647348
      H      -1.994386      1.920466     -0.930411
      H       1.855460      3.628562      0.766887
      H       2.530816      3.143907     -0.818184
      H       2.550239      2.018886      0.537650
      C       0.630731      2.249810     -0.396740
      O       0.507440      1.701279     -1.472173
      O       4.620082      0.427618      0.529648
      O       3.980040     -0.893849      0.724382
Rotational constants (GHz):    0.6328800    0.2580200    0.2101300
Vibrational harmonic frequencies (cm-1):
    -1729.1878                  15.7234                  34.2286
      41.6139                   59.0608                  82.0196
      87.7201                   98.1003                 101.3964
     125.5476                  146.0231                 165.7340
     185.8439                  196.2352                 216.5952
     233.1603                  255.5673                 268.7270
     278.9102                  294.5741                 296.4674
     359.4567                  370.4692                 378.1259
     415.6588                  441.5721                 467.7213
     479.9912                  502.2789                 518.2253
     560.0272                  597.7325                 607.9249
     652.3025                  722.8241                 734.0345
     751.6476                  773.7964                 799.7937
     835.5832                  854.5586                 883.6248
     903.8028                  918.0337                 924.7337
     946.0105                  955.2554                 961.1044
     963.9504                  988.4068                 998.4741
    1023.3434                 1027.2153                1032.4767
    1042.9170                 1057.2087                1117.8282
    1120.7474                 1129.1217                1161.1855
    1171.7205                 1174.8602                1199.9838
    1210.6504                 1213.9662                1222.1831
    1233.4515                 1243.2045                1261.1348
    1273.8479                 1279.5103                1317.1459
    1338.4894                 1347.6737                1377.6207
    1387.3220                 1393.3779                1397.2942
    1402.1645                 1418.0795                1422.2505
    1448.4873                 1451.0418                1464.0984
    1475.8741                 1476.9249                1477.6289
    1484.0393                 1487.3650                1489.4459
    1496.2256                 1507.0058                1511.8947
    1514.3298                 1703.0414                1778.6066
    2086.5390                 3001.6589                3008.8423
```

```
    3014.5177                3018.6962                3020.0454
    3021.7867                3024.4473                3026.8807
    3035.2893                3036.5250                3051.6047
    3065.7378                3066.6324                3071.9693
    3076.2870                3078.8352                3079.9077
    3089.4681                3091.4794                3093.6854
    3127.6345                3155.9650                3229.5586
Zero-point correction (Hartree): 0.357190
```

TS19a: B3LYP/6-311G**

```
TS-rp-Dio-2a-B3LYP
------------------
E(UB+HF-LYP/6-311G(d,p)) (Hartree): -811.737801247
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       1.109934     -1.049057       0.600519
     C       1.681364      0.018150      -0.395623
     C       2.455107     -1.814229       0.446661
     C       3.126818     -0.506536      -0.076700
     C       3.831671      0.261256       1.047670
     C       4.053157     -0.653890      -1.281558
     C      -0.221887     -1.709487       0.329318
     C      -1.296674     -1.432108       1.364041
     C      -2.753113     -1.633721       0.948566
     C      -0.419903     -2.483038      -0.747400
     C      -3.182556     -0.627173      -0.148383
     C      -0.100325      1.808909      -0.805101
     C       1.303678      1.484679      -0.209657
     C      -0.557974      4.226489       0.008345
     H       1.078005     -0.598846       1.597388
     H       1.430495     -0.294059      -1.415454
     H       2.400821     -2.578076      -0.332036
     H       2.869192     -2.265083       1.352170
     H       4.738597     -0.269591       1.353563
     H       3.202329      0.372483       1.934533
     H       4.129823      1.262489       0.721564
     H       4.971023     -1.185780      -1.009226
     H       4.345501      0.324558      -1.678599
     H       3.569934     -1.211874      -2.088774
     H      -1.176353     -0.401614       1.717522
     H      -1.088308     -2.062002       2.241216
     H      -3.411312     -1.462183       1.805617
     H      -2.952442     -2.638242       0.569786
     H      -1.365169     -2.960946      -0.959767
     H       0.372260     -2.654886      -1.468312
     H      -3.001900      0.404869       0.224830
     H       0.019371      2.249708      -1.799377
     H      -0.688238      0.897824      -0.920416
     H       2.056603      2.125803      -0.680294
     H       1.323878      1.723831       0.859156
     H      -1.054180      4.767357       0.812948
     H      -0.902570      4.614975      -0.956157
     H       0.522486      4.393028       0.050391
     C      -0.883028      2.749154       0.093141
     O      -1.720513      2.331626       0.868711
     O      -4.441438     -0.776179      -0.622558
     O      -2.621481     -0.854216      -1.368066
Rotational constants (GHz):    0.4967400    0.2971000    0.2146600
Vibrational harmonic frequencies (cm-1):
    -1153.1442                27.8873                33.2145
```

```
      37.7353                53.2927                59.4255
      86.0695                88.3798                96.8456
     118.2763               129.5782               157.6979
     188.1942               213.9155               225.5657
     239.0443               249.5725               264.4005
     270.6082               279.1054               301.2916
     349.8935               377.9441               385.7333
     434.4263               448.9906               474.5958
     491.7544               529.1645               543.6692
     564.7136               607.2541               611.2654
     683.6290               742.6958               781.5450
     795.0723               808.1971               845.3106
     868.0205               881.4281               905.4039
     906.8533               917.8507               938.8322
     954.2129               966.8730               974.9008
     979.6004               993.8015              1017.1942
    1019.4352              1029.2194              1050.6795
    1054.0183              1059.1261              1062.8194
    1111.8132              1125.1444              1163.2664
    1179.5885              1187.6718              1204.9021
    1211.8844              1219.3469              1224.8476
    1236.7781              1241.5835              1259.6396
    1267.6746              1278.6722              1296.0093
    1306.6071              1328.1246              1330.8301
    1359.0988              1384.3554              1391.8661
    1401.8226              1403.9380              1417.4323
    1424.1470              1448.5790              1462.5725
    1468.0145              1476.5595              1485.3568
    1486.0652              1489.0123              1493.0427
    1499.6760              1505.1534              1507.1543
    1509.8168              1664.8631              1769.3331
    2804.5486              2987.7094              3009.1698
    3016.7918              3022.7683              3024.0622
    3027.4275              3033.8240              3040.2178
    3043.4874              3045.2265              3048.3115
    3058.1490              3067.0879              3078.4107
    3079.5612              3084.5621              3090.8799
    3098.5011              3101.4907              3110.9066
    3140.2687              3146.4975              3238.7844
Zero-point correction (Hartree): 0.359488
```

TS19b: B3LYP/6-311G**

```
TS-rp-Dio-2b-B3LYP
------------------
E(UB+HF-LYP/6-311G(d,p)) (Hartree): -811.736760107
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.857131     -0.810600      -0.153285
     C      -1.921118      0.203786       0.366592
     C      -2.009484     -1.846846      -0.371546
     C      -3.053149     -0.697598      -0.262157
     C      -3.529058     -0.241252      -1.646502
     C      -4.250240     -0.964106       0.648363
     C       0.305929     -1.287865       0.682232
     C       1.321756     -2.139977      -0.052457
     C       2.254689     -1.350557      -0.989781
     C       0.439491     -1.038585       1.986006
     C       3.269624     -0.487025      -0.202339
     C      -0.868356      2.576056       0.721748
     C      -1.881823      1.681064      -0.030791
```

```
      C       1.019974      2.856458      -1.044902
      H      -0.489220     -0.478589      -1.130949
      H      -2.000178      0.132995       1.455969
      H      -2.072140     -2.543248       0.467987
      H      -2.001872     -2.415424      -1.304754
      H      -4.165361     -1.012517      -2.091683
      H      -2.697293     -0.067580      -2.334911
      H      -4.117617      0.679443      -1.590954
      H      -4.911354     -1.723296       0.216980
      H      -4.844469     -0.055561       0.796526
      H      -3.929022     -1.319788       1.631422
      H       0.800810     -2.888236      -0.662744
      H       1.932259     -2.695771       0.664244
      H       1.694884     -0.683207      -1.651327
      H       2.840494     -2.028103      -1.614550
      H       1.274808     -1.438719       2.550051
      H      -0.252771     -0.412933       2.534701
      H       2.735396      0.214125       0.473365
      H      -1.129361      3.622269       0.520563
      H      -0.942967      2.412859       1.799019
      H      -2.876350      2.100358       0.160467
      H      -1.725496      1.776327      -1.110073
      H       0.326122      2.537305      -1.826244
      H       2.025349      2.497799      -1.263297
      H       1.028215      3.952057      -1.055087
      C       0.590517      2.384604       0.333018
      O       1.390012      1.908241       1.110847
      O       4.184072      0.129756      -0.992857
      O       4.239342     -1.186487       0.439521
Rotational constants (GHz):    0.5910900    0.2750700    0.2239700
Vibrational harmonic frequencies (cm-1):
    -1448.7506                  21.5035                  32.2571
      42.3991                   54.6666                  65.5955
      76.0909                   87.8610                 103.4320
     109.9813                  118.8134                 130.2956
     182.1104                  191.9275                 228.7609
     240.7109                  266.3580                 275.8298
     286.5858                  315.1598                 344.9789
     364.2230                  383.5186                 392.8583
     427.3416                  435.0361                 459.9150
     486.3346                  500.8889                 531.7167
     561.7491                  593.3978                 647.5937
     718.1842                  727.3092                 759.2714
     789.2210                  802.8062                 845.4033
     856.3871                  877.8962                 897.9089
     923.4882                  932.8169                 935.8272
     949.2069                  965.9464                 972.1984
     984.5814                  992.3102                1008.1846
    1018.4294                 1028.6996                1040.5899
    1047.0027                 1048.8864                1070.1771
    1110.2594                 1115.2929                1150.7214
    1170.7515                 1185.0633                1197.8450
    1207.0640                 1222.8576                1226.8433
    1238.2944                 1254.6163                1257.0137
    1260.0526                 1265.0766                1278.4748
    1313.8533                 1334.5551                1338.7600
    1348.1026                 1362.4066                1382.2434
    1387.3713                 1401.4312                1409.9445
    1419.8293                 1452.5238                1465.6066
    1474.0480                 1476.8180                1481.2334
    1484.5880                 1486.9421                1487.6216
```

1492.0253	1497.3616	1507.7511
1509.5811	1696.6449	1777.2470
2788.4563	3009.3664	3012.0134
3012.3861	3014.6454	3019.6924
3024.2639	3031.2102	3037.8325
3043.0017	3046.9389	3057.0323
3067.4991	3070.3969	3079.1409
3081.0495	3085.9275	3089.9834
3092.2638	3095.8492	3100.8314
3138.1455	3143.9143	3223.4829

Zero-point correction (Hartree): 0.359146

TS20

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.740494599
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.442509	0.774832	0.293384
C	-1.372939	-0.580401	-0.513368
C	-2.956079	0.510150	0.511601
C	-2.766052	-0.977302	0.103674
C	-2.674900	-1.888607	1.334108
C	-3.782296	-1.533264	-0.892659
C	-1.018147	2.093702	-0.319194
C	0.444375	2.326589	-0.650406
C	1.411997	2.367294	0.554895
C	-1.893311	3.079766	-0.541314
C	2.511327	1.310084	0.554833
C	-0.225969	-1.575490	-0.321312
C	3.501834	-2.108485	-0.761690
H	-0.896625	0.633510	1.231474
H	-1.508734	-0.373327	-1.581905
H	-3.574559	1.038565	-0.216134
H	-3.353614	0.701171	1.511645
H	-3.656289	-1.955348	1.814714
H	-1.970381	-1.508783	2.078456
H	-2.368653	-2.905004	1.068083
H	-4.771965	-1.629533	-0.432902
H	-3.486551	-2.526706	-1.248339
H	-3.880382	-0.879876	-1.764360
H	0.515334	3.270994	-1.194255
H	0.808666	1.569809	-1.349083
H	0.882407	2.312790	1.509812
H	1.936983	3.330207	0.566358
H	-1.570299	4.029209	-0.955329
H	-2.947942	2.992121	-0.313547
H	3.207228	1.410544	1.402852
H	-0.561966	-2.554125	-0.682051
H	-0.027712	-1.687006	0.742929
H	3.846161	-1.633039	-1.682774
H	3.195094	-3.131131	-1.004250
H	4.312875	-2.121221	-0.036042
C	2.339553	-1.329573	-0.247389
O	2.374448	-1.144061	1.029482
O	1.539641	-0.094625	1.441076
O	2.917768	0.760349	-0.503233
C	1.083216	-1.214985	-1.070963
H	1.222441	-1.873525	-1.933180
H	1.033023	-0.209462	-1.475978

Rotational constants (GHz): 0.5913400 0.3375300 0.2517400

Vibrational harmonic frequencies (cm-1):

-327.9013	37.9924	58.9999
69.1712	118.1627	133.0030
160.4840	162.0696	171.3577
190.1639	211.5825	222.8438
235.1125	252.0095	272.3537
281.5498	290.8177	299.4159
324.9443	350.9033	372.4338
379.6325	406.8975	418.5650
438.7693	492.2020	500.4345
508.5443	546.0218	564.4595
617.5428	630.0744	672.8380
697.7662	744.9692	767.5064
796.6253	813.8560	870.0809
886.4115	904.6848	912.7524
922.4245	924.9980	930.3502
950.6085	957.9698	971.8376
992.5930	1004.1724	1012.6447
1026.5658	1035.1381	1043.1393
1049.1201	1061.8821	1092.3885
1102.4138	1131.3090	1160.0904
1191.7234	1202.2549	1212.6045
1218.6497	1222.7577	1231.6437
1252.9805	1269.5886	1280.2527
1291.1360	1318.5035	1334.9311
1344.3841	1354.8749	1372.3436
1375.2773	1382.7457	1399.1514
1402.7918	1409.5632	1418.6923
1429.9793	1452.0836	1470.0801
1472.9185	1477.9149	1482.1574
1486.7099	1489.9528	1496.0139
1504.8165	1506.9231	1511.2409
1512.6064	1549.9269	1687.2968
2958.6442	3006.5895	3010.1333
3017.5062	3021.6256	3023.4134
3035.9649	3040.9469	3044.7801
3054.8784	3056.1320	3063.8624
3071.4156	3074.9939	3079.6253
3082.9289	3090.8754	3096.8208
3102.3337	3122.3976	3137.3545
3150.1107	3151.2150	3217.8097

Zero-point correction (Hartree): 0.364246

TS21

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.742556552
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.283787	0.863192	0.336742
C	-1.452395	-0.479300	-0.478783
C	-2.822222	0.881282	0.536995
C	-2.902916	-0.613103	0.127428
C	-2.995032	-1.521615	1.360060
C	-3.993458	-0.977867	-0.878872
C	-0.632111	2.087307	-0.271642
C	0.826509	2.043419	-0.691787
C	1.874723	2.156231	0.443274
C	-1.305041	3.233280	-0.421185
C	2.272320	0.860265	1.121847
C	-0.560266	-1.717376	-0.308184

C	2.638776	-2.361527	0.531857
H	-0.772441	0.626584	1.272429
H	-1.546339	-0.245221	-1.546090
H	-3.323979	1.516057	-0.195928
H	-3.191651	1.138939	1.532922
H	-3.973451	-1.393793	1.834279
H	-2.235401	-1.281247	2.108564
H	-2.892591	-2.579912	1.101552
H	-4.987717	-0.902726	-0.425258
H	-3.874090	-2.006062	-1.239453
H	-3.970460	-0.313106	-1.747137
H	0.995964	2.884959	-1.368172
H	1.028026	1.144917	-1.274381
H	1.490477	2.818056	1.232372
H	2.784321	2.626493	0.063102
H	-0.825387	4.111327	-0.841536
H	-2.339340	3.350988	-0.123353
H	3.090988	0.955904	1.852258
H	-1.173698	-2.577978	-0.596134
H	-0.310696	-1.853464	0.744390
H	2.981474	-3.234503	-0.040897
H	1.922041	-2.701150	1.277052
H	3.486189	-1.885325	1.013135
C	1.993189	-1.431977	-0.436588
O	1.473888	-0.101914	1.217014
C	0.737471	-1.807395	-1.163061
H	0.862422	-2.845287	-1.492242
H	0.655219	-1.187820	-2.058336
O	3.603754	0.145560	-0.202059
O	2.640551	-0.475588	-1.006424

Rotational constants (GHz): 0.6234100 0.3353300 0.2551900

Vibrational harmonic frequencies (cm-1):

-277.4873	32.1347	62.9368
73.1158	122.0423	144.2360
156.1004	174.0911	176.1500
190.5172	210.1700	227.4702
238.1664	245.9060	276.5593
281.5149	291.4761	303.3925
346.7870	353.9894	365.8966
374.0724	407.4012	417.5089
448.9035	478.2219	491.4376
515.0277	559.9889	568.3255
598.3689	625.6378	691.3325
708.6724	749.9382	783.0099
804.8703	816.5472	866.7351
883.9547	891.4490	903.4006
922.3808	927.5731	929.5782
945.8433	948.4427	971.3101
989.8164	994.2720	1008.3620
1018.3395	1030.5229	1036.0391
1044.6170	1052.9103	1085.2374
1092.7425	1126.0371	1166.1246
1198.7096	1200.9704	1206.6867
1222.6683	1230.7879	1250.8631
1269.1798	1280.3661	1292.5801
1296.0535	1313.5217	1343.3209
1354.3317	1362.1536	1369.0895
1371.4066	1379.3280	1393.2077
1402.2332	1402.6073	1419.8256
1433.6863	1450.4511	1458.3613
1473.5882	1478.8271	1487.3316

1488.1955	1490.9497	1497.9751
1499.0174	1508.3568	1511.1244
1511.9464	1570.3960	1684.0438
2969.6102	3003.5618	3006.8517
3008.7425	3011.9021	3017.0240
3020.5509	3034.1571	3043.6061
3052.3505	3063.6136	3069.4825
3076.0372	3079.3065	3082.3708
3086.4104	3090.6156	3096.3989
3104.6826	3118.9486	3125.5061
3134.9403	3191.3123	3214.8959

Zero-point correction (Hartree): 0.364403

TS22

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.737182156
Electronic state : 1-A
Cartesian coordinates (Angs):

C	1.767869	0.789221	-0.391778
C	1.059632	-0.558550	-0.029448
C	3.120947	0.161873	0.054362
C	2.478883	-1.255008	0.020899
C	2.872029	-2.016616	-1.247870
C	2.732459	-2.120763	1.254964
C	1.386473	2.122695	0.242522
C	-0.015003	2.362876	0.766047
C	-1.108879	2.490440	-0.354372
C	2.305729	3.084517	0.365791
C	-2.240511	1.535158	-0.194996
C	-0.032026	-1.088479	-0.978908
C	-3.271420	-1.915555	1.163451
H	1.758662	0.906578	-1.482591
H	0.665988	-0.501223	0.986091
H	3.383210	0.472275	1.068438
H	3.985463	0.322850	-0.594816
H	3.934249	-2.278850	-1.207075
H	2.715347	-1.423816	-2.153726
H	2.306560	-2.947540	-1.355215
H	3.786817	-2.411023	1.323166
H	2.138194	-3.040622	1.222034
H	2.472377	-1.587076	2.173515
H	-0.011169	3.283924	1.351181
H	-0.299536	1.551903	1.434396
H	-0.673143	2.335715	-1.342433
H	-1.519423	3.505425	-0.334213
H	2.067001	4.047352	0.805199
H	3.330145	2.942835	0.038338
H	-2.993016	1.616024	0.578451
H	0.429646	-1.715415	-1.746769
H	-0.472365	-0.257368	-1.529799
H	-3.991037	-1.233673	1.614170
H	-2.859912	-2.558623	1.949443
H	-3.772429	-2.547838	0.428590
C	-2.140002	-1.122001	0.541892
O	-3.328960	-0.293646	-0.879947
O	-2.478307	0.772485	-1.192587
O	-1.741372	-0.071599	1.115296
C	-1.167820	-1.907073	-0.339305
H	-1.738883	-2.424517	-1.113155
H	-0.743794	-2.691631	0.305184

Rotational constants (GHz): 0.5594100 0.3487200 0.2534400
Vibrational harmonic frequencies (cm-1):

-283.2121	24.8107	45.5026
57.2318	114.2134	125.5460
149.3885	171.0036	173.1402
184.4986	214.2633	221.1297
227.8099	255.5311	271.3601
296.6084	302.7620	318.0444
320.9023	339.7819	365.4103
393.3301	408.4187	416.9235
440.3461	461.6858	498.1321
514.0479	525.9970	559.7494
564.7969	594.6169	644.1943
701.7934	728.2073	760.9897
795.0167	821.8444	863.9444
887.2247	904.0632	916.2344
926.0377	931.2312	938.2784
949.2369	955.8839	976.7242
982.4992	995.2904	1003.5046
1006.1350	1012.4095	1035.0150
1045.9154	1072.8586	1088.6339
1110.3096	1122.0592	1163.4435
1184.6088	1200.2778	1202.9696
1224.3784	1228.8794	1238.6336
1263.2569	1266.9348	1286.4686
1294.0259	1300.6202	1306.1483
1339.6126	1344.1443	1356.6790
1373.8650	1382.1599	1393.6696
1400.3472	1401.4381	1418.0727
1445.6182	1456.2406	1465.9750
1469.9120	1479.9756	1486.1158
1487.5128	1494.3163	1498.1720
1502.3334	1508.8825	1509.2596
1516.0664	1554.1208	1683.9798
2988.8940	3002.9879	3007.4146
3016.1102	3030.0176	3036.4892
3040.4091	3056.0094	3064.4484
3067.7560	3074.5196	3077.8499
3080.1846	3082.9706	3087.6407
3092.9260	3099.7614	3101.2552
3104.3594	3127.1655	3127.8750
3140.5808	3205.6236	3206.3501

Zero-point correction (Hartree): 0.364008

TS23

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.732694763
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.511008	0.877268	0.364098
C	-1.541023	-0.503196	-0.392570
C	-3.059861	0.856807	0.389488
C	-3.041577	-0.664108	0.066448
C	-3.221773	-1.505868	1.336248
C	-4.008637	-1.132436	-1.019193
C	-0.796079	2.063673	-0.236289
C	0.679736	1.885462	-0.508907
C	1.519059	1.854007	0.785167
C	-1.412465	3.213329	-0.519692
C	2.809873	1.105162	0.835669

C	-0.583266	-1.656442	-0.064308
C	3.186339	-2.356205	-0.099959
H	-1.123438	0.699683	1.374466
H	-1.534025	-0.315455	-1.473079
H	-3.484773	1.433145	-0.435364
H	-3.550469	1.159883	1.318013
H	-4.247926	-1.403939	1.704094
H	-2.551447	-1.191147	2.140439
H	-3.042233	-2.568548	1.149084
H	-5.046963	-1.068461	-0.675632
H	-3.817465	-2.175127	-1.296314
H	-3.916077	-0.522853	-1.922603
H	1.041682	2.694127	-1.148092
H	0.849273	0.968227	-1.062642
H	0.938980	1.475409	1.629800
H	1.792250	2.882639	1.068175
H	-0.869674	4.050285	-0.946904
H	-2.470002	3.364972	-0.339685
H	3.407807	1.257849	1.733900
H	-1.125157	-2.580829	-0.293074
H	-0.390709	-1.672770	1.010927
H	3.375992	-2.613576	-1.142004
H	2.956399	-3.276194	0.452671
H	4.079524	-1.910070	0.336314
C	2.005855	-1.417956	0.047291
O	1.877758	-0.757815	1.111553
C	0.770912	-1.730096	-0.812705
H	0.908218	-2.740431	-1.209917
H	0.780144	-1.075900	-1.688208
O	3.553798	0.664263	-0.110436
O	2.851390	0.067635	-1.164753

Rotational constants (GHz): 0.6507100 0.3048500 0.2367700

Vibrational harmonic frequencies (cm-1):

-328.1851	21.6074	41.7129
82.1880	119.7543	133.0840
152.0607	164.2180	187.7006
211.9253	215.4712	226.2455
233.7872	242.2485	257.0977
272.8834	285.3589	288.4876
294.7909	338.2258	360.5165
374.3945	401.5280	410.9786
431.5020	482.5585	492.9532
509.9805	519.7182	562.9262
615.5791	626.0675	697.2475
718.7477	743.0010	765.0986
789.2647	801.5785	865.0505
868.7860	878.6463	889.5617
903.2372	924.1406	926.3079
949.5883	958.3113	965.9237
988.8087	1000.4549	1008.3854
1008.6217	1025.1521	1033.4334
1044.7965	1054.2768	1086.5246
1105.9427	1128.7810	1163.1590
1189.6104	1195.7418	1202.8162
1208.4953	1230.8563	1249.3324
1261.3691	1280.0090	1283.8742
1296.7752	1318.9707	1323.8327
1348.2935	1361.4286	1371.4767
1376.9149	1394.4938	1396.1636
1400.1219	1402.6853	1419.1793
1445.0900	1452.4671	1458.8556

1468.5365	1477.0044	1482.2418
1485.4611	1488.1318	1496.6914
1505.6045	1507.6628	1509.5938
1513.6560	1565.7687	1698.9574
2983.4176	3007.0248	3008.8283
3015.3472	3016.3883	3020.6412
3021.6173	3041.6538	3042.6022
3062.9719	3064.5236	3072.5472
3075.3727	3078.9479	3079.6548
3084.9372	3088.9989	3093.1511
3099.3181	3133.0044	3136.3297
3141.4696	3171.1231	3212.5199

Zero-point correction (Hartree): 0.363757

TS24-from SOZ1 to Acid

E(UB+HF-LYP/6-311G(d,p)) (Hartree): -811.731037994
Electronic state : 1-A
Cartesian coordinates (Angs):

C	1.300466	0.636692	-0.586937
C	0.918056	-0.743046	0.094654
C	2.750128	0.103968	-0.797614
C	2.457468	-1.112675	0.123410
C	2.910081	-2.465441	-0.421872
C	3.025350	-0.900885	1.532210
C	1.157261	1.985444	0.126893
C	-0.067561	2.339429	0.965080
C	-1.425457	2.511792	0.220184
C	2.101873	2.921560	-0.014828
C	-1.783567	1.198303	-0.454338
C	-0.026341	-1.666683	-0.729813
C	-3.287123	-1.321897	1.416229
H	0.773114	0.734002	-1.539953
H	0.523033	-0.637162	1.106347
H	3.567404	0.749283	-0.472089
H	2.936307	-0.187550	-1.834555
H	4.003950	-2.519202	-0.416711
H	2.582671	-2.629068	-1.451743
H	2.538380	-3.296036	0.188495
H	4.119329	-0.953164	1.524894
H	2.655170	-1.667967	2.221305
H	2.741975	0.076332	1.932265
H	0.138993	3.284657	1.473164
H	-0.212951	1.587676	1.743918
H	-1.356936	3.291286	-0.539945
H	-2.188193	2.789237	0.950959
H	1.991779	3.903212	0.433788
H	3.005639	2.757416	-0.588315
H	-2.960962	0.862506	-0.801704
H	0.504497	-2.589055	-0.980797
H	-0.282311	-1.197354	-1.681541
H	-2.679208	-1.359665	2.321650
H	-3.779409	-2.283196	1.259451
H	-4.048903	-0.548485	1.528596
C	-2.408970	-0.997356	0.192534
O	-3.131410	-0.807127	-0.917901
O	-1.374463	1.008587	-1.660558
O	-1.676546	0.192503	0.525260
C	-1.323006	-2.132361	-0.044105
H	-1.804500	-2.918708	-0.628121
H	-1.101460	-2.541773	0.946108

Rotational constants (GHz): 0.5783500 0.3782100 0.2768100
Vibrational harmonic frequencies (cm-1):

-1961.1803	37.4529	51.3842
73.4286	103.5491	148.5494
171.1531	180.2572	200.0379
228.3247	242.4453	253.1765
262.1442	265.9273	280.1733
306.0699	320.0755	330.2460
346.8550	367.2188	373.5315
401.0930	416.5843	427.1885
460.1620	486.5528	488.3221
516.9806	561.3859	569.5581
617.3810	628.5116	667.5833
706.9232	756.6395	770.8494
802.2281	828.6469	848.2812
863.0144	872.1040	896.0913
918.2444	927.2449	927.8562
936.2838	949.3791	958.1540
974.4495	977.1339	990.2281
1002.2373	1017.7646	1020.7075
1028.7788	1050.4395	1062.6862
1080.8230	1085.3126	1107.6212
1132.5736	1150.4157	1170.5191
1179.7525	1208.4904	1210.9487
1217.5633	1235.4135	1238.3856
1268.0038	1272.7219	1283.3034
1296.4111	1318.6569	1324.7749
1339.5963	1357.7257	1364.8947
1374.3341	1387.0484	1393.5410
1402.3256	1419.9502	1450.0023
1469.4099	1478.3255	1480.2661
1481.6103	1484.8678	1487.5419
1489.3956	1491.1171	1496.2675
1506.5984	1515.3927	1677.7688
1696.4297	3008.2465	3013.7597
3020.4776	3039.3938	3042.4802
3045.9288	3047.7109	3048.9089
3060.4686	3062.0732	3065.6744
3071.2366	3084.6709	3086.8633
3088.3481	3089.1293	3097.9602
3101.5381	3116.7843	3122.8470
3126.9650	3136.4461	3216.3054

Zero-point correction (Hartree): 0.359244

TS25-from SOZ2 to Acid

E(UB+HF-LYP/6-311G(d,p)) (Hartree): -811.741731198
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-1.246365	0.768163	0.778682
C	-1.127719	-0.520700	-0.115098
C	-2.673565	0.968518	0.186614
C	-2.701603	-0.528196	-0.230951
C	-3.407449	-1.388993	0.824555
C	-3.254164	-0.838960	-1.620216
C	-0.322922	1.970880	0.772989
C	0.218764	2.545461	-0.529978
C	1.700544	2.184052	-0.863642
C	-0.059419	2.603203	1.920896
C	1.783886	0.677418	-1.030996

```
      C      -0.422487     -1.806802      0.369308
      C       2.552175     -1.577561      1.714318
      H      -1.345829      0.447629      1.820107
      H      -0.744813     -0.248800     -1.101258
      H      -2.659496      1.627710     -0.686129
      H      -3.446292      1.319707      0.875442
      H      -4.480557     -1.172076      0.824798
      H      -3.033306     -1.200038      1.834356
      H      -3.290387     -2.457609      0.620335
      H      -4.336064     -0.671492     -1.662283
      H      -3.072243     -1.884544     -1.893269
      H      -2.786167     -0.209856     -2.382772
      H       0.159382      3.636249     -0.485115
      H      -0.396754      2.230943     -1.377704
      H       2.363157      2.510451     -0.061735
      H       1.987449      2.671609     -1.797213
      H       0.526312      3.516956      1.950094
      H      -0.415599      2.226148      2.873573
      H       2.881915      0.144697     -1.271450
      H      -1.069207     -2.651463      0.105600
      H      -0.379377     -1.812886      1.464831
      H       2.989675     -2.575207      1.739443
      H       1.676677     -1.547159      2.364946
      H       3.280735     -0.841791      2.050820
      C       2.105448     -1.230788      0.274394
      O       1.649858      0.118272      0.271880
      C       0.966896     -2.153653     -0.218437
      H       1.226123     -3.183585      0.046855
      H       0.931510     -2.097848     -1.306255
      O       1.173021      0.170364     -2.050591
      O       3.272251     -1.264886     -0.463869
Rotational constants (GHz):    0.5686800    0.3699700    0.3028500
Vibrational harmonic frequencies (cm-1):
    -1931.7949                 57.2039                 70.0892
      81.8980                132.5752                144.6876
     159.5998                176.1063                185.0889
     195.2587                224.6597                229.3393
     236.6176                252.2589                265.4742
     276.7326                308.1081                318.9277
     342.0850                352.6854                377.7650
     399.6248                420.6289                441.9913
     446.3443                477.4998                505.4180
     533.2412                566.9474                591.4952
     619.6433                629.6492                674.7097
     714.0593                729.9506                777.0112
     789.1734                805.6480                835.4153
     841.0862                868.3312                900.1719
     902.3692                908.4080                922.2467
     932.1533                945.0329                951.8876
     973.9101                978.4050                986.7943
     994.2936               1002.4803               1019.8781
    1037.8786               1042.5723               1068.2715
    1096.4727               1115.4213               1133.1717
    1151.4940               1163.8687               1173.1835
    1192.8768               1202.4944               1215.1618
    1221.5863               1233.7918               1262.4942
    1272.3710               1283.3986               1292.4897
    1307.4881               1329.8411               1332.2549
    1339.6928               1360.2385               1367.3206
    1368.0726               1376.7129               1390.4151
    1404.2623               1420.4782               1454.3678
```

```
    1470.2616                1474.4650                1477.1975
    1481.5542                1483.2751                1485.9960
    1491.8147                1493.9374                1496.8920
    1507.0267                1508.3535                1681.1940
    1730.8752                3008.0967                3010.3059
    3019.6313                3032.8081                3033.7113
    3035.5480                3038.1295                3045.1752
    3054.2451                3057.4855                3064.1509
    3065.4252                3075.4131                3077.9146
    3079.1688                3084.9809                3087.8648
    3114.3905                3121.2323                3124.2055
    3134.1044                3151.4105                3199.5934
Zero-point correction (Hartree): 0.358996



CCCCCCCCCCCCCCCCCCCCCCCCC

CCCCCCCCCCCCCCCCCCCCCCCCC
```

SOZ-1

```
--------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.795054198
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.401555      0.773972       0.358396
     C      -1.306866     -0.565772      -0.463456
     C      -2.929631      0.541972       0.502017
     C      -2.754897     -0.933348       0.052154
     C      -2.782272     -1.885014       1.255260
     C      -3.717907     -1.422753      -1.028427
     C      -0.952618      2.090325      -0.237180
     C       0.436869      2.214511      -0.828875
     C       1.600989      2.378139       0.177897
     C      -1.754307      3.160019      -0.241557
     C       2.337896      1.101453       0.547784
     C      -0.236210     -1.640296      -0.228218
     C       3.599802     -1.892091      -0.504519
     H      -0.898089      0.629280       1.318899
     H      -1.369275     -0.341191      -1.535152
     H      -3.498307      1.120574      -0.228973
     H      -3.367171      0.701918       1.490796
     H      -3.794410     -1.916219       1.671727
     H      -2.109292     -1.560703       2.053332
     H      -2.508289     -2.907547       0.979611
     H      -4.737093     -1.513191      -0.636759
     H      -3.420849     -2.408240      -1.404756
     H      -3.745210     -0.733651      -1.877479
     H       0.440514      3.093078      -1.478215
     H       0.659590      1.360006      -1.472008
     H       1.266589      2.865617       1.098288
     H       2.357755      3.034708      -0.261653
     H      -1.425878      4.106887      -0.658023
     H      -2.754781      3.139124       0.173211
     H       3.273333      1.315615       1.081402
     H      -0.707771     -2.585079      -0.521913
     H      -0.029018     -1.737386       0.838503
     H       3.780674     -1.948163      -1.579891
     H       3.461938     -2.905493      -0.121447
     H       4.463022     -1.435785      -0.020155
```

```
     C       2.357044     -1.054417      -0.246308
     O       2.192832     -1.011022       1.180589
     O       1.525560      0.269160       1.363893
     O       2.616198      0.312372      -0.595194
     C       1.107684     -1.586520      -0.995230
     H       1.345466     -2.609057      -1.301972
     H       1.015712     -1.010260      -1.920100
Rotational constants (GHz):    0.6151300    0.3496000    0.2603200
Vibrational harmonic frequencies (cm-1):
      32.6656                 59.8236                 64.4490
     104.2900                148.0079                169.0927
     185.8628                208.8063                220.9832
     236.2871                238.1532                250.3567
     263.8896                277.7725                289.1346
     304.8684                344.9609                366.7264
     373.7540                382.9800                404.8550
     423.9858                439.0544                492.8383
     504.5364                557.1486                577.8102
     585.5097                635.6697                644.4841
     692.0779                734.9365                748.6356
     781.3258                801.6919                818.0450
     857.7002                864.5107                885.8314
     897.4563                900.4026                907.8441
     924.0699                924.8421                945.1532
     949.6520                959.7052                968.1785
     993.3810               1010.5273               1023.8643
    1030.8278               1047.6905               1053.4928
    1062.9021               1087.6853               1112.4388
    1135.1795               1150.6903               1166.2006
    1182.1431               1202.8946               1206.2410
    1210.8341               1220.1518               1230.1878
    1247.3196               1269.9124               1279.1570
    1292.6756               1310.2340               1326.1978
    1346.4383               1360.9795               1371.1342
    1375.6403               1379.5878               1388.2108
    1397.1654               1402.2194               1407.7164
    1410.7614               1419.5456               1451.9754
    1474.4731               1479.5025               1483.5141
    1486.1077               1487.1041               1489.7121
    1492.7125               1497.8085               1506.7900
    1508.8869               1511.4411               1686.5165
    2998.9055               3006.0302               3009.9531
    3011.8386               3019.7361               3039.4617
    3041.5782               3042.6511               3047.3129
    3050.3314               3052.9881               3063.5029
    3073.1923               3075.9335               3078.4146
    3081.8214               3086.2186               3090.3277
    3092.6942               3097.2386               3117.1358
    3132.0779               3133.6082               3212.0649
Zero-point correction (Hartree): 0.368322
```

SOZ-2

```
--------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.795615428
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -1.303508      0.842933       0.335537
     C      -1.505394     -0.478682      -0.505338
     C      -2.831077      0.840700       0.610045
     C      -2.918387     -0.645995       0.167581
```

```
      C      -2.934428     -1.588422      1.377240
      C      -4.057820     -0.995551     -0.788826
      C      -0.675572      2.074833     -0.281847
      C       0.817126      2.082935     -0.563462
      C       1.715811      2.025752      0.700432
      C      -1.384756      3.175392     -0.551771
      C       2.419946      0.700977      0.973979
      C      -0.564342     -1.686336     -0.447883
      C       2.719610     -2.427402      0.273835
      H      -0.756678      0.588141      1.247688
      H      -1.655420     -0.199922     -1.555398
      H      -3.377917      1.484450     -0.080735
      H      -3.150666      1.073654      1.629062
      H      -3.887838     -1.490378      1.906383
      H      -2.138517     -1.357539      2.090381
      H      -2.827835     -2.636388      1.080938
      H      -5.028110     -0.935722     -0.283710
      H      -3.951585     -2.014742     -1.177075
      H      -4.082343     -0.312553     -1.642868
      H       1.047640      3.000774     -1.108347
      H       1.087733      1.265742     -1.231911
      H       1.126261      2.273748      1.589625
      H       2.501515      2.784704      0.637610
      H      -0.911050      4.052856     -0.979399
      H      -2.446100      3.254358     -0.355095
      H       2.885387      0.711262      1.966040
      H      -1.103936     -2.521722     -0.908945
      H      -0.391029     -1.975822      0.590784
      H       3.099689     -3.019030     -0.561713
      H       2.052517     -3.050309      0.874411
      H       3.558018     -2.110236      0.894560
      C       1.969427     -1.207992     -0.246344
      O       1.540026     -0.403252      0.862196
      C       0.790055     -1.538327     -1.175178
      H       1.034729     -2.463785     -1.702141
      H       0.726587     -0.758322     -1.937542
      O       3.504353      0.400812      0.086131
      O       2.836723     -0.334073     -0.979652
 Rotational constants (GHz):    0.6566800    0.3331600    0.2553600
 Vibrational harmonic frequencies (cm-1):
       29.0531                57.2353                67.0249
      119.1496               146.4520               154.1080
      178.2267               206.6324               215.2343
      219.5708               235.5354               239.4154
      246.9246               285.8812               294.4642
      327.8592               347.9101               352.7263
      370.6350               376.3877               407.8738
      423.9875               452.9591               500.9251
      517.5585               540.5654               555.8147
      580.6403               612.6525               640.4102
      700.6503               749.5507               789.2997
      796.2426               811.1402               819.0360
      842.9368               867.4552               881.7138
      890.5717               893.6922               909.9868
      924.8504               933.3804               944.1094
      949.4046               954.6582               973.7913
      990.7592              1007.5096              1017.2147
     1021.1089              1027.6592              1041.7289
     1063.8602              1083.4142              1106.7585
     1130.6390              1140.4924              1152.2159
     1176.0781              1204.2599              1212.3921
```

```
    1222.9161                1224.3811                1233.3137
    1246.0144                1266.5404                1278.7077
    1282.1925                1301.7274                1316.6579
    1330.5008                1351.8167                1358.7002
    1365.7515                1375.0270                1381.4480
    1396.9206                1402.4748                1402.8179
    1408.2090                1418.0129                1451.8844
    1472.4390                1480.9738                1482.7802
    1486.2519                1487.8549                1489.6335
    1496.6334                1497.3437                1506.9784
    1508.3274                1510.7836                1688.3004
    3007.1674                3011.1650                3015.9755
    3020.5940                3025.4598                3041.9181
    3042.9045                3045.4236                3051.8767
    3056.1407                3058.0775                3064.3671
    3073.8833                3075.2621                3078.5483
    3079.7876                3086.5336                3087.9156
    3099.1112                3112.2831                3112.3506
    3129.5822                3138.4217                3218.8571
Zero-point correction (Hartree): 0.368084
```

POZ-3: B3LYP

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.702006790
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.001914	-0.569175	-0.613977
C	-1.279829	-0.542823	0.317551
C	-0.065222	-2.120616	-0.576685
C	-1.516578	-2.061872	-0.034465
C	-2.536067	-2.300888	-1.155200
C	-1.827727	-2.960636	1.160899
C	1.400610	0.012039	-0.279787
C	1.692655	1.487324	-0.656456
C	1.333060	2.599216	0.360274
C	-0.034344	2.362874	0.930628
C	-1.197257	2.537274	0.296976
C	-2.403896	1.780275	0.786396
C	-2.473113	0.399070	0.092332
C	-1.358590	3.290187	-0.998060
H	-0.271601	-0.200030	-1.608346
H	-0.972485	-0.482381	1.367479
H	0.637134	-2.537234	0.148210
H	0.090783	-2.636200	-1.525499
H	-2.484997	-3.345121	-1.479047
H	-2.340072	-1.677426	-2.031696
H	-3.561573	-2.107435	-0.827733
H	-1.826942	-4.016155	0.869212
H	-2.814290	-2.735193	1.581006
H	-1.087806	-2.835984	1.957141
H	1.175128	1.686539	-1.599176
H	2.764825	1.536350	-0.867392
H	1.405898	3.561047	-0.155756
H	2.076409	2.634105	1.161338
H	-0.061358	1.814969	1.871249
H	-3.333511	2.325543	0.587627
H	-2.342407	1.632025	1.869406
H	-3.369664	-0.112548	0.462108
H	-2.633770	0.538967	-0.981886
H	-1.693825	2.632698	-1.808174
H	-0.439327	3.778403	-1.322062
H	-2.128062	4.062774	-0.887987
C	1.944927	-0.363246	1.139711
H	1.198739	-0.838465	1.775937
H	2.371149	0.506289	1.643902
O	2.954889	-1.342193	0.909258
O	3.474269	-0.923431	-0.373121
O	2.268509	-0.794323	-1.138722

Rotational constants (GHz): 0.4729000 0.4306000 0.2679900
Vibrational harmonic frequencies (cm-1):

49.6717	67.0118	74.1908
84.8075	124.7504	158.5074
159.3900	202.4858	205.7186
217.5783	228.6730	255.2328
265.2988	277.2205	303.2539
314.0231	328.9515	360.1061
375.8858	393.0966	403.0911
419.7996	447.9317	489.8540
511.8749	523.4431	554.1080
572.5026	599.8054	650.1467
705.1307	722.3207	741.0813
780.9365	805.7038	811.4873

```
     836.6624                866.0575                888.9024
     901.7586                914.1101                922.5283
     926.7511                949.7008                951.1028
     967.3616                974.6090                987.8263
     992.9721               1002.5335               1011.0733
    1013.7220               1036.5232               1054.7914
    1064.1386               1075.0483               1092.0813
    1112.8777               1141.7526               1156.3128
    1169.0863               1188.0676               1208.1634
    1221.8029               1229.3562               1242.3346
    1254.1500               1261.2750               1270.5341
    1281.5765               1302.0214               1308.6501
    1325.8645               1346.3073               1357.3322
    1364.5427               1366.9006               1380.8913
    1387.6060               1400.9896               1403.4642
    1419.7388               1420.7570               1478.1413
    1480.5648               1485.6759               1488.0582
    1489.3792               1493.0406               1496.8645
    1497.8500               1507.2688               1509.5447
    1511.2264               1516.0502               1733.0645
    3009.0026               3009.6654               3013.9729
    3019.4458               3021.7624               3024.5324
    3035.2980               3038.8877               3041.2771
    3045.6849               3054.1225               3058.7759
    3059.9078               3063.0955               3064.8780
    3067.9705               3077.5561               3080.9029
    3084.2171               3090.0293               3105.8019
    3109.7070               3115.1873               3127.0921
Zero-point correction (Hartree): 0.367339

POZ-3: MPW1B95
--------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.150854279

Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.153593     -0.519655      -0.616665
     C      -1.360645     -0.217054       0.329111
     C      -0.555141     -2.005096      -0.561719
     C      -1.943941     -1.615299      -0.035683
     C      -2.957797     -1.573824      -1.171369
     C      -2.484840     -2.418431       1.130222
     C       1.335855     -0.295683      -0.288969
     C       1.981800      1.043665      -0.678996
     C       1.928794      2.184067       0.345939
     C       0.562645      2.270436       0.943032
     C      -0.532995      2.670428       0.292429
     C      -1.874118      2.269578       0.818434
     C      -2.305666      0.963327       0.142655
     C      -0.511228      3.305255      -1.064343
     H      -0.348325     -0.092309      -1.606234
     H      -1.025156     -0.241346       1.373416
     H       0.037121     -2.540105       0.185537
     H      -0.507010     -2.569081      -1.493696
     H      -3.164438     -2.590080      -1.515217
     H      -2.585962     -1.007195      -2.028582
     H      -3.905866     -1.129370      -0.860005
     H      -2.747662     -3.433101       0.820111
     H      -3.385152     -1.955324       1.544692
     H      -1.746263     -2.494926       1.931860
     H       1.506942      1.368791      -1.608270
```

```
      H       3.024896      0.818992      -0.916430
      H       2.212115      3.111253      -0.158929
      H       2.677345      2.031803       1.125645
      H       0.422673      1.801023       1.915443
      H      -2.630003      3.040023       0.639522
      H      -1.817963      2.109071       1.898763
      H      -3.279715      0.670898       0.550060
      H      -2.470386      1.135800      -0.925628
      H      -0.810846      2.591271      -1.839238
      H       0.472813      3.686916      -1.333526
      H      -1.220728      4.135112      -1.110496
      C       1.747268     -0.767102       1.131184
      H       0.899748     -1.062986       1.749389
      H       2.341096     -0.011708       1.647659
      O       2.512803     -1.936078       0.915391
      O       3.109245     -1.655498      -0.343863
      O       1.976995     -1.301061      -1.106205
Rotational constants (GHz):    0.4894800    0.4437100    0.2789500
Vibrational harmonic frequencies (cm-1):
      59.9188                86.2945                98.5839
     107.0408               139.0108               160.0403
     196.5364               210.5302               221.9273
     225.9476               240.8515               264.5720
     275.3542               294.9888               314.3186
     323.7801               344.5892               362.1297
     389.9687               398.2016               404.8229
     425.1336               451.8529               495.1736
     529.0615               529.5431               562.4366
     576.2107               611.0772               668.2410
     735.1360               754.9382               789.2798
     815.9425               818.9513               829.0557
     856.5836               877.6325               899.1428
     920.2465               935.5102               948.3664
     959.8226               971.1308               981.4224
     991.3966               993.2143              1008.5560
    1017.1307              1021.1627              1027.1136
    1048.6905              1059.8186              1061.4474
    1091.0267              1101.0053              1127.8073
    1135.3618              1147.3983              1158.8363
    1185.3383              1204.8519              1227.5005
    1233.2622              1239.8112              1249.4773
    1256.0399              1265.0745              1280.8505
    1303.1005              1315.1124              1325.3270
    1336.3461              1351.4258              1360.2579
    1369.0025              1374.8527              1385.1131
    1393.4256              1407.1935              1414.0091
    1424.1632              1431.3088              1474.7900
    1483.6150              1488.4531              1490.4975
    1493.1182              1497.0061              1498.7106
    1504.8299              1514.1547              1516.0398
    1519.7590              1527.6257              1773.5012
    3053.5772              3055.0518              3056.3720
    3058.2272              3066.4689              3070.1286
    3079.3880              3083.4413              3090.7235
    3096.5485              3104.7916              3110.8099
    3120.5739              3124.0578              3126.8879
    3132.7058              3141.3334              3143.1517
    3145.3118              3148.5536              3157.0273
    3167.8204              3172.8291              3175.7012
Zero-point correction (Hartree): 0.373273
```

POZ-4: B3LYP

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.699665973
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.208311	0.497530	-0.607661
C	0.945711	0.982284	0.361280
C	-0.738226	1.957699	-0.641535
C	0.589605	2.471235	-0.025372
C	1.496324	3.089980	-1.096837
C	0.451844	3.425776	1.159976
C	-1.293096	-0.578077	-0.306045
C	-0.984360	-2.036159	-0.745010
C	-0.223697	-2.945318	0.252667
C	0.922464	-2.205600	0.876917
C	2.082393	-1.893352	0.293103
C	2.873499	-0.737893	0.849410
C	2.418447	0.580375	0.179710
C	2.570951	-2.479086	-1.006146
H	0.226008	0.239187	-1.578209
H	0.656485	0.819845	1.405749
H	-1.591834	2.109548	0.020047
H	-1.007138	2.345050	-1.625863
H	1.060863	4.033238	-1.441476
H	1.603871	2.441819	-1.970894
H	2.497497	3.309492	-0.714849
H	0.048580	4.392625	0.840376
H	1.421933	3.612592	1.634273
H	-0.221100	3.021671	1.922198
H	-0.421856	-1.985383	-1.681826
H	-1.947001	-2.495362	-0.981164
H	0.105281	-3.836749	-0.288892
H	-0.909784	-3.303390	1.025912
H	0.703818	-1.716549	1.824541
H	3.949394	-0.866454	0.685080
H	2.719416	-0.661260	1.930593
H	3.031139	1.390286	0.593477
H	2.657092	0.545256	-0.888621
H	2.620922	-1.721435	-1.796610
H	1.943216	-3.295187	-1.365505
H	3.588376	-2.867204	-0.883182
C	-1.914723	-0.479952	1.120189
H	-1.599908	0.431415	1.633990
H	-1.716324	-1.350719	1.741284
O	-3.320025	-0.465040	0.900719
O	-3.403605	0.383029	-0.253604
O	-2.445356	-0.229111	-1.150652

Rotational constants (GHz): 0.4712000 0.4347000 0.2688900
Vibrational harmonic frequencies (cm-1):

47.7155	60.5682	74.7303
84.9456	116.5585	159.6127
168.9789	192.1509	203.7933
215.6777	230.7148	254.8414
267.5379	270.2415	294.1488
316.8960	320.5279	356.8145
383.1637	397.9468	406.3408
413.6265	438.6656	479.1037
495.9757	527.4507	553.1757
576.6917	600.0341	651.5640
709.5067	722.5586	745.0610
775.3470	795.5586	816.2481

```
     840.2891                869.5872                878.7002
     896.4129                907.5026                918.2261
     925.2252                950.5971                961.6762
     966.3355                978.0010                986.1029
    1000.8119               1007.7154               1012.6559
    1016.4744               1037.9656               1051.3995
    1063.0813               1074.6204               1090.7106
    1116.7364               1138.7587               1157.5523
    1175.2404               1185.0536               1206.5553
    1225.1170               1232.0802               1250.4388
    1255.3706               1264.0949               1270.2536
    1279.1909               1284.2847               1311.9474
    1328.8186               1345.1177               1355.4395
    1364.3717               1367.5309               1381.3082
    1389.5435               1402.6692               1404.7427
    1421.7577               1424.6283               1479.5504
    1483.0706               1484.9444               1488.0339
    1489.8096               1494.4000               1495.5100
    1498.6029               1504.8967               1508.7743
    1510.4312               1515.7640               1735.9353
    3007.8776               3009.2335               3013.3392
    3017.5667               3020.1570               3023.0167
    3034.3774               3038.0008               3043.3286
    3046.0293               3054.1551               3055.4285
    3062.1785               3063.4287               3063.8300
    3066.9467               3076.2178               3079.3244
    3088.0576               3088.9199               3110.4363
    3113.3764               3116.2036               3147.7040
Zero-point correction (Hartree): 0.367300

POZ-4: MPW1B95
---------------
E(RmPW+HF-B95/6-31+G(d,p)) (Hartree): -811.148305986
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.129017     -0.505002      -0.606472
     C      -1.322936     -0.252704       0.372063
     C      -0.510239     -1.996593      -0.607846
     C      -1.889232     -1.649868      -0.026670
     C      -2.939828     -1.594845      -1.127626
     C      -2.376296     -2.503178       1.127677
     C       1.364966     -0.247080      -0.315360
     C       1.944269      1.105922      -0.771379
     C       1.896949      2.255075       0.243669
     C       0.553806      2.313116       0.894621
     C      -0.580112      2.668819       0.286205
     C      -1.880571      2.230598       0.879408
     C      -2.302478      0.906986       0.232610
     C      -0.638343      3.286097      -1.077364
     H      -0.356010     -0.051921      -1.577398
     H      -0.970159     -0.300759       1.410164
     H       0.096484     -2.569145       0.095390
     H      -0.484340     -2.509554      -1.570071
     H      -3.137158     -2.604901      -1.494533
     H      -2.606036     -0.996939      -1.979280
     H      -3.886091     -1.179091      -0.774064
     H      -2.626399     -3.513083       0.792444
     H      -3.273344     -2.073459       1.583187
     H      -1.612712     -2.588135       1.904779
     H       1.409000      1.402683      -1.677099
     H       2.979377      0.920607      -1.063285
```

```
      H       2.137012      3.184279      -0.279618
      H       2.681146      2.127321       0.992919
      H       0.463411      1.861465       1.880669
      H      -2.669272      2.974411       0.731440
      H      -1.766931      2.082094       1.956902
      H      -3.248419      0.590090       0.685874
      H      -2.522603      1.070985      -0.826889
      H      -0.955403      2.555914      -1.829723
      H       0.322118      3.689590      -1.395932
      H      -1.370729      4.096872      -1.098842
      C       1.796509     -0.663232       1.108088
      H       1.013415     -1.236452       1.610555
      H       2.114401      0.166956       1.733277
      O       2.933807     -1.471490       0.900672
      O       2.505370     -2.225536      -0.214285
      O       2.103893     -1.206035      -1.121464
Rotational constants (GHz):    0.4841800    0.4507000    0.2799500
Vibrational harmonic frequencies (cm-1):
      46.9159                  71.5923                  93.7625
      98.8517                 134.2435                 159.8339
     193.9550                 201.2864                 218.9526
     228.1516                 232.4709                 264.9939
     280.6813                 292.3575                 308.9339
     324.1894                 347.7413                 357.9116
     394.0404                 402.9265                 409.7088
     423.3774                 450.1078                 483.8848
     502.2340                 537.6902                 556.7285
     574.8674                 612.2282                 667.2272
     727.6353                 765.5278                 789.3026
     809.3054                 819.7912                 828.3426
     858.1830                 880.6212                 894.9523
     918.2925                 926.9981                 936.9314
     958.8372                 971.8390                 977.9929
     989.6331                1000.4793                1007.9502
    1018.3863                1023.2736                1038.5567
    1049.8465                1057.7585                1058.9404
    1081.9858                1099.8665                1127.6486
    1137.4888                1145.4330                1158.6628
    1185.3058                1204.3048                1229.3224
    1233.7234                1236.9095                1254.7301
    1258.4474                1261.1331                1277.5118
    1296.1795                1305.3761                1326.8233
    1335.4724                1357.6334                1361.5787
    1366.1513                1374.3781                1393.0389
    1397.7474                1408.6994                1413.8333
    1423.8401                1435.3232                1476.4020
    1484.8423                1488.2743                1489.2451
    1491.9331                1497.0049                1499.9364
    1511.8810                1512.0772                1515.3717
    1518.4492                1532.1459                1775.7136
    3050.0730                3054.9812                3055.9954
    3057.6373                3065.7479                3069.5402
    3078.2159                3087.5196                3092.4019
    3093.1512                3105.0298                3108.3108
    3120.8864                3123.8707                3126.9234
    3133.2259                3140.2914                3144.1529

    3148.5161                3148.9572                3164.6357
    3165.4432                3175.0516                3198.3329
Zero-point correction (Hartree): 0.373100
```

TS27

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.671172266
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.424129	0.161102	0.758792
C	0.222960	1.285023	-0.333739
C	1.897167	0.606564	0.918232
C	1.617728	1.894409	0.095862
C	1.534304	3.131313	0.997940
C	2.577288	2.152064	-1.065522
C	0.251369	-1.397152	0.655584
C	-1.167362	-2.037867	0.857312
C	-2.240120	-2.009263	-0.259018
C	-2.307944	-0.666469	-0.928802
C	-2.737444	0.475232	-0.384641
C	-2.274875	1.775221	-0.988807
C	-0.973601	2.250236	-0.297104
C	-3.509020	0.567440	0.906043
H	-0.155507	0.432538	1.649421
H	0.316984	0.876462	-1.345947
H	2.586566	-0.076176	0.423124
H	2.248272	0.748992	1.942326
H	2.527397	3.355115	1.400320
H	0.866103	2.976156	1.849416
H	1.190917	4.017940	0.456545
H	3.572228	2.425299	-0.698128
H	2.222332	2.971042	-1.701661
H	2.688914	1.261638	-1.690836
H	-1.569111	-1.524820	1.737350
H	-0.971392	-3.069002	1.160495
H	-3.195809	-2.288333	0.196810
H	-2.035540	-2.785660	-1.002133
H	-1.797191	-0.586914	-1.885710
H	-3.033311	2.560743	-0.893225
H	-2.082069	1.641929	-2.058272
H	-0.664913	3.183800	-0.781928
H	-1.194459	2.516309	0.742011
H	-2.933793	1.077559	1.686878
H	-3.806609	-0.408205	1.291998
H	-4.418423	1.159712	0.754428
C	0.688436	-1.951018	-1.118074
H	0.301002	-1.255536	-1.851850
H	0.265843	-2.947493	-1.057229
O	2.012717	-1.908469	-1.053010
O	2.460550	-2.776047	-0.159028
O	1.158417	-2.025997	1.310968

Rotational constants (GHz): 0.4716400 0.4345200 0.2753600
Vibrational harmonic frequencies (cm-1):

-410.6785	33.8036	48.5390
88.4261	99.7012	123.7941
156.7758	170.4732	173.1089
202.0732	215.9478	231.9197
255.4787	258.6608	267.1851
288.6935	294.8548	316.8449
332.6405	351.4302	386.0946
397.0687	406.9083	442.6141
484.9105	495.8938	502.3017
523.2887	543.9417	564.1097
595.0036	609.5277	615.4217
720.7518	751.8059	811.4310

```
     816.8928                850.0325                871.7347
     884.1893                887.4547                896.6186
     923.6835                946.5868                954.9863
     972.1405                979.6500                988.0492
     997.1738               1006.8100               1029.2850
    1034.6173               1043.3720               1062.2419
    1066.4061               1075.9424               1102.8855
    1108.6203               1137.9433               1157.1322
    1173.7743               1199.0139               1203.3554
    1226.8779               1232.8612               1240.9732
    1246.9974               1254.4137               1258.0551
    1278.7869               1282.9958               1297.2739
    1316.0050               1333.3643               1348.4142
    1354.0585               1363.1647               1378.3608
    1396.9637               1399.9819               1404.1356
    1421.6346               1423.3073               1473.9359
    1479.4466               1483.0350               1486.6954
    1487.4634               1488.6367               1491.7822
    1496.7164               1498.0832               1509.4700
    1510.6835               1511.1914               1732.2576
    3007.2524               3008.5582               3011.4305
    3014.0478               3018.0058               3020.8684
    3022.4704               3027.7188               3033.6851
    3044.0034               3055.5315               3056.8416
    3062.0185               3062.4956               3065.5366
    3077.1079               3080.9717               3087.2604
    3088.5019               3112.3822               3120.7716
    3123.8316               3126.4927               3251.9149
Zero-point correction (Hartree): 0.364096
```

TS26

```
--------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.676870756
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.352269     -0.557507      -0.665221
     C      -1.427698      0.010880       0.346671
     C      -1.118832     -1.908759      -0.668227
     C      -2.344482     -1.227450      -0.003117
     C      -3.445199     -0.939867      -1.032098
     C      -2.931677     -1.949403       1.208488
     C       1.157479     -0.647434      -0.417331
     C       2.086988      0.524960      -0.762383
     C       2.339968      1.625639       0.292951
     C       1.044089      2.094275       0.897053
     C       0.049943      2.714130       0.253917
     C      -1.344079      2.604212       0.813683
     C      -2.073629      1.396250       0.174655
     C       0.182650      3.358653      -1.101850
     H      -0.476814     -0.048989      -1.628301
     H      -1.068902     -0.098727       1.374704
     H      -0.650464     -2.651134      -0.021090
     H      -1.280744     -2.368511      -1.645210
     H      -3.891941     -1.883703      -1.359983
     H      -3.059718     -0.435508      -1.922441
     H      -4.246783     -0.322903      -0.616730
     H      -3.421218     -2.882120       0.909467
     H      -3.681136     -1.329959       1.713275
     H      -2.156217     -2.198954       1.938385
     H       1.642446      0.988406      -1.650418
     H       3.039868      0.083948      -1.052803
```

```
     H       2.886399      2.435317      -0.201187
     H       3.006357      1.235011       1.065008
     H       0.821861      1.724458       1.895153
     H      -1.934528      3.508481       0.625921
     H      -1.302238      2.464098       1.898433
     H      -3.075594      1.344582       0.616525
     H      -2.231486      1.594266      -0.890673
     H      -0.400143      2.832661      -1.867138
     H       1.216880      3.412230      -1.443377
     H      -0.209154      4.381363      -1.065101
     C       1.594732     -1.229203       1.331124
     H       0.761946     -1.913353       1.558128
     H       1.490238     -0.232731       1.777672
     O       2.771650     -1.709558       1.239042
     O       2.864840     -2.062111      -0.781484
     O       1.577658     -1.835141      -0.959821
Rotational constants (GHz):    0.4873800    0.4090500    0.2707900
Vibrational harmonic frequencies (cm-1):
    -434.9555                  51.3771                  65.4886
      92.4286                  99.0088                 130.6512
     156.3917                 164.3760                 180.3498
     194.9216                 231.1622                 239.0265
     253.7791                 272.4448                 279.9306
     298.0188                 307.7556                 318.0307
     340.6432                 355.3841                 378.4938
     399.8690                 406.1460                 425.8672
     459.6297                 487.1223                 512.0789
     539.0126                 551.7212                 561.0491
     588.5584                 613.5354                 672.4884
     731.5735                 752.7064                 807.4965
     821.3472                 848.5395                 856.2670
     881.5929                 897.3645                 906.2023
     926.8193                 952.4965                 960.7105
     971.7458                 984.8894                 986.6072
     996.1530                1006.9275                1029.9607
    1035.9475                1059.4135                1074.4499
    1084.0225                1106.5720                1125.0049
    1138.1298                1150.3632                1160.4311
    1182.2533                1195.1915                1207.3629
    1210.7364                1228.0307                1233.3060
    1248.9420                1255.8460                1263.6430
    1283.0651                1302.0781                1310.2629
    1324.3573                1349.4936                1358.6051
    1370.0928                1374.4826                1382.6523
    1387.9174                1402.2640                1405.1173
    1422.1309                1423.6990                1470.8385
    1479.0370                1485.0810                1486.5843
    1488.8514                1492.4959                1497.6292
    1499.2014                1507.9739                1509.9560
    1512.6974                1539.0564                1727.4235
    2944.6829                3011.0595                3011.3205
    3012.6959                3013.5996                3020.4109
    3025.5117                3027.6077                3033.3470
    3037.5542                3038.7350                3048.5522
    3053.5047                3060.9199                3065.8477
    3070.3618                3081.6529                3082.8930
    3083.1966                3091.0328                3111.4516
    3112.3611                3118.8857                3127.0328
Zero-point correction (Hartree): 0.364468
```

TS28

```
------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.671377448
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.282047     -0.493174       0.741820
     C       1.376808     -0.197050      -0.356932
     C       0.806296     -1.941257       0.855811
     C       2.065056     -1.570753       0.022373
     C       3.310361     -1.449312       0.908606
     C       2.358815     -2.479763      -1.170856
     C      -1.294789     -0.390676       0.668930
     C      -1.999267      0.983450       0.883340
     C      -2.050850      2.048049      -0.238627
     C      -0.712827      2.223911      -0.900981
     C       0.398412      2.709257      -0.340131
     C       1.727357      2.339348      -0.946940
     C       2.273914      1.050270      -0.286457
     C       0.436538      3.451214       0.970593
     H       0.526080      0.076126       1.645864
     H       0.962772     -0.277104      -1.367918
     H       0.151121     -2.662181       0.362539
     H       0.981013     -2.309708       1.868557
     H       3.595199     -2.440791       1.274673
     H       3.133807     -0.817848       1.783305
     H       4.166595     -1.039885       0.364470
     H       2.681950     -3.471947      -0.838679
     H       3.154463     -2.064050      -1.799124
     H       1.473818     -2.614264      -1.800518
     H      -1.505150      1.420007       1.758685
     H      -3.015220      0.732871       1.195592
     H      -2.413141      2.982055       0.203791
     H      -2.802351      1.762782      -0.980421
     H      -0.593552      1.749767      -1.873005
     H       2.467521      3.138711      -0.826195
     H       1.611838      2.166997      -2.021974
     H       3.223772      0.806362      -0.776266
     H       2.525677      1.259266       0.758693
     H       0.962542      2.882681       1.746075
     H      -0.558145      3.691424       1.347303
     H       0.985426      4.391985       0.850302
     C      -1.679561     -0.948519      -1.117128
     H      -0.990613     -1.783658      -1.166699
     H      -1.566861     -0.129597      -1.814982
     O      -2.952350     -1.283965      -0.953991
     O      -3.063686     -2.307648      -0.124146
     O      -1.852518     -1.340883       1.321314
Rotational constants (GHz):    0.4708900    0.4185700    0.2676900
Vibrational harmonic frequencies (cm-1):
    -407.8898                  46.1698                  67.7334
      69.8875                  92.1820                 118.5751
     160.2317                 164.0243                 183.6817
     202.0007                 214.2695                 226.1928
     251.8735                 260.2808                 266.4349
     274.4898                 292.8842                 305.0187
     333.9954                 354.9866                 390.9569
     398.7479                 410.9306                 446.3203
     471.6551                 491.5696                 494.6649
     531.3421                 550.8942                 561.9739
     594.6660                 596.7300                 633.1266
     724.1229                 751.8855                 802.8606
     815.9842                 845.8507                 863.6136
```

```
     887.0010                892.7901                903.4585
     924.1804                946.4068                953.9127
     971.2698                982.3760                987.7444
     997.7841               1005.1748               1030.0785
    1038.2180               1042.7264               1061.1513
    1072.5284               1079.2422               1097.4628
    1106.3991               1132.4145               1159.1393
    1173.8882               1199.4766               1200.8276
    1227.1248               1232.2163               1245.8984
    1249.3207               1252.6978               1261.0554
    1271.0109               1280.9222               1293.3324
    1311.1552               1332.7938               1351.1121
    1358.7144               1364.9925               1380.4683
    1397.8863               1402.4578               1413.2138
    1421.1517               1422.8340               1472.6490
    1476.6507               1479.9341               1485.3037
    1486.9673               1489.5238               1493.9499
    1496.3501               1500.8173               1508.7408
    1510.9589               1513.4177               1730.5636
    3007.9907               3009.9819               3014.1858
    3017.9199               3019.6489               3023.4169
    3024.6878               3028.2816               3030.7727
    3044.8208               3055.2687               3056.0332
    3060.1600               3062.2036               3067.9998
    3074.5832               3078.9681               3089.8729
    3090.2629               3097.5355               3112.6535
    3116.5972               3131.1884               3260.9678
Zero-point correction (Hartree): 0.364053
```

TS29

```
------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -811.671674832
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.641151      0.028694      -0.624646
     C      -0.192529      1.269793       0.254107
     C      -2.110024      0.497891      -0.415388
     C      -1.605686      1.906671      -0.025155
     C      -1.635600      2.866984      -1.222211
     C      -2.272135      2.554033       1.187048
     C      -0.268394     -1.457796      -0.423035
     C       1.146203     -1.959789      -0.745100
     C       2.213798     -1.957100       0.377972
     C       2.323127     -0.579628       0.962581
     C       2.812087      0.490560       0.329005
     C       2.324769      1.853198       0.740355
     C       1.021102      2.172645      -0.032705
     C       3.652830      0.435075      -0.920555
     H      -0.338487      0.222975      -1.663024
     H      -0.175008      0.970430       1.306981
     H      -2.573244     -0.018289       0.422582
     H      -2.772197      0.420847      -1.277665
     H      -2.674322      3.088053      -1.486370
     H      -1.157486      2.443199      -2.109918
     H      -1.143787      3.818358      -0.999775
     H      -3.301346      2.849193       0.957541
     H      -1.733883      3.455363       1.501833
     H      -2.305532      1.865333       2.035882
     H       1.527081     -1.352319      -1.572747
     H       1.027051     -2.979020      -1.122934
     H       3.152812     -2.295527      -0.069739
```

H	1.960142	-2.690414	1.146114
H	1.760307	-0.406930	1.876212
H	3.065515	2.633075	0.532113
H	2.118061	1.880185	1.814992
H	0.726786	3.195406	0.229515
H	1.228201	2.193183	-1.108042
H	3.137544	0.883159	-1.778107
H	3.943803	-0.579283	-1.194898
H	4.569933	1.016625	-0.773981
C	-0.857125	-1.981691	1.327405
H	-0.496325	-1.061724	1.812894
H	-0.222419	-2.865809	1.487386
O	-2.116032	-2.153610	1.246208
O	-2.382201	-2.179280	-0.789798
O	-1.100620	-2.357525	-1.029525

Rotational constants (GHz): 0.4763400 0.4272700 0.2742800

Vibrational harmonic frequencies (cm-1):

-425.2497	43.7018	66.8442
84.8488	127.4910	153.6063
156.5695	162.1809	170.6846
194.1104	217.7545	219.8087
245.4913	258.1778	263.5943
275.6153	299.2904	327.2775
352.7247	355.5174	373.9114
389.2556	414.7975	428.0316
456.9883	488.2828	509.8893
526.1910	542.4634	558.6327
583.0859	593.0408	654.3243
720.2230	757.4098	807.0549
822.0161	850.7632	870.2674
892.3243	897.0675	910.5241
930.8118	942.3025	952.8805
974.5820	978.9561	988.7186
997.1141	1008.6147	1027.6862
1036.7698	1059.4454	1073.3039
1094.2417	1107.4973	1125.8151
1142.7760	1155.6398	1158.1388
1179.9635	1182.3940	1200.4388
1212.4242	1229.8088	1233.0113
1248.3148	1253.5881	1263.8813
1283.8665	1297.7809	1310.0712
1327.0229	1345.1003	1356.3509
1369.2173	1372.1554	1387.1997
1388.1619	1400.8861	1405.4839
1418.3623	1423.2690	1476.8087
1479.0918	1485.6722	1486.3818
1488.2781	1492.9493	1497.7812
1505.0911	1509.6414	1510.1885
1510.7572	1538.7510	1728.2156
2934.8911	2993.2320	3001.4967
3009.9839	3012.8126	3014.2550
3021.4163	3024.9991	3028.8610
3031.4116	3044.4533	3048.3192
3053.6442	3065.6283	3067.5853
3073.2370	3079.6901	3081.1991
3083.4165	3087.2912	3088.1845
3113.0218	3136.0208	3142.6955

Zero-point correction (Hartree): 0.364081

CI-3

E(RB+HF-LYP/6-311G(d,p)) (Hartree): -697.190567154
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.505274	-0.570596	0.760704
C	1.148337	0.352115	-0.360942
C	1.845260	-1.360993	0.792292
C	2.563047	-0.186215	0.067907
C	3.298121	0.720065	1.062899
C	3.487544	-0.572764	-1.084142
C	-0.752119	-1.320566	0.457755
C	-2.095824	-1.035114	1.043996
C	-3.021280	-0.283400	0.028946
C	-2.159691	0.646881	-0.784972
C	-1.609376	1.795274	-0.375089
C	-0.394392	2.329641	-1.096490
C	0.916110	1.865503	-0.408858
C	-2.019202	2.533808	0.874009
H	0.355767	0.001996	1.677903
H	0.898005	-0.088210	-1.331478
H	1.788830	-2.254025	0.169205
H	2.216702	-1.636519	1.781817
H	4.176030	0.200149	1.458655
H	2.671522	0.999457	1.914805
H	3.646312	1.641809	0.588173
H	4.382572	-1.083331	-0.713236
H	3.819569	0.311327	-1.639296
H	2.985754	-1.243431	-1.786891
H	-1.958505	-0.426329	1.939910
H	-2.548483	-1.997778	1.302826
H	-3.804355	0.231845	0.590172
H	-3.489721	-1.023726	-0.616215
H	-1.792722	0.216583	-1.715093
H	-0.400562	3.425434	-1.128155
H	-0.392962	1.977852	-2.132928
H	1.755918	2.310740	-0.956808
H	0.968214	2.282102	0.602755
H	-1.204631	2.580035	1.606111
H	-2.885682	2.087777	1.363279
H	-2.271905	3.571816	0.629244
O	-1.764938	-2.941003	-0.789309
O	-0.633376	-2.254922	-0.394797

Rotational constants (GHz): 0.6852300 0.4651000 0.3307400
Vibrational harmonic frequencies (cm-1):

44.6299	54.8066	71.2537
116.4949	154.5262	159.8081
182.3486	203.8977	220.0375
233.5453	261.9595	281.6552
289.1429	298.5692	310.3795
337.8614	343.3537	354.2324
400.4202	421.7969	433.7099
455.2994	493.7189	549.4797
555.0173	579.8773	614.8912
675.7204	747.1835	769.1798
811.1971	818.5789	842.3501
865.9470	896.5239	901.0855
917.0841	932.4426	945.8365
954.8027	966.0994	979.4302
999.7815	1005.5900	1013.4121
1032.9118	1036.0074	1061.6791
1076.4960	1101.7465	1133.0797
1160.0454	1167.4958	1188.2050

```
    1194.3593                1210.8366                1226.5586
    1237.9901                1251.9022                1256.0387
    1257.1879                1283.5848                1313.4719
    1325.6873                1331.3377                1349.0347
    1362.2385                1378.2399                1391.9384
    1396.7242                1405.6802                1420.2657
    1421.9989                1455.1522                1477.7914
    1484.5762                1484.8540                1487.1225

    1489.7503                1495.6237                1497.8647
    1504.5915                1510.2528                1510.7705
    1526.5445                1725.1328                3007.4364
    3011.5023                3012.3908                3018.6946
    3022.0670                3034.6398                3035.0307
    3045.7890                3051.2054                3055.6375
    3056.3287                3065.2815                3070.5355
    3073.7282                3081.4657                3085.7156
    3087.0261                3097.5403                3113.0223
    3117.0086                3119.7440                3136.6523
Zero-point correction (Hartree): 0.333720
```

CI-4

```
-----------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -697.187936905
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.393515     -0.433051       0.765326
     C       0.961658      0.506594      -0.373750
     C       1.857700     -0.886257       1.080809
     C       2.410933      0.282568       0.209766
     C       2.941367      1.431775       1.073725
     C       3.446622     -0.126125      -0.836126
     C      -0.603626     -1.485595       0.439879
     C      -1.988762     -1.538492       1.040581
     C      -3.039120     -0.930746       0.049115
     C      -2.358494      0.119534      -0.794927
     C      -2.028106      1.362405      -0.427090
     C      -0.948593      2.092264      -1.193058
     C       0.434576      1.938592      -0.506672
     C      -2.557579      2.052435       0.803786
     H      -0.012648      0.168622       1.579892
     H       0.886760     -0.017415      -1.326662
     H       2.079987     -1.862389       0.658309
     H       2.118104     -0.861828       2.141635
     H       3.864355      1.120752       1.573463
     H       2.233356      1.730271       1.852676
     H       3.173192      2.317275       0.474376
     H       4.387929     -0.420943      -0.359136
     H       3.667478      0.704022      -1.516837
     H       3.081818     -0.969502      -1.425301
     H      -1.982720     -0.963029       1.967993
     H      -2.245837     -2.572781       1.282484

     H      -3.886767     -0.543464       0.619301
     H      -3.419629     -1.728257      -0.591989
     H      -1.919954     -0.257699      -1.716300
     H      -1.178080      3.161104      -1.276778
     H      -0.885023      1.694633      -2.210354
     H       1.162620      2.506473      -1.098591
     H       0.407650      2.423229       0.475376
     H      -1.751024      2.325611       1.493165
```

```
     H      -3.279111      1.446315       1.352966
     H      -3.052433      2.989277       0.523285
     O       0.771327     -2.428072      -1.151573
     O      -0.394148     -2.410138      -0.406071
Rotational constants (GHz):    0.7270200    0.4740900    0.3525800
Vibrational harmonic frequencies (cm-1):
      43.4919                 67.3500                 73.2934
     101.8595                147.1429                163.8936
     188.5922                202.1832                211.4917
     242.1910                268.3786                274.0408
     281.0215                291.9193                304.8096
     335.7739                351.0170                382.7384
     393.5857                397.6362                445.4220
     458.3936                490.5906                534.1752
     562.7067                581.4031                608.5576
     686.5393                742.8889                750.9670
     811.1251                821.5786                862.5977
     872.7497                886.3374                908.5238
     913.7775                922.5075                932.3455
     949.1013                966.6705                971.8489
     996.9374               1000.0963               1014.9005
    1029.0029               1040.4637               1060.9675
    1075.2443               1097.4783               1133.0873
    1155.8886               1180.8790               1192.9420
    1197.2565               1208.7931               1226.5012
    1234.9570               1248.6603               1256.7094
    1265.1205               1284.1613               1313.8984
    1320.2975               1341.4639               1349.7572
    1360.0279               1381.4004               1397.2595
    1399.6247               1407.7987               1415.6933
    1420.6441               1472.8678               1474.9344
    1478.9359               1486.5068               1488.0125
    1492.9685               1494.1528               1496.6573
    1505.4714               1507.0522               1515.7898
    1528.2751               1724.6298               3008.7861
    3009.3459               3014.3741               3017.2014
    3021.9679               3043.6911               3049.8450
    3052.8619               3055.4472               3056.8434
    3062.7720               3067.3480               3072.7759
    3076.6126               3082.2800               3087.2222
    3099.0971               3105.7114               3108.1235
    3110.4247               3127.4961               3150.4632
Zero-point correction (Hartree): 0.333884
```

beta-nocaryophyllone

```
-------------------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -622.087215309
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.470600     -0.764919       0.643294
     C       0.979716      0.361632      -0.344587
     C       1.916563     -1.328743       0.656522
     C       2.458457     -0.000943       0.055409
     C       3.052731      0.904368       1.140700
     C       3.431104     -0.140028      -1.113932
     C      -0.599679     -1.730427       0.141178
     C      -2.011901     -1.669696       0.735436
     C      -2.990016     -0.975720      -0.257919
     C      -2.282422      0.197149      -0.889653
     C      -1.949931      1.347660      -0.294710
     C      -0.828554      2.174837      -0.877247
```

```
      C       0.528480      1.820957      -0.214657
      C      -2.506725      1.811850       1.027022
      H       0.180261     -0.333157       1.603679
      H       0.807394      0.011971      -1.367895
      H       1.996533     -2.162338      -0.043192
      H       2.315157     -1.629217       1.628604
      H       3.990690      0.475330       1.507450
      H       2.384547      1.013331       1.999700
      H       3.274640      1.905545       0.759398
      H       4.392044     -0.545665      -0.779290
      H       3.628508      0.830371      -1.583258
      H       3.032891     -0.810829      -1.880061
      H      -1.998945     -1.118524       1.678816
      H      -2.338212     -2.693889       0.936921
      H      -3.902201     -0.691403       0.273631
      H      -3.277060     -1.691909      -1.030171
      H      -1.819885     -0.016457      -1.850618
      H      -1.013298      3.247510      -0.745739
      H      -0.753443      1.990619      -1.953535
      H       1.297588      2.451260      -0.677999
      H       0.506324      2.108448       0.842012
      H      -1.726716      1.882945       1.793750
      H      -3.292744      1.158132       1.406781
      H      -2.929561      2.817667       0.922733
      O      -0.345632     -2.530950      -0.735356
Rotational constants (GHz):    0.8759000    0.4941000    0.3782800
Vibrational harmonic frequencies (cm-1):
      50.3439                56.9878                84.9034
     110.1279               157.7444               169.6033
     198.4210               210.6209               228.7445
     233.7909               261.9368               280.2903
     288.0362               297.1993               325.9079
     356.6552               395.1164               404.5990
     436.9710               444.0319               489.3504
     542.1412               558.9786               584.0333
     603.3578               688.9533               745.6699
     761.3917               815.9841               823.1196
     862.9872               874.5852               900.1279
     912.3324               918.4773               935.5416
     953.6205               961.7022               972.5614
     994.0203              1002.1138              1009.2057
    1033.2570              1035.5107              1061.0394
    1070.2503              1100.9392              1103.5314
    1137.0689              1166.7918              1176.0614
    1195.3721              1209.1155              1213.9645
    1226.7268              1245.9847              1253.8474
    1255.2994              1281.7129              1309.5697
    1326.8103              1329.9797              1345.0095
    1358.6716              1364.3303              1386.5490
    1397.0648              1404.7906              1420.3853
    1421.1802              1476.2457              1478.4419
    1483.5802              1486.0898              1488.4071
    1489.9527              1495.2945              1497.3330
    1505.0437              1507.5043              1509.1446
    1726.6387              1768.6720              3005.6258
    3008.9653              3011.6396              3017.2293
    3020.5397              3031.6961              3038.8061
    3042.8836              3047.2659              3047.7171
    3052.1541              3062.4628              3064.7344
    3066.2132              3077.4520              3081.2218
    3084.1717              3085.6714              3098.1416
```

```
    3109.4829                3111.0774                3131.0738
Zero-point correction (Hartree): 0.330201
```

TS30

```
---------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -697.154819296
Electronic state : 1-A
Cartesian coordinates (Angs):
     C       0.551922     -0.646417       0.760232
     C       1.148086      0.362874      -0.320348
     C       1.880150     -1.441283       0.669402
     C       2.574717     -0.208029       0.023177
     C       3.330933      0.617724       1.071126
     C       3.466709     -0.488159      -1.183663
     C      -0.741554     -1.298414       0.432344
     C      -2.044374     -0.994934       0.905300
     C      -3.002906     -0.255040      -0.094272
     C      -2.155028      0.742724      -0.847415
     C      -1.608119      1.858846      -0.352128
     C      -0.351540      2.409384      -0.983153
     C       0.920777      1.879054      -0.265741
     C      -2.043324      2.509542       0.936084
     H       0.437711     -0.135182       1.718384
     H       0.867211     -0.011181      -1.310303
     H       1.795211     -2.276781      -0.026417
     H       2.291044     -1.804637       1.613729
     H       4.214475      0.067656       1.409369
     H       2.719761      0.830313       1.952812
     H       3.672419      1.573379       0.663410
     H       4.380298     -1.011974      -0.883417
     H       3.767710      0.442649      -1.676574
     H       2.951112     -1.108927      -1.921713
     H      -2.007386     -0.465425       1.855788
     H      -2.364672     -2.293631       0.494211
     H      -3.797226      0.207661       0.494147
     H      -3.465810     -0.958288      -0.785600
     H      -1.759886      0.367533      -1.790624
     H      -0.332773      3.505149      -0.948293
     H      -0.305648      2.121225      -2.038325
     H       1.789413      2.356278      -0.736837
     H       0.925497      2.220350       0.774869
     H      -1.265769      2.449370       1.707257
     H      -2.951830      2.066469       1.344791
     H      -2.235548      3.576270       0.773865
     O      -1.947148     -2.919974      -0.525168
     O      -0.663353     -2.330714      -0.373609
Rotational constants (GHz):    0.6845300    0.4652400    0.3256400
Vibrational harmonic frequencies (cm-1):
    -1573.5287                 50.4487                 57.8202
      74.8330                131.1962                157.2613
     167.0136                191.4932                211.2752
     220.3824                225.3154                262.7849
     276.6082                299.6308                304.6095
     321.3586                344.6247                360.8329
     399.3757                419.2492                430.4582
     465.8780                493.8782                549.3082
     555.7572                580.1924                658.7849
     685.5443                728.0472                759.4859
     791.2522                827.0372                835.8938
     859.2391                893.0828                903.4528
     906.2936                922.9378                938.2659
```

```
     944.1565                952.9616                958.8335
     984.3276                992.8964               1002.8527
    1021.8121               1031.3820               1048.8817
    1060.1102               1071.8167               1098.3586
    1127.8738               1151.5500               1167.3845
    1184.1469               1208.0627               1223.6009
    1237.7665               1241.6657               1250.2873
    1257.8556               1282.0710               1298.1068
    1311.6121               1316.8787               1330.9195
    1342.7273               1360.2141               1379.9079
    1395.4737               1403.7878               1415.8679

    1416.4498               1421.7687               1476.8446
    1479.4977               1485.3720               1486.8746
    1487.5819               1492.0049               1495.9209
    1500.1220               1508.2644               1509.7598
    1511.4106               1719.0288               1858.0841
    3005.0332               3008.0943               3011.6034
    3016.7636               3022.0512               3033.2968
    3044.3339               3048.6235               3057.7794
    3062.7201               3067.1059               3070.1632
    3074.4718               3082.3024               3084.4220
    3087.7787               3101.5458               3110.4447
    3112.9293               3117.4861               3123.6809
Zero-point correction (Hartree): 0.329215
```

TS31

```
---------------
E(RB+HF-LYP/6-311G(d,p)) (Hartree): -697.147523382
Electronic state : 1-A
Cartesian coordinates (Angs):
     C      -0.362654      0.392313      0.722744
     C      -0.967221     -0.513220     -0.417553
     C      -1.809396      0.685133      1.238142
     C      -2.414091     -0.283215      0.173911
     C      -3.095415     -1.505098      0.794527
     C      -3.348809      0.407516     -0.820812
     C       0.591811      1.460502      0.265768
     C       1.922977      1.616651      0.956889
     C       3.040872      0.939897      0.075276
     C       2.416099     -0.154942     -0.760159
     C       2.028521     -1.368575     -0.350694
     C       0.979844     -2.111224     -1.149189
     C      -0.438866     -1.949377     -0.534935
     C       2.462944     -2.005647      0.944427
     H       0.182309     -0.203845      1.456514
     H      -0.876109     -0.004634     -1.379686
     H      -2.083586      1.726885      1.103691
     H      -1.970902      0.379972      2.275475
     H      -4.008181     -1.192973      1.312125
     H      -2.461216     -2.010033      1.528520
     H      -3.383267     -2.238994      0.035325
     H      -4.284082      0.704427     -0.333423
     H      -3.603274     -0.264066     -1.648902
     H      -2.871950      1.302324     -1.226335
     H       1.887168      1.145613      1.939905
     H       2.130803      2.681830      1.086324
     H       3.828898      0.579691      0.739606
     H       3.485340      1.693032     -0.576449
     H       2.054640      0.179356     -1.728765
     H       1.208557     -3.182445     -1.201040
```

```
     H       0.966716     -1.733751      -2.176001
     H      -1.136173     -2.516632      -1.162382
     H      -0.461784     -2.435487       0.446136
     H       1.613005     -2.212401       1.603821
     H       3.177511     -1.394746       1.497631
     H       2.937009     -2.972853       0.742019
     O      -0.802578      2.705124      -0.532457
     O       0.506188      2.083058      -0.863062
Rotational constants (GHz):    0.7389800    0.4814300    0.3527200
Vibrational harmonic frequencies (cm-1):
    -423.5339                  43.2647                  78.6885
      91.8862                 114.5473                 155.3110
     163.1602                 204.2854                 209.9701
     218.0347                 263.4715                 271.8929
     283.9923                 290.7898                 295.9619
     321.9766                 344.9423                 380.7559
     397.2196                 400.4427                 436.1718
     459.0645                 480.5469                 524.3430
     558.8826                 560.4271                 602.1944
     678.7677                 738.1553                 743.3854
     805.7093                 809.9915                 826.9198
     843.4504                 869.9918                 878.4809
     901.1277                 912.0293                 931.1501
     954.2372                 960.3730                 980.6089
     992.1758                 999.2636                1015.6986
    1031.5449                1035.4098                1060.7958
    1066.8027                1086.6129                1126.4857
    1131.9379                1167.1536                1182.4562
    1192.9717                1203.5822                1210.3828
    1229.7941                1241.9435                1251.5825
    1259.5680                1284.4601                1305.9266
    1309.4735                1330.9151                1341.7249
    1358.6613                1374.8700                1389.2827
    1398.4838                1401.1219                1419.1062
    1420.5736                1464.8794                1476.5163
    1479.0994                1486.1007                1487.0726
    1492.4863                1494.9556                1498.1408
    1500.6802                1507.0442                1508.7275
    1521.1025                1721.4576                3005.5415
    3010.1863                3014.9419                3017.9781
    3023.9748                3045.1507                3045.9783
    3054.7712                3056.2186                3062.4399
    3063.9582                3065.6519                3070.6385
    3076.6097                3077.9072                3086.4674
    3097.6482                3101.4253                3109.7565
    3117.7498                3141.6061                3160.3126
Zero-point correction (Hartree): 0.332504
```

Rad-3

```
----------------
E(UB+HF-LYP/6-311G(d,p)) (Hartree): -621.422411136
Electronic state : 2-A
Cartesian coordinates (Angs):
     C      -0.611533      0.849509       0.721779
     C      -0.949080     -0.340330      -0.270936
     C      -2.073322      1.323040       0.556559
     C      -2.472848     -0.084908       0.024040
     C      -3.038707     -0.967822       1.142715
     C      -3.390222     -0.116721      -1.196187
     C       0.512036      1.750139       0.234912
     C       1.840022      1.479118       0.790649
```

C	2.970834	1.192558	-0.158475
C	2.362317	-0.006215	-0.879007
C	2.097746	-1.205251	-0.333448
C	0.963502	-2.033703	-0.889590
C	-0.370390	-1.757309	-0.133767
C	2.742775	-1.722143	0.926058
H	-0.404619	0.468721	1.725178
H	-0.752161	0.030531	-1.282691
H	-2.129256	2.087991	-0.220394
H	-2.583100	1.677561	1.455504
H	-4.029918	-0.607886	1.436165
H	-2.408756	-0.958835	2.036604
H	-3.147885	-2.007822	0.820616
H	-4.399153	0.222055	-0.937270
H	-3.478017	-1.131353	-1.600863
H	-3.012356	0.532552	-1.990720
H	1.888724	1.026443	1.776912
H	3.903423	0.979558	0.365439
H	3.137702	2.012768	-0.858400
H	1.831009	0.257913	-1.789327
H	1.184537	-3.104873	-0.816391
H	0.817178	-1.806462	-1.950148
H	-1.113844	-2.460418	-0.529746
H	-0.252075	-2.017566	0.923584
H	2.007394	-1.878981	1.723258
H	3.518847	-1.057746	1.307566
H	3.203342	-2.697886	0.733673
O	0.340026	2.534244	-0.692545

Rotational constants (GHz): 0.9185800 0.4856600 0.3796300

Vibrational harmonic frequencies (cm-1):

58.9055	70.2649	104.9023
136.1977	165.7162	179.4495
205.1040	213.6812	226.8911
240.4529	266.3425	286.0611
297.1063	307.9402	313.8316
352.3022	385.0774	402.2443
434.0700	435.5242	489.6581
525.5299	558.0062	585.0807
623.7552	669.2614	733.1277
750.1556	762.9650	820.2499
840.8779	883.4954	894.4115
913.9354	929.5274	934.3741
948.0215	952.5842	985.7749
987.4962	999.8776	1012.7923
1029.0759	1052.2691	1061.2370
1063.9049	1097.2056	1111.7298
1132.4616	1164.7903	1178.7509
1189.6889	1208.1360	1226.3207
1237.9399	1243.5759	1255.2859
1260.3689	1282.2677	1308.8559
1330.4600	1356.2213	1361.6270
1379.5668	1395.4669	1398.9254
1404.8113	1417.2678	1419.5528
1474.7596	1478.5153	1485.0094
1487.2860	1490.2207	1493.1144
1497.0994	1500.9451	1507.9417
1510.1492	1666.1256	1681.6412
3006.3145	3009.1220	3012.6784
3018.8966	3021.5149	3027.4013
3045.0238	3048.1863	3053.3433
3059.3230	3064.4836	3065.5262

3067.3979 3078.4081 3084.1058
3086.6671 3106.6200 3108.8956
3113.9814 3146.8504 3155.4213
Zero-point correction (Hartree): 0.316902

Ester $CH_3C(O)OCH_3$

E(RB+HF-LYP/CBSB7) (Hartree): -268.467105133
Electronic state : 1-A
Cartesian coordinates (Angs):

C	-0.462493	0.179445	-0.000014
O	0.548713	-0.719222	-0.000020
O	-0.290182	1.371439	-0.000001
C	-1.799096	-0.519426	0.000005
H	-2.595021	0.222029	-0.000264
H	-1.884073	-1.160696	-0.880065
H	-1.884265	-1.160215	0.880414
C	1.874934	-0.161634	0.000013
H	2.549722	-1.014801	0.000016
H	2.032678	0.452828	-0.887826
H	2.032640	0.452808	0.887872

Rotational constants (GHz): 10.2157000 4.1474400 3.0624800
Vibrational harmonic frequencies (cm-1):
50.8520 121.2861 180.4749
282.3992 423.1571 606.7493
645.2878 858.5963 982.8974
1065.7800 1070.1374 1173.6199
1208.9474 1264.4403 1396.7738
1471.3790 1474.8110 1477.1089
1483.4773 1500.8411 1816.6629
3047.5606 3050.9079 3110.9711
3117.7114 3154.4319 3157.7604
Zero-point correction (Hartree): 0.089293

TS of CO_2-elimination

E(RHF/6-31+(d')) (Hartree): -266.637262537
E(CCSD(T)/6-31+(d')) (Hartree): -267.50706344
E(MP2/6-31+(d')) (Hartree): -267.44663873
E(MP3/6-31+(d')) (Hartree): -267.44694226
Electronic state : 1-A
Cartesian coordinates (Angs):

C	0.085994	-0.430323	0.000016
O	-0.046492	-0.888325	1.150501
O	-0.046299	-0.888421	-1.150449
C	1.242043	0.840549	0.000058
H	1.169060	1.424687	-0.910432
H	1.169790	1.423534	0.911346
H	2.141506	0.229347	-0.000733
C	-1.241194	0.919838	-0.000110
H	-1.088728	1.459578	0.923214
H	-1.089370	1.458405	-0.924224
H	-2.080987	0.238031	0.000637

Rotational constants (GHz): 5.2093893 5.0630342 4.7965546
Vibrational harmonic frequencies (cm-1):
-348.6615 124.6903 186.0628
272.0867 290.7115 356.9734
362.0994 462.1389 641.9806
784.6271 801.6118 927.7804
981.7468 1156.9650 1225.1395
1314.7584 1426.3859 1447.6377

```
    1460.1689                1471.7139                1629.6463
    3080.4111                3116.3792                3187.0429
    3217.8083                3269.5699                3285.6003
Zero-point correction (Hartree): 0.083112
```