Electronic Supplementary Information for

Fragmentation of a Dioxolanyl Radical via Nonstatistical Reaction Dynamics: Characterization of the Vinyloxy Radical by ns Time-Resolved Laser Flash Photolysis

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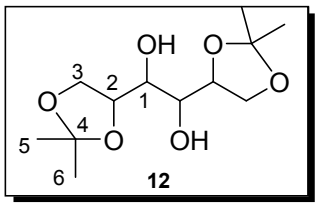
Synthesis of compounds

General Information

All commercial reagents were used without further purification. Solvents were dried with the appropriate desiccants and distilled prior to use. ^{1}H NMR and ^{13}C NMR were recorded on Bruker 200 MHz or 400 MHz (Avance) machines using the deuterated solvent as the lock and residual protiated solvent as the internal reference (CD_3Cl: δ_H = 7.26 ppm and δ_C = 77.0 ppm). The following abbreviations were utilized to describe peak patterns: s = singlet, d = doublet, t = triplet, dd = doublet of doublet, td = triplet of doublet, dt = doublet of triplet, br = broad, bs = broad singlet, bd = broad doublet and m = multiplet. The numbering of the carbon atoms in the molecular formulae (*vide infra*) is used only for the assignments of the NMR signals and thus is not necessarily in accordance with IUPAC nomenclature. Melting points were measured on a Büchi SMP-20 instrument. Infrared spectra were recorded using a Varian 1000 FT-IR instrument. Elemental analysis was done on the EA 3000 CHNS.

Synthesis of Model Compounds

[D]-1,2,5,6-Diisopropylidenemannitol (12)



12

D-mannitol (36.0 g, 190 mmol) was added to a vigorously stirring dry acetone (150 mL) containing fused zinc chloride (75.0 g, 550 mmol) at 0 °C. A solution of potassium carbonate in water (100 g in 100 mL) was added slowly to the reaction mixture after 3 h. The precipitate was filtered and the filtrate was extracted with chloroform (3 × 300 mL). The combined organic layers were dried over Na_2SO_4 (anhyd.) and concentrated.

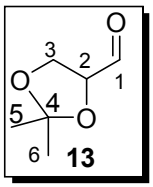
Yield: 37.0 g (0.141 mol) of a white solid, 72%.

Melting Point: 120-122 °C (Lit:[1] 118-120 °C)

IR (NaCl): $\tilde{\nu}$ (cm^{-1}) = 3404 (b, OH), 3283, 2989 (s, CH), 2935, 2895, 1381, 1265, 1213, 1160, 1126, 1069, 1009, 943, 858, 800, 666, 516.

^{1}H-NMR ($CDCl_3$, 200 MHz): δ (ppm) = 1.34 (s, 6H, 5-H), 1.39 (s, 6H, 6-H), 2.82 (m, 2H, OH), 3.71 (t, *J* = 6.6 Hz, 2H, 1-H), 3.91-4.13 (m, 6H, 2,3-H).

[D]-2,3-Isopropylideneglyceraldehyde (12)[2]



13

Sodium metaperiodate (12.5 g, 58.3 mmol) was added to [D]-1,2,5,6-diisopropylidenemannitol (10.0 g, 38.1 mmol) in dichloromethane (100 mL) and 4.40 mL of saturated sodium bicarbonate. The reaction was stirred at room temperature for 5 h, filtered and concentrated at temperature lower than 45 °C. The crude product was purified by distillation under reduced pressure.

Yield: 6.20 g (47.6 mmol) of a colourless liquid, 62%.

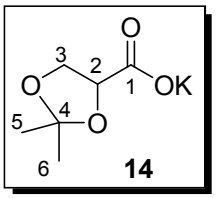
Boiling Point: 42-44 °C/11 mbar (Lit:[3] 31 °C/1 torr)

IR (NaCl): $\tilde{\nu}$ (cm^{-1}) = 3451 (m, OH), 2990 (s, CH), 2892, 2819, 1735 (s, C=O), 1456, 1375, 1255, 1220, 1151, 1073, 842.

^{1}H-NMR ($CDCl_3$, 200 MHz): δ (ppm) = 1.39 (s, 3H, 5-H), 1.46 (s, 3H, H-6), 4.03-4.19 (m, 2H, 3-H), 4.33-4.40 (m, 1H, 2-H), 9.68 (s, 1H, 1-H).

^{13}C-NMR ($CDCl_3$, 50 MHz): δ (ppm) = 26.3 (C-5), 27.2 (C-6), 66.6 (C-3), 80.7 (C-2), 112.3 (C-4), and 202.8 (C-1).

Potassium-[D]-2,3-isopropylideneglycerate[2] **(14)**



14

Potassium permanganate (10.3 g, 70.0 mmol) in water (250 mL) was added slowly to the crude [D]-2,3-isopropylidene acetaldehyde (6.50 g, 49.9 mmol) and potassium hydroxide (5.70 g, 100 mmol) in 100 ml of water at 0 °C. The solution was neutralized to pH 8 after 3 h. Water was removed by distillation producing a brown mass, which upon extraction with hot ethanol yielded a yellow oil. The oil, when precipitated with acetone (100 mL), furnished a white solid.

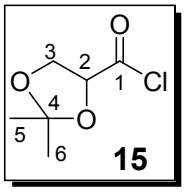
Yield: 6.50 g (35.3 mmol) of a white solid, 46%.

Melting Point: softens above 60° C.

IR (NaCl): $\tilde{\nu}$ (cm^{-1}) = 2992 (m, CH), 2958, 2881, 1620 (bs, C=O), 1372, 1259, 1218, 1149, 1067, 970, 846, 788, 512.

^{1}H-NMR (D_2O, 200 MHz): δ (ppm) = 1.23 (s, 3H), 1.29 (s, 3H), 3.75 (dd, *J* = 8.2 Hz, *J* = 6.8 Hz, 1H, 2-H), 4.12 (t, *J* = 8.2 Hz, 1H, 3a-H), 4.31 (dd, *J* = 7.4 Hz, *J* = 6.8 Hz, 1H, 3b-H).

[D]-2,3-Isopropylideneglyceryl chloride (15)



Oxalyl chloride (4.50 ml, 52.5 mmol), potassium [D]-2,3-isopropylideneglycerate (4.60 g, 24.8 mmol) and 100 µl of pyridine in 50 ml dry ether were stirred at room temperature for 20 h. The reaction mixture was then filtered and concentrated. The crude product was purified by distillation under reduced pressure.

Yield: 1.80 g (10.9 mmol) of a colourless liquid, 43%.

Boiling Point: 71-72 °C/25 mbar (Lit:[2] 70 °C/25 mbar).

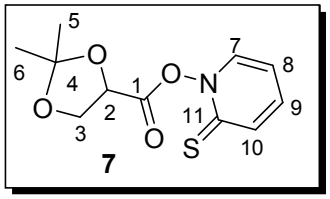
IR (NaCl): $\tilde{\nu}$ (cm^{-1}) = 2992 (m), 2941, 2891, 1820 (s, C=O), 1777, 1456, 1385, 1226, 1113, 1074, 889, 839, 752, 642.

^{1}H-NMR ($CDCl_3$, 200 MHz): δ (ppm) = 1.38 (s, 3H, 5-H), 1.48 (s, 3H, H-6), 4.32 (d, *J* = 5.4 Hz, 2H, 3-H), 4.82 (t, *J* = 5.7 Hz, 1H, 2-H).

^{13}C-NMR ($CDCl_3$, 50 MHz): δ (ppm) = 26.3 (C-5), 26.6 (C-6), 67.9 (C-3), 82.1 (C-2), 114.0 (C-4), and 174.2 (C-1).

DEPT-135 ($CDCl_3$, 50 MHz): δ (ppm) = 26.3 (C-5), 26.6 (C-6), and 82.1 (C-2). Signal at 67.9 (C-3) inverted due to secondary nature of the carbon, while signals at 114.0 (C-4) and 174.2 (C-1) disappeared due to the quaternary nature of the carbons.

2,2-Dimethyl-[1,3]dioxolane-4-carboxylic acid 2-thio-2*H*-pyridin-1yl-ester (7)



N-2-thiopyridineoxide sodium salt (1.67 g, 10 µmol), [D]-2,3-diisopropylideneglyceryl chloride (1.77 g, 10 µmol) and catalytic amount of DMAP were stirred in 50 mL of dry ether was stirred for 30 minutes in dark. The reaction mixture was filtered through a bed of celite and concentrated below 45 °C.

Yield: 2.28 g (8.93 mmol) of a cream-coloured solid, 83%.
Melting point: 62 °C

IR (NaCl): $\tilde{\nu}$ (cm^{-1}) = 3100 (w), 2992 (w), 1810 (s), 1736 (b), 1605 (s), 1527 (s), 1448 (s), 1372 (s), 1227 (b), 1132 (b), 1076 (bs), 963 (s), 840 (s), 740 (s).

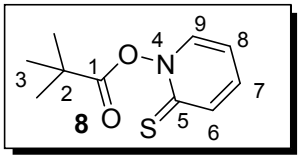
^{1}H-NMR ($CDCl_3$, 200 MHz): δ (ppm) = 1.37 (s, 3H, 5-H), 1.49 (s, 3H, 6-H), 4.31 (dd, *J* = 9.1 Hz, *J* = 7.4 Hz 1H, 2-H), 4.65 (dd, *J* = 9.1 Hz, *J* = 4.7 Hz, 1H, 3-H), 4.86 (dd, *J* = 7.4 Hz, *J* = 4.7 Hz, 1H, 3-H), 6.67 (td, *J* = 6.9 Hz, *J* = 2.0 Hz, 1H, 8-H), 7.12-7.21 (m, 1H, 9-H), 7.58 (dd, *J* = 9.1 Hz, *J* = 2.0 Hz, 1H, 10-H), 7.66 (dd, *J* = 7.0 Hz, *J* = 1.6 Hz, 1H, 7-H).

^{13}C-NMR ($CDCl_3$, 50 MHz): δ (ppm) = 26.7 (C-5), 26.8 (C-6), 66.7 (C-4), 68.2 (C-3), 74.5 (C-2), 134.0 (C-10), 137.7 (C-7), 138.8 (C-8, 9), 171.2 (C-1), 172.9 (C-11).

DEPT-135 ($CDCl_3$, 50 MHz): δ (ppm) = 26.7 (C-5), 26.8 (C-6), 74.5 (C-2), 134.0 (C-10), 137.7 (C-7), 138.8 (C-8, 9). Signal at 68.2 (C-3) inverted due to the secondary nature of the carbon while signals at 66.7 (C-4), 171.2 (C-1) and 172.9 (C-11) disappeared due to the quaternary nature of the carbon.

Elemental analysis: Calcd. C = 51.75, H = 5.13, N = 5.49, S = 12.56
Found C = 51.06, H = 5.15, N = 5.56, S = 13.18

2,2-Dimethyl-propanoic acid 2-thioxo-2*H*-pyridin-1-yl-ester (8)[4]



Pivalylchloride (2.0 g, 17 mmol) was added dropwise to a suspension of *N*-hydroxy-2-pyridinethione sodium salt (2.5 g, 17 mmol) and catalytic amount DMAP (100 mg) in 50 mL of dry ether at room temperature. After 45 min the reaction mixture was poured into water and extracted with ether (3 × 50 mL). The combined organic layer was then passed through celite (285) and washed with water (3 × 100 mL) and dried over Na_2SO_4 (anhyd.) and concentrated at 40 °C.

Yield: 3.1 g (15 mmol) of cream coloured solid, 93%.

Melting point: 93-94 °C

IR (NaCl): $\tilde{\nu}$ (cm^{-1}) = 3069, 2975, 2931, 1789 (C=O), 1606, 1526, 1452, 1414, 1368, 1285, 1227, 1176, 1137, 1092, 1057, 1015, 941, 864, 840, 797, 759, 711, 524, 502.

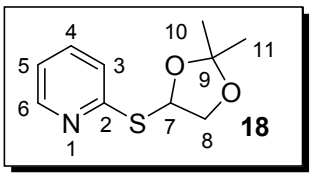
^{1}H-NMR ($CDCl_3$, 200 MHz): δ (ppm) = 1.45 (s, 9H, 3-H), 6.62 (td, *J* = 6.9 Hz, *J* = 1.7 Hz, 1H, 8-H), 7.19 (td, *J* = 6.9 Hz, *J* = 1.7 Hz, *J* = 1.5 Hz, 1H, 7-H), 7.48 (dd, *J* = 7.0 Hz, *J* = 1.5 Hz, 1H, H-6), 7.67 (dd, *J* = 7.0 Hz, *J* = 1.7 Hz, 1H, 9-H).

^{13}C-NMR ($CDCl_3$, 50 MHz): δ (ppm) = 27.1 (C-3), 38.8 (C-2), 112.6 (C-9), 133.4 (C-6), 137.4 (C-7), 137.6 (C-8).

HRMS: $C_{10}H_{13}NO_2S$, Calculated: 211.0667, Found: 211.0670

Synthesis of Reference Compounds

2-(2,2-Dimethyl-[1,3]dioxolan-4-ylsulfanyl)-pyridine (18)



A solution of **7** (0.50 g, 2.0 mmol) in 25 mL of benzene (dry) was photolyzed (300 W UV-Lamp) for about 20 min. The reaction mixture was concentrated and purified by column chromatography with hexane - ethyl acetate as eluent. The pure product was collected as the second fraction with 20% ethyl acetate in hexane.

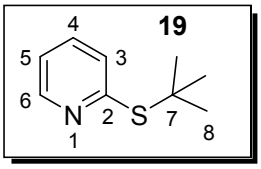
Yield: 0.3 g (1.4 mmol) of colourless oil, 73%.

IR (NaCl): $\tilde{\nu}$ (cm^{-1}) = 3046 (w), 2988 (m), 2937, 2872, 1578 (s), 1453 (s), 1417, 1374 (s), 1220 (b), 1148 (b), 1127, 1072 (bs), 989, 949, 838 (s), 760 (s), 725, 639, 514.

^{1}H-NMR ($CDCl_3$, 200 MHz): δ (ppm) = 1.44 (s, 3H, 10-H), 1.53 (s, 3H, 11-H), 4.12 (dd, ^3J = 9.4 Hz, ^2J = 4.7 Hz 1H, 8-H), 4.46 (dd, ^3J = 9.4 Hz, ^2J = 6.4 Hz, 1H, 8-H), 6.34 (dd, ^3J = 6.4 Hz, ^3J = 4.7 Hz, 1H, 7-H), 7.00-7.06 (m, 1H, 5-H), 7.24-7.29 (m, 1H, 3-H), 7.45-7.55 (m, 1H, 4-H), 8.44-8.49 (m, 1H, 6-H).

^{13}C-NMR ($CDCl_3$, 50 MHz): δ (ppm) = 26.0 (C-10), 26.0 (C-11), 70.0 (C-8), 80.1 (C-7), 115.5 (C-9), 120.2 (C-5), 122.1 (C-3), 136.4 (C-6,4), 149.7 (C-6).

2-*tert*-Butylsulphanyl-pyridine[90] (19)



A solution of **78** (0.4 g, 2.0 mmol) in 25 mL of benzene (dry) was photolyzed (300 W UV-Lamp) for about 20 min. The reaction mixture was concentrated and purified by column chromatography with hexane - ethyl acetate as eluent. The pure product was collected as second fraction with 20% ethyl acetate in hexane (R_f = 0.72).

Yield: 0.25 g (1.5 mmol) of colourless oil, 80%.

IR (NaCl): $\tilde{\nu}$ (cm^{-1}) = 3045 (w), 2961 (m), 2922, 1727, 1578 (s), 1556, 1449 (s), 1413, 1361 (s), 1278 (b), 1122 (b), 1072 (bs), 1044, 986, 758 (s), 724, 623.

^{1}H-NMR ($CDCl_3$, 200 MHz): δ (ppm) = 1.50 (s, 9H, 8-H), 7.04-7.10 (m, 1H, 5-H), 7.33 (dd, J = 7.9 Hz, J = 0.7 Hz, 1H, 3-H), 7.51 (td, J = 7.7 Hz, J = 2.0 Hz, 1H, 4-H), 8.51 (dt, J = 4.2 Hz, J = 0.7 Hz, 1H, 6-H).

^{13}C-NMR ($CDCl_3$, 50 MHz): δ (ppm) = 30.9 (C-8), 47.5 (C-7), 120.7 (C-5), 127.4 (C-3), 135.9 (C-6,4), 149.4 (C-2).

Acid stability of 7

General Information

As the idea of generating ethenol radical cation from **7** would require acidic conditions, it was necessary to evaluate the acid sensitivity of **7**. Using the absorption band at λ_{max} = 360 nm, any change by protonation can easily be followed by monitoring the absorbance changes.

Testing Compound 7

An increasing amount of trifluoroacetic acid (38.5 mM: stock solution) was added stepwise to a solution of **7** (0.10 mM). After adding an equimolar quantity of TFA to **7**, a very small decrease in absorption was observed at λ_{max} = 360 nm (Figure S1a). A further increase in acid concentration not only decreased the absorption at λ_{max} = 360 nm but additionally led to a 12 nm shift of the chromophore to λ_{max} = 348 nm (Figure S1c).

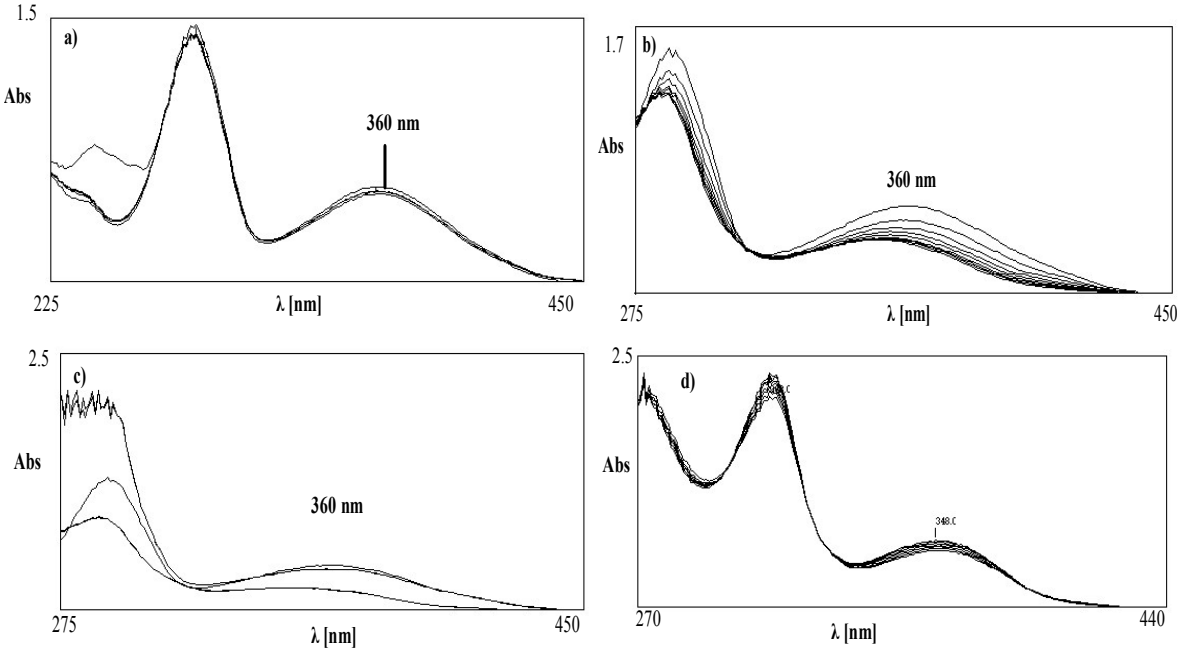


Figure S1: Addition of TFA to **7**, a) 1 eq. of TFA followed by addition of 1.1eq. pyridine, b) serial addition of up to 70eq. of TFA, c) addition of 70 eq. of TFA followed by addition of 1.1 eq. of pyridine, d) time dependent measurement (over 5 h) over the decay of **7** with 56 eq. of TFA.

Interestingly, a plateau was reached after the addition of 28 equivalents of TFA to Barton ester **7** (Figure S2). The original spectrum of the acid-free **7** was retained after the addition of a slight excess

of pyridine as base (dilution factor taken into account) to the acidified solution clearly showing a reversible protonation of the chromophore.

The above experiments with the addition of TFA to **7** clearly showed that it was not very sensitive to the TFA at low concentrations. The process of protonation was reversible in the time frame of about 3-4 h.

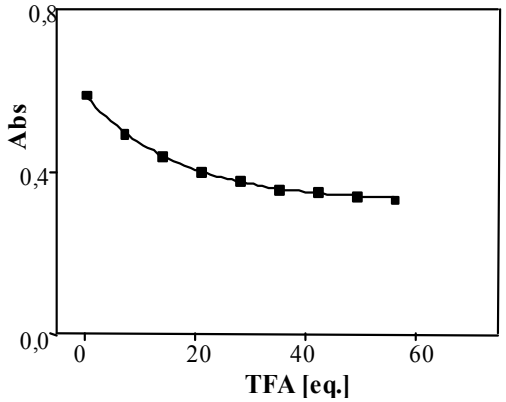


Figure S2: Absorbance changes at 360 nm upon addition of TFA to **7** (0 - 56 equiv. of TFA).

Photolysis

Steady State Photolysis

Photolysis of **8** (568 µM) in the presence of an equimolar concentration of ferrocene and TFA showed a decrease in the 370 nm band but no formation of any long absorbing species above 400 nm. Even with 9 eq. of TFA (5.19 mM) no formation of any long absorbing species was observed.

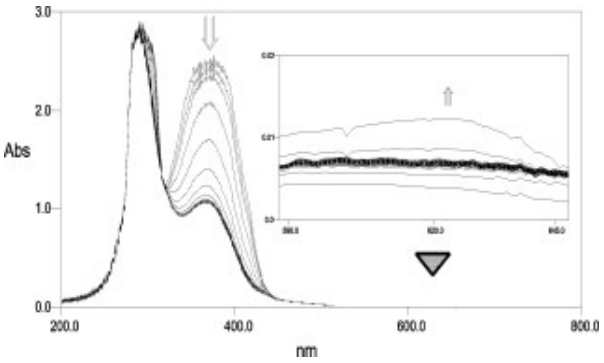


Figure S3: UV-Vis changes observed during the photolysis of **8** (568 µM) in presence of both ferrocene (567.9 µM) and TFA (5.19 mM). The overall UV-vis spectrum is an overlay of measurements made at every second over a period of 90 s.

Product Analysis after Steady State Photolysis

Preparative scale photolysis was carried out for **7** and **8** in dry benzene. The photolysis products were purified by column chromatography with hexane and ethyl acetate as eluent. Alkyl-2-pyridylsulfides **18** (20% ethyl acetate in hexane, R_f = 0.35) and **19** (10% ethyl acetate in hexane, R_f = 0.72) were obtained. A substantial amount of **6** was also obtained as a by-product when photolysis was carried out at high concentrations of the Barton ester due to the involvement of radical **5** in the radical chain propagation step.

Photolysis of Barton ester **7** (1.57 mM) was carried out both in the absence and in the presence of an equimolar amount of TFA (1.57 mM) and the products were analyzed by HPLC. The chromatograms typically had four peaks at 4.78, 5.24 (**18**), 7.26 and 9.25 min (**6**) (both in acid and in absence of acid). Interestingly, the peak area for **6** remained more or less unchanged in both the experiments. Based on calibration curves the overall conversion of **7**→**18** in the absence of acid was calculated as 89% and as 59% in the presence of TFA.

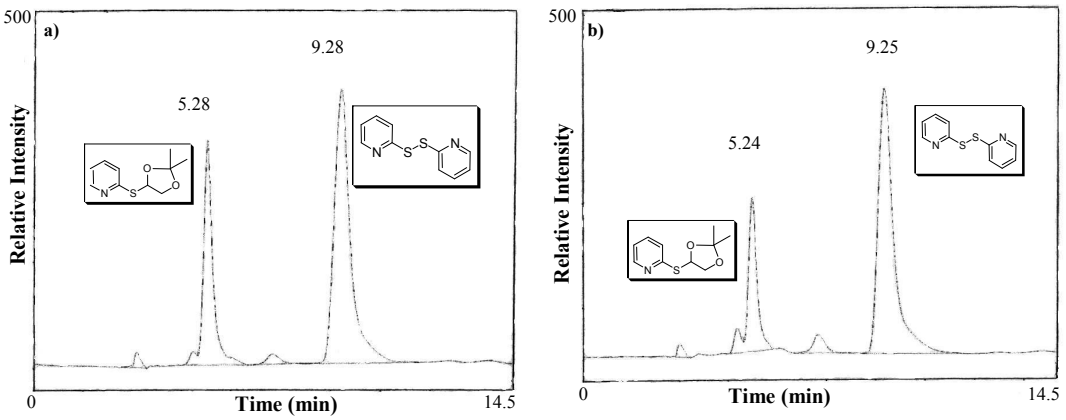


Figure S4: HPLC chromatograms after photolysis of **7** (1.57 mM) for 15 min: a) without TFA, b) with TFA (1.57 mM).

Time resolved EPR

The time resolved EPR spectrum of **3** was observed upon photolysis (308 nm, XeCl excimer laser) of **7** in benzene. The EPR results show equivalence of the β-protons due to fast torsional oscillations. For **3** the literature reported g value is 2.0032.[5] The spectrum shows a doublet and a triplet, as expected for **3**. The g value is found to be 2.0035, which is in close agreement to the reported value, with a coupling constant of 11.2 G (d) and 27.2 G (t).

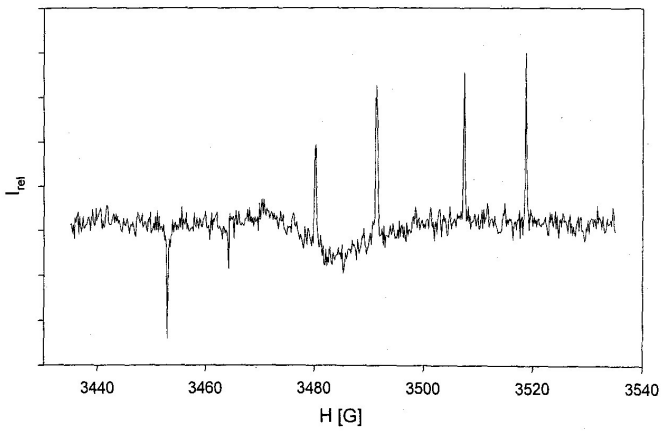


Figure S5: Time resolved EPR spectrum of **3** obtained by photolysis of **7** in benzene.

Laser flash photolysis

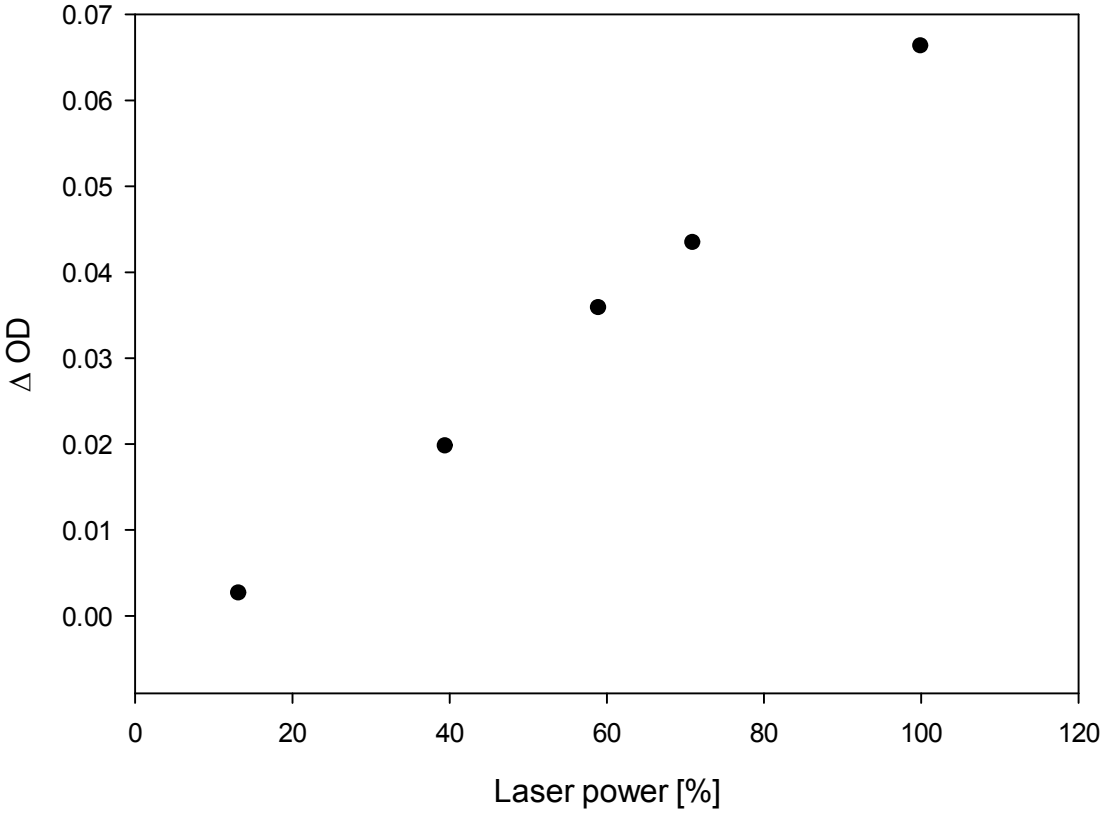


Figure S6: Plot of transient intensity @500 nm vs laser power (100% = 90 mJ / pulse), for the short-lived transient **C** observed after LFP (355 nm) of **7** in benzene.

Computations on stationary points

Calculated geometries of stationary points:

Dioxolanyl radical 3, optimized geometry (M06-2X/cc-pVQZ):

6	-0.574591000	0.002279000	0.013988000
8	0.282239000	0.096356000	1.130641000
6	1.609152000	0.223675000	0.642911000
6	1.507011000	-0.305841000	-0.757933000
8	0.213608000	-0.646531000	-0.991330000
1	1.936136000	1.268451000	0.676484000
1	2.270843000	-0.360338000	1.284106000
1	2.244810000	-0.909746000	-1.259342000
6	-0.977843000	1.380853000	-0.482183000
1	-1.539624000	1.899372000	0.291356000
1	-1.592535000	1.292554000	-1.375121000
1	-0.090755000	1.962637000	-0.727648000
6	-1.747096000	-0.879746000	0.359663000
1	-2.325069000	-0.421032000	1.158518000
1	-1.385424000	-1.849563000	0.690090000
1	-2.384962000	-1.008250000	-0.511603000

E(M06-2X): -346.3343515

E(CCSD(T)/cc-pVTZ//M06-2X/cc-pVQZ): -345.7716978

Dioxolanyl radical 3, optimized geometry (M06-2X/cc-pVQZ, polarizable continuum model, benzene):

6	-0.575695000	0.002652000	0.014103000
8	0.281833000	0.120980000	1.129019000
6	1.608865000	0.244826000	0.635236000
6	1.508790000	-0.330876000	-0.747104000
8	0.213870000	-0.676785000	-0.972060000
1	1.925193000	1.292977000	0.633972000
1	2.276899000	-0.312248000	1.292696000
1	2.246870000	-0.953346000	-1.225055000
6	-0.971286000	1.369223000	-0.518848000
1	-1.537238000	1.907820000	0.237717000
1	-1.581928000	1.259805000	-1.412198000
1	-0.081840000	1.943542000	-0.773270000
6	-1.752956000	-0.864410000	0.379819000
1	-2.331452000	-0.381370000	1.163824000
1	-1.398542000	-1.827748000	0.736593000
1	-2.389883000	-1.011487000	-0.489192000

E(M06-2X): -346.3362931

Transition state 3 → 20, optimized geometry (M06-2X/cc-pVQZ):

6	0.764043000	0.095505000	-0.154879000
8	-0.145073000	0.404041000	-1.077905000
6	-1.496614000	0.626415000	-0.529771000
6	-1.649328000	-0.556321000	0.350525000
8	-0.678257000	-0.747932000	1.104990000
1	-1.493965000	1.572821000	0.013633000
1	-2.175210000	0.671678000	-1.374031000
1	-2.386602000	-1.334832000	0.141434000
6	1.227786000	1.145052000	0.792471000
1	2.026490000	1.737964000	0.338699000
1	1.613730000	0.683134000	1.698264000
1	0.418349000	1.817016000	1.066155000
6	1.647810000	-1.043688000	-0.506982000
1	2.381582000	-0.747925000	-1.263389000
1	1.052619000	-1.857657000	-0.915975000
1	2.187468000	-1.392843000	0.370348000

E(M06-2X): -346.2956589

E(CCSD(T)/cc-pVTZ//M06-2X/cc-pVQZ): -345.7334140

Transition state 3 → 20, optimized geometry (M06-2X/cc-pVQZ, polarizable continuum model, benzene):

6	0.765790000	0.094799000	-0.153548000
8	-0.142700000	0.398879000	-1.077026000
6	-1.496159000	0.630325000	-0.528944000
6	-1.654991000	-0.554658000	0.345065000
8	-0.684739000	-0.753607000	1.103667000
1	-1.485875000	1.575015000	0.016268000
1	-2.173407000	0.681590000	-1.373526000
1	-2.391828000	-1.330607000	0.127585000
6	1.225284000	1.146097000	0.793654000
1	2.021350000	1.739403000	0.335942000
1	1.617714000	0.686828000	1.697913000
1	0.415217000	1.816935000	1.067576000
6	1.654607000	-1.041045000	-0.503768000
1	2.387542000	-0.739834000	-1.258638000
1	1.064906000	-1.858165000	-0.914436000
1	2.196701000	-1.386445000	0.373439000

E(M06-2X): -346.2982552

Radical 20, optimized geometry (M06-2X/cc-pVQZ):

6	-2.004921000	0.040699000	-0.136116000
1	-2.992343000	0.458456000	0.147554000
8	-1.745959000	-0.227440000	-1.270234000
6	-1.064633000	-0.135084000	1.033842000
1	-1.550986000	-0.802979000	1.747822000
1	-0.972492000	0.839348000	1.529995000
8	0.167395000	-0.696330000	0.715457000
6	1.009163000	0.013175000	-0.113766000
6	2.257448000	-0.744111000	-0.378237000
1	2.025226000	-1.773027000	-0.646896000
1	2.912188000	-0.773107000	0.502557000
1	2.815193000	-0.287576000	-1.192779000
6	1.018367000	1.498485000	-0.015485000
1	1.745344000	1.897917000	-0.717949000
1	1.301012000	1.848280000	0.987241000
1	0.052820000	1.943874000	-0.260764000

E(M06-2X): -346.3160194

E(CCSD(T)/cc-pVTZ//M06-2X/cc-pVQZ): -345.7532995

Radical 20, optimized geometry (M06-2X/cc-pVQZ, polarizable continuum model, benzene):

6	-2.011616000	0.037192000	-0.133215000
1	-2.987813000	0.502165000	0.103543000
8	-1.769069000	-0.376734000	-1.229109000
6	-1.061938000	-0.009740000	1.038790000
1	-1.547725000	-0.586143000	1.828457000
1	-0.955697000	1.013065000	1.418737000
8	0.163327000	-0.617227000	0.773136000
6	1.012954000	-0.001328000	-0.121518000
6	2.259980000	-0.787361000	-0.297181000
1	2.027775000	-1.838073000	-0.462292000
1	2.906271000	-0.727544000	0.588296000
1	2.827343000	-0.417018000	-1.147940000
6	1.035944000	1.486720000	-0.171341000
1	1.765721000	1.807256000	-0.910367000

1	1.323821000	1.929135000	0.792276000
1	0.074289000	1.915944000	-0.456134000

E(M06-2X): -346.3196703

Transition state 20 → 2 + 22 (M06-2X/cc-pVQZ):

6	-1.788068000	0.459650000	0.032874000
1	-2.509017000	0.994282000	-0.603531000
8	-1.193851000	1.032142000	0.932571000
6	-1.440038000	-0.901799000	-0.332811000
1	-1.968278000	-1.355123000	-1.158454000
1	-1.217788000	-1.566708000	0.491696000
8	0.117673000	-0.669380000	-1.007214000
6	0.997694000	-0.177090000	-0.226671000
6	1.372396000	-0.886854000	1.030002000
1	1.272110000	-1.964042000	0.914855000
1	2.393684000	-0.648696000	1.319973000
6	1.619864000	1.137534000	-0.553802000
1	1.064954000	1.625759000	-1.349349000
1	2.654282000	0.999787000	-0.878905000
1	1.637514000	1.780538000	0.327033000
1	0.710875000	-0.556538000	1.836277000

E(M06-2X): -346.2959304

E(CCSD(T)/cc-pVTZ//M06-2X/cc-pVQZ): -345.7322772

Transition state 20 → 2 + 22 (M06-2X/cc-pVQZ, polarizable continuum model, benzene):

6	-1.802524000	0.445734000	0.022843000
1	-2.517668000	0.973331000	-0.624379000
8	-1.236551000	1.022879000	0.941621000
6	-1.424928000	-0.905275000	-0.346939000
1	-1.943583000	-1.362768000	-1.176229000
1	-1.195772000	-1.571281000	0.474858000
8	0.123191000	-0.638280000	-1.013686000
6	1.004937000	-0.165982000	-0.220361000
6	1.372403000	-0.902835000	1.021840000
1	1.276621000	-1.977530000	0.882378000
1	2.390213000	-0.666427000	1.324126000
6	1.641990000	1.145009000	-0.530044000
1	1.073816000	1.667207000	-1.294260000
1	2.662207000	0.994663000	-0.892611000
1	1.705461000	1.762165000	0.366693000
1	0.704320000	-0.596059000	1.831912000

E(M06-2X): -346.2990042

Transition state 3 → 21, optimized geometry (M06-2X/cc-pVQZ):

6	-0.615665000	0.048571000	0.084889000
8	0.037452000	0.209774000	1.261429000
6	1.949448000	0.423832000	0.327626000
6	1.527105000	-0.612322000	-0.455879000
8	0.276095000	-0.776426000	-0.803332000
1	1.512485000	1.405625000	0.299787000
1	2.901044000	0.329916000	0.830370000
1	2.179429000	-1.422202000	-0.759110000
6	-0.937810000	1.329654000	-0.677159000
1	-1.569735000	1.955112000	-0.050414000
1	-1.467922000	1.100298000	-1.599372000
1	-0.040606000	1.887804000	-0.930995000
6	-1.852140000	-0.806044000	0.299569000
1	-2.562848000	-0.257852000	0.913828000

1	-1.569476000	-1.721072000	0.811912000
1	-2.316372000	-1.046552000	-0.655056000

E(M06-2X): -346.2818005

E(CCSD(T)/cc-pVTZ//M06-2X/cc-pVQZ): -345.7198528

Transition state 3 → 21, optimized geometry (M06-2X/cc-pVQZ, polarizable continuum model, benzene):

6	-0.618622000	0.049812000	0.086130000
8	0.024850000	0.210534000	1.268683000
6	1.961700000	0.422925000	0.322379000
6	1.528937000	-0.616699000	-0.450595000
8	0.276228000	-0.786324000	-0.787901000
1	1.516766000	1.401281000	0.304307000
1	2.922074000	0.331995000	0.808725000
1	2.181604000	-1.422849000	-0.762771000
6	-0.925383000	1.329916000	-0.683324000
1	-1.563232000	1.959380000	-0.066569000
1	-1.446846000	1.099208000	-1.610050000
1	-0.023916000	1.884583000	-0.928797000
6	-1.863712000	-0.795835000	0.288947000
1	-2.577454000	-0.241589000	0.894176000
1	-1.595062000	-1.713858000	0.803874000
1	-2.320067000	-1.032542000	-0.670369000

E(M06-2X): -346.2849989

Radical 21, optimized geometry (M06-2X/cc-pVQZ):

1	1.742927000	1.137065000	0.831101000
6	2.243396000	0.357116000	0.279823000
1	3.318649000	0.394550000	0.211958000
6	1.618226000	-0.660633000	-0.294598000
1	2.170911000	-1.439109000	-0.802786000
8	0.291488000	-0.931468000	-0.359450000
6	-0.655035000	0.047398000	0.066031000
6	-2.002685000	-0.694806000	0.088531000
1	-2.156593000	-1.130927000	-0.894915000
1	-2.801987000	0.000784000	0.322335000
1	-1.966984000	-1.486126000	0.831487000
6	-0.690314000	1.219990000	-0.923770000
1	-0.935470000	0.831924000	-1.909271000
1	0.275789000	1.712629000	-0.966366000
1	-1.446582000	1.933384000	-0.610076000
8	-0.451762000	0.485397000	1.320754000

E(M06-2X): -346.3038954

E(CCSD(T)/cc-pVTZ//M06-2X/cc-pVQZ): -345.7415363

Radical 21, optimized geometry (M06-2X/cc-pVQZ, polarizable continuum model, benzene):

1	1.741620000	1.145269000	0.818833000
6	2.243604000	0.358933000	0.277830000
1	3.319436000	0.394035000	0.215582000
6	1.619860000	-0.660062000	-0.296933000
1	2.174614000	-1.440761000	-0.799562000
8	0.292804000	-0.929211000	-0.367325000
6	-0.655080000	0.047161000	0.066385000
6	-2.004863000	-0.693474000	0.079473000
1	-2.159267000	-1.113053000	-0.911069000
1	-2.802343000	0.000908000	0.322120000
1	-1.971922000	-1.495715000	0.810729000
6	-0.690775000	1.230501000	-0.910057000
1	-0.931922000	0.852219000	-1.900212000
1	0.272284000	1.729426000	-0.943996000

```
1       -1.452223000      1.936027000     -0.591329000
8       -0.451149000      0.465872000      1.327165000
```

E(M06-2X): -346.306014

Transition state 21 → 2 + 22, optimized geometry (M06-2X / cc-pVQZ):

```
1        1.774629000      1.469119000      0.000000000
6        2.296792000      0.533383000      0.000000000
1        3.375987000      0.513755000      0.000001000
6        1.665394000     -0.692078000     -0.000001000
1        2.295030000     -1.581572000     -0.000002000
8        0.415090000     -0.964928000     -0.000002000
6       -0.754540000      0.228930000      0.000000000
6       -1.486397000     -0.205015000      1.283258000
1       -1.749165000     -1.257704000      1.258052000
1       -2.386976000      0.401887000      1.345942000
1       -0.854450000      0.007064000      2.140768000
6       -1.486399000     -0.205012000     -1.283257000
1       -1.749167000     -1.257701000     -1.258054000
1       -0.854454000      0.007069000     -2.140767000
1       -2.386979000      0.401890000     -1.345938000
8       -0.274284000      1.381797000      0.000001000
```

E(M06-2X): -346.2827097

E(CCSD(T)/cc-pVTZ//M06-2X/cc-pVQZ): -345.7200203

Transition state 21 → 2 + 22, optimized geometry (M06-2X / cc-pVQZ, polarizable continuum model, benzene):

```
1        1.791472000      1.463645000     -0.000324000
6        2.303855000      0.522864000     -0.000231000
1        3.382525000      0.490467000     -0.000293000
6        1.658425000     -0.695540000     -0.000027000
1        2.274592000     -1.592989000      0.000050000
8        0.403283000     -0.954329000      0.000092000
6       -0.743757000      0.221669000      0.000022000
6       -1.488698000     -0.200700000      1.281015000
1       -1.765137000     -1.250054000      1.256501000
1       -2.382639000      0.416126000      1.338376000
1       -0.858553000      0.003717000      2.142046000
6       -1.488902000     -0.201048000     -1.280737000
1       -1.765334000     -1.250396000     -1.255897000
1       -0.858896000      0.003141000     -2.141923000
1       -2.382855000      0.415761000     -1.338120000
8       -0.263373000      1.381468000     -0.000175000
```

E(M06-2X): -346.2857094

Acetone 2, optimized geometry (M06-2X/cc-pVQZ):

```
6        0.000000000      0.000000000      0.186637000
8        0.000000000      0.000000000      1.389338000
6        0.000000000      1.282798000     -0.610224000
1       -0.875756000      1.317296000     -1.258325000
1        0.876864000      1.318058000     -1.256796000
1       -0.000895000      2.136352000      0.059203000
6        0.000000000     -1.282798000     -0.610224000
1        0.000895000     -2.136352000      0.059203000
1        0.875756000     -1.317296000     -1.258325000
1       -0.876864000     -1.318058000     -1.256796000
```

E(M06-2X): -193.1502932

E(CCSD(T)/cc-pVTZ//M06-2X/cc-pVQZ): -192.8362077

Acetone 2, optimized geometry (M06-2X/cc-pVQZ, polarizable continuum model, benzene):

6	0.000000000	0.000000000	0.185097000
8	0.000000000	0.000000000	1.390878000
6	0.000000000	1.281076000	-0.610114000
1	-0.822442000	1.279476000	-1.324740000
1	0.923170000	1.348463000	-1.186226000
1	-0.081283000	2.135853000	0.052849000
6	0.000000000	-1.281076000	-0.610114000
1	0.081283000	-2.135853000	0.052849000
1	0.822442000	-1.279476000	-1.324740000
1	-0.923170000	-1.348463000	-1.186226000

E(M06-2X): -193.1532946

Vinyloxy radical 22, optimized geometry (M06-2X/cc-pVQZ):

1	0.791286000	-1.587072000	0.000000000
6	1.047636000	-0.538891000	0.000000000
1	2.083916000	-0.239571000	0.000000000
6	0.000000000	0.429059000	0.000000000
1	0.300916000	1.488268000	0.000000000
8	-1.182742000	0.124670000	0.000000000

E(M06-2X): -153.1688471

E(CCSD(T)/cc-pVTZ//M06-2X/cc-pVQZ): -152.9242974

Vinyloxy radical 22, optimized geometry (M06-2X/cc-pVQZ, polarizable continuum model, benzene):

1	0.800752000	-1.584911000	0.000000000
6	1.049909000	-0.534948000	0.000000000
1	2.083945000	-0.228904000	0.000000000
6	0.000000000	0.428351000	0.000000000
1	0.295846000	1.487559000	0.000000000
8	-1.185000000	0.120730000	0.000000000

E(M06-2X): -153.1718991

Complex of vinyloxy radical 22 and benzene, optimized geometry (M06-2X/cc-pVTZ):

6	-3.138468000	1.094951000	-0.000224000
1	-2.952694000	2.158447000	-0.000515000
1	-4.153752000	0.726415000	0.000068000
6	-2.061993000	0.157449000	-0.000222000
1	-1.038372000	0.563401000	-0.000517000
8	-2.247477000	-1.053190000	0.000093000
1	1.364049000	-0.059997000	2.469695000
6	1.366354000	-0.061188000	1.387969000
6	1.366568000	-0.062401000	-1.387830000
6	1.775627000	1.071273000	0.693591000
6	0.955875000	-1.191085000	0.694779000
6	0.955981000	-1.191691000	-0.693717000
6	1.775734000	1.070667000	-0.694377000
1	2.095052000	1.951854000	1.234611000
1	0.615805000	-2.065002000	1.232420000
1	0.615992000	-2.066076000	-1.230648000
1	2.095243000	1.950775000	-1.236116000
1	1.364428000	-0.062149000	-2.469556000

E(M06-2X): -385.386763

Complex of vinyloxy radical 22 and diphenylether (M06-2X/cc-pVTZ):

6	3.485710000	2.157388000	-0.265896000
1	4.265718000	1.501033000	-0.620105000

1	3.736509000	3.038070000	0.307090000
6	2.113370000	1.881731000	-0.547587000
1	1.899089000	0.963207000	-1.115933000
8	1.202953000	2.612794000	-0.178665000
1	4.074456000	-1.086792000	1.139056000
6	3.059819000	-1.141439000	0.769874000
6	0.447750000	-1.287058000	-0.167362000
6	2.790563000	-1.723394000	-0.462748000
6	2.011156000	-0.640349000	1.529179000
6	0.703497000	-0.709601000	1.071123000
6	1.489908000	-1.795655000	-0.935021000
1	3.596580000	-2.125324000	-1.061868000
1	2.207842000	-0.188466000	2.492040000
1	-0.109122000	-0.316551000	1.664530000
1	1.257004000	-2.245681000	-1.889846000
8	-0.810027000	-1.446114000	-0.677493000
6	-1.826419000	-0.587597000	-0.313095000
6	-3.977833000	1.043148000	0.291820000
6	-3.061752000	-1.156285000	-0.047238000
6	-1.649290000	0.788737000	-0.285543000
6	-2.732939000	1.597013000	0.023652000
6	-4.138631000	-0.334380000	0.251202000
1	-3.161400000	-2.231930000	-0.085017000
1	-0.681775000	1.229526000	-0.489135000
1	-2.595920000	2.669443000	0.049351000
1	-5.104567000	-0.775303000	0.456450000
1	-4.817271000	1.681779000	0.528491000

E(M06-2X): -691.6462595

Carbonyloxy radical 4, optimized geometry (M06-2X/cc-pVQZ):

6	-0.573734000	0.006114000	0.012400000
8	0.286223000	0.236103000	1.105227000
6	1.604477000	0.330890000	0.593740000
6	1.532819000	-0.552558000	-0.608521000
8	0.228207000	-0.674889000	-0.967326000
1	1.854515000	1.373702000	0.351606000
1	2.298745000	-0.018147000	1.356015000
1	2.254637000	-0.604565000	-1.407483000
6	-1.051063000	1.314475000	-0.593117000
1	-1.647451000	1.860188000	0.134908000
1	-1.652924000	1.119452000	-1.477965000
1	-0.198048000	1.926326000	-0.881798000
6	-1.698161000	-0.898087000	0.452000000
1	-2.279119000	-0.406962000	1.229429000
1	-1.283889000	-1.823109000	0.844139000
1	-2.347927000	-1.121597000	-0.391081000

E(M06-2X): -346.3338106

Carbonyloxy radical 4, optimized geometry (M06-2X/cc-pVQZ, polarizable continuum model, benzene):

6	-1.347935000	0.161587000	-0.041033000
8	-0.769743000	-0.615514000	-1.072008000
6	0.143434000	-1.499553000	-0.462186000
6	0.723945000	-0.620246000	0.643531000
8	-0.336356000	0.236009000	0.983521000
1	-0.357576000	-2.368510000	-0.031901000
1	0.879055000	-1.821696000	-1.192321000
1	1.058465000	-1.188487000	1.510526000
6	-2.574666000	-0.514813000	0.541166000
1	-3.356483000	-0.571413000	-0.212834000
1	-2.940440000	0.056635000	1.391056000
1	-2.333540000	-1.520472000	0.879514000
6	-1.629989000	1.544666000	-0.575235000
1	-2.359952000	1.486713000	-1.379443000
1	-0.711413000	1.984878000	-0.954989000
1	-2.028143000	2.171563000	0.219089000
6	1.919087000	0.166449000	0.131577000
8	2.956983000	-0.301550000	-0.250927000
8	1.742463000	1.473836000	0.132463000

E(M06-2X): -534.9049057

Transition state for decarboxylation of 4, optimized geometry (M06-2X/cc-pVQZ):

6	-1.364651000	0.147303000	-0.040958000
8	-0.761803000	-0.621185000	-1.064415000
6	0.185716000	-1.463394000	-0.452788000
6	0.716478000	-0.562725000	0.657174000
8	-0.386418000	0.201320000	1.016191000
1	-0.280321000	-2.350908000	-0.015219000
1	0.936039000	-1.759202000	-1.178011000
1	1.112300000	-1.096990000	1.520162000
6	-2.607657000	-0.531960000	0.499657000
1	-3.372782000	-0.569244000	-0.272427000
1	-2.988468000	0.022263000	1.354379000
1	-2.376745000	-1.545920000	0.820092000
6	-1.626794000	1.537407000	-0.568890000
1	-2.318424000	1.486374000	-1.406891000
1	-0.694367000	1.985724000	-0.901578000
1	-2.062312000	2.153185000	0.214538000
6	1.965843000	0.219712000	0.108538000
8	2.949937000	-0.371786000	-0.238465000
8	1.752217000	1.491233000	0.117759000

E(M06-2X): -534.8998848

Transition state for decarboxylation of 4, optimized geometry (M06-2X/cc-pVQZ, polarizable continuum model, benzene):

6	-1.368985000	0.145540000	-0.033547000
8	-0.762004000	-0.588994000	-1.079927000
6	0.186321000	-1.447645000	-0.490589000
6	0.720363000	-0.574461000	0.640455000
8	-0.378183000	0.189558000	1.014793000
1	-0.278817000	-2.344103000	-0.072666000
1	0.932347000	-1.728684000	-1.226063000
1	1.114137000	-1.130985000	1.490103000
6	-2.596201000	-0.565051000	0.501987000
1	-3.367252000	-0.595943000	-0.264453000
1	-2.978881000	-0.034443000	1.370746000
1	-2.348373000	-1.582203000	0.798613000
6	-1.656240000	1.543972000	-0.523776000
1	-2.360341000	1.504545000	-1.351919000
1	-0.734918000	2.013017000	-0.859211000
1	-2.088966000	2.134364000	0.280392000
6	1.968938000	0.218655000	0.114688000

8	2.979083000	-0.356236000	-0.190189000
8	1.734339000	1.485470000	0.077716000

E(M06-2X): -534.9035696

Complex of thiyl radical 5 and benzene, optimized geometry (M06-2X/cc-pVTZ):

1	-2.229031000	-1.547712000	-2.075537000
6	-2.052978000	-0.932555000	-1.201880000
7	-1.595616000	0.654909000	1.049671000
6	-1.249954000	0.193447000	-1.284746000
6	-2.617715000	-1.252378000	0.019062000
6	-2.357123000	-0.423332000	1.111883000
6	-1.041241000	0.967135000	-0.135514000
1	-0.778507000	0.486564000	-2.212676000
1	-3.251281000	-2.121503000	0.137997000
1	-2.790590000	-0.648849000	2.081089000
16	-0.038406000	2.380035000	-0.224392000
1	3.240557000	1.196040000	-0.499321000
6	2.624889000	0.355024000	-0.204322000
6	1.030396000	-1.790660000	0.550579000
6	2.293132000	-0.623514000	-1.133672000
6	2.160878000	0.259038000	1.102566000
6	1.362504000	-0.813956000	1.478996000
6	1.497637000	-1.696323000	-0.755539000
1	2.653015000	-0.546597000	-2.152404000
1	2.411846000	1.026469000	1.824255000
1	0.988736000	-0.879362000	2.493234000
1	1.234941000	-2.457896000	-1.480194000
1	0.401580000	-2.623627000	0.841662000

E(M06-2X): -878.0533031

Radical 23, optimized geometry (M06-2X/6-311++G(2df,p), polarizable continuum model, benzene)

1	5.534225000	-2.913563000	0.449973000
6	4.545636000	-2.481322000	0.359382000
7	2.055533000	-1.384080000	0.115008000
6	4.391261000	-1.210364000	-0.169855000
6	3.428281000	-3.185197000	0.783659000
6	2.182782000	-2.593630000	0.640859000
6	3.106580000	-0.683481000	-0.283063000
1	5.240091000	-0.619071000	-0.484881000
1	3.511377000	-4.173905000	1.213346000
1	1.262350000	-3.075843000	0.945896000
16	2.856669000	0.931068000	-0.968878000
8	0.288260000	-1.040646000	-1.019195000
6	-0.702958000	-1.252357000	-0.222186000
8	-0.688542000	-1.590294000	0.939782000
6	-2.044438000	-1.045425000	-0.976987000
6	-2.952881000	-2.281709000	-0.851164000
1	-2.991017000	-2.874031000	-1.762634000
1	-2.639130000	-2.905455000	-0.010193000
1	-1.854511000	-0.775669000	-2.016458000
6	2.022902000	1.757937000	0.448065000
1	2.574528000	1.462175000	1.339403000
6	2.047374000	3.279980000	0.178944000
1	2.298127000	3.497764000	-0.865154000
1	2.746906000	3.802992000	0.828263000
8	0.680068000	1.452637000	0.634357000
8	0.736919000	3.688922000	0.485769000
6	-0.109962000	2.576625000	0.248361000
6	-1.303129000	2.659917000	1.166105000
1	-1.909475000	3.527025000	0.902350000
1	-0.961795000	2.755268000	2.195986000
1	-1.901127000	1.755843000	1.055024000
6	-0.495093000	2.476304000	-1.218997000
1	-1.037589000	3.374460000	-1.516174000

1	-1.138241000	1.608537000	-1.363087000
1	0.386545000	2.363464000	-1.850820000
8	-2.781684000	-0.013987000	-0.359596000
8	-4.226477000	-1.715926000	-0.624689000
6	-4.018703000	-0.541738000	0.131755000
6	-3.897384000	-0.846976000	1.615490000
1	-3.064778000	-1.525268000	1.798138000
1	-4.826037000	-1.289935000	1.977228000
1	-3.705994000	0.076277000	2.163838000
6	-5.120670000	0.442469000	-0.181449000
1	-5.162300000	0.613856000	-1.256164000
1	-4.925717000	1.386339000	0.327995000
1	-6.077813000	0.048352000	0.160180000

E(M06-2X): -1527.0782942

Radical 24, optimized geometry (M06-2X/6-311++G(2df,p), polarizable continuum model, benzene)

1	3.970247000	-3.277289000	-0.153668000
6	3.060716000	-2.691142000	-0.110946000
7	0.767320000	-1.200654000	-0.017059000
6	3.048329000	-1.392239000	-0.592795000
6	1.903342000	-3.225272000	0.434599000
6	0.763408000	-2.436366000	0.463113000
6	1.863037000	-0.660459000	-0.534701000
1	3.935390000	-0.930984000	-1.004715000
1	1.874780000	-4.231653000	0.829255000
1	-0.177277000	-2.778518000	0.876186000
16	1.817082000	0.993975000	-1.175037000
6	1.598080000	2.016285000	0.360482000
6	2.635925000	1.625464000	1.404810000
1	3.647763000	1.700968000	1.003183000
1	2.475888000	0.606657000	1.762904000
1	2.551420000	2.297539000	2.263238000
6	1.843018000	3.442441000	-0.130584000
1	2.854535000	3.559399000	-0.522452000
1	1.713804000	4.132770000	0.706230000
1	1.130975000	3.718209000	-0.910965000
6	0.187893000	1.884665000	0.922413000
1	-0.008134000	0.876230000	1.286872000
1	-0.555381000	2.127100000	0.161090000
1	0.073943000	2.580701000	1.759190000
8	-1.132211000	-0.471622000	-0.761928000
6	-1.974013000	-0.551515000	0.215366000
8	-1.773185000	-1.011210000	1.321855000
6	-3.363713000	0.027215000	-0.170658000
6	-4.349472000	-1.143419000	-0.123016000
1	-5.357760000	-0.777238000	-0.330711000
1	-4.341931000	-1.612590000	0.860843000
1	-4.100176000	-1.897190000	-0.873024000
6	-3.719106000	1.058933000	0.902968000
1	-4.717167000	1.456893000	0.704274000
1	-3.012856000	1.892293000	0.897465000
1	-3.709037000	0.603522000	1.892530000
6	-3.377594000	0.676538000	-1.552453000
1	-4.374858000	1.076149000	-1.751008000
1	-3.134083000	-0.042901000	-2.334791000
1	-2.660575000	1.496804000	-1.612926000

E(M06-2X): -1149.9900933

Radical 24, complex with benzene, optimized geometry (M06-2X/6-311++G(2df,p), polarizable continuum model, benzene)

1	-2.986546000	0.917152000	3.039658000
6	-2.141815000	0.581518000	2.456282000
7	0.030794000	-0.276932000	0.940075000
6	-1.130436000	1.464042000	2.090089000

6	-2.020334000	-0.769177000	2.056884000
6	-0.945302000	-1.180400000	1.345148000
6	-0.035687000	1.065114000	1.353949000
1	-1.180379000	2.509798000	2.366472000
1	-2.786185000	-1.494410000	2.296658000
1	-0.796113000	-2.191885000	0.996293000
16	1.233449000	2.165765000	0.860151000
6	0.686723000	2.757426000	-0.818215000
6	-0.654773000	3.468860000	-0.711094000
1	-0.590669000	4.325002000	-0.037368000
1	-1.429526000	2.795448000	-0.339923000
1	-0.959565000	3.826430000	-1.699174000
6	1.782583000	3.733186000	-1.237767000
1	1.856633000	4.569882000	-0.540514000
1	1.549583000	4.131952000	-2.228249000
1	2.753022000	3.235349000	-1.289550000
6	0.609023000	1.585298000	-1.786906000
1	-0.097837000	0.829846000	-1.442264000
1	1.582764000	1.104517000	-1.898407000
1	0.285443000	1.941657000	-2.770143000
8	1.342943000	-0.814991000	0.998992000
6	1.740779000	-1.417399000	-0.156932000
8	1.002348000	-1.618925000	-1.074764000
6	3.214857000	-1.781058000	-0.081756000
6	3.465810000	-2.656974000	1.152569000
1	4.518968000	-2.943354000	1.175769000
1	2.866597000	-3.569200000	1.116042000
1	3.231769000	-2.123345000	2.073160000
6	3.590920000	-2.535500000	-1.353367000
1	4.651405000	-2.791089000	-1.319601000
1	3.406342000	-1.926731000	-2.238957000
1	3.013901000	-3.455891000	-1.450945000
6	4.022370000	-0.479580000	0.025343000
1	5.086374000	-0.723226000	0.052997000
1	3.761820000	0.075194000	0.926155000
1	3.841563000	0.166639000	-0.836728000
1	-4.381486000	-3.269353000	-0.365046000
6	-3.957221000	-2.310980000	-0.639810000
6	-2.874693000	0.145046000	-1.350471000
6	-2.782392000	-2.257093000	-1.378585000
6	-4.588474000	-1.135522000	-0.251268000
6	-4.046486000	0.092687000	-0.606275000
6	-2.238989000	-1.028672000	-1.733040000
1	-2.283801000	-3.172159000	-1.675103000
1	-5.502702000	-1.177439000	0.328628000
1	-4.535736000	1.009897000	-0.300985000
1	-1.311594000	-0.991522000	-2.290849000
1	-2.455886000	1.103520000	-1.633460000

E(M06-2X): -1382.1878021

TS for N-O cleavage of radical 24, complex with benzene, optimized geometry (M06-2X/6-311++G(2df,p), polarizable continuum model, benzene)

1	-2.772109000	0.683041000	3.431918000
6	-2.001513000	0.440387000	2.713958000
7	-0.010614000	-0.177391000	0.879138000
6	-1.097555000	1.406464000	2.288793000
6	-1.894646000	-0.848925000	2.176257000
6	-0.904231000	-1.137570000	1.283189000
6	-0.104053000	1.103597000	1.377019000
1	-1.164739000	2.428579000	2.638735000
1	-2.600407000	-1.626249000	2.437447000
1	-0.775587000	-2.104155000	0.817432000
16	1.038103000	2.315747000	0.805255000
6	0.378916000	2.762821000	-0.873391000
6	-1.062080000	3.241395000	-0.755966000
1	-1.131111000	4.113730000	-0.103760000
1	-1.708235000	2.458869000	-0.353938000

1	-1.436858000	3.517773000	-1.746137000
6	1.287242000	3.902147000	-1.330114000
1	1.220385000	4.757905000	-0.656027000
1	0.981114000	4.225228000	-2.328163000
1	2.328585000	3.577863000	-1.381850000
6	0.494347000	1.577547000	-1.824601000
1	-0.078802000	0.719168000	-1.474393000
1	1.534716000	1.263956000	-1.927956000
1	0.121371000	1.866925000	-2.812550000
8	1.456029000	-0.703459000	0.994719000
6	1.848386000	-1.346593000	-0.112521000
8	1.108212000	-1.657351000	-1.007813000
6	3.353340000	-1.611770000	-0.085223000
6	3.751231000	-2.265887000	1.242398000
1	4.822415000	-2.477363000	1.230040000
1	3.220658000	-3.208895000	1.390427000
1	3.536685000	-1.612030000	2.087057000
6	3.713074000	-2.523135000	-1.254380000
1	4.790477000	-2.699770000	-1.256559000
1	3.430373000	-2.071038000	-2.204985000
1	3.203608000	-3.484455000	-1.174390000
6	4.057759000	-0.255219000	-0.231466000
1	5.139147000	-0.408279000	-0.220444000
1	3.787599000	0.417995000	0.582386000
1	3.791773000	0.223070000	-1.176867000
1	-4.154818000	-3.439093000	-0.147646000
6	-3.775775000	-2.496708000	-0.524823000
6	-2.811225000	-0.084019000	-1.501246000
6	-2.654897000	-2.477479000	-1.345657000
6	-4.409458000	-1.307828000	-0.185146000
6	-3.926844000	-0.100458000	-0.673852000
6	-2.168840000	-1.270373000	-1.831154000
1	-2.152998000	-3.402692000	-1.602289000
1	-5.280112000	-1.322373000	0.459528000
1	-4.420482000	0.827556000	-0.410610000
1	-1.281031000	-1.255325000	-2.451106000
1	-2.439944000	0.855960000	-1.891035000

E(M06-2X): -1382.1856539

Radical 27, optimized geometry (M06-2X/6-311++G(2df,p), polarizable continuum model, benzene)

1	-2.763502000	2.971894000	1.109546000
6	-1.886907000	2.428999000	0.779594000
7	0.281406000	1.054265000	-0.047670000
6	-1.476698000	1.321682000	1.467253000
6	-1.185339000	2.857679000	-0.362364000
6	-0.098067000	2.141040000	-0.753248000
6	-0.343001000	0.570751000	1.071949000
1	-2.010613000	0.965459000	2.336512000
1	-1.487070000	3.724177000	-0.931078000
1	0.511641000	2.358669000	-1.617756000
16	0.171799000	-0.837290000	1.837899000
8	1.345658000	0.365138000	-0.552200000
6	2.545657000	0.639780000	0.108522000
8	2.622271000	1.505579000	0.917118000
16	-0.714039000	-2.379342000	-0.244806000
6	-2.128822000	-1.372045000	-0.462061000
6	-4.314721000	0.244470000	-0.798884000
7	-2.109047000	-0.449373000	-1.435462000
6	-3.231781000	-1.515989000	0.392708000
6	-4.331107000	-0.695543000	0.222486000
6	-3.181464000	0.319543000	-1.596842000
1	-3.200532000	-2.266157000	1.171052000
1	-5.191797000	-0.791631000	0.873446000
1	-3.129192000	1.043657000	-2.404652000
1	-5.155040000	0.902101000	-0.978132000

6	3.628019000	-0.286397000	-0.399510000
6	3.252357000	-1.728874000	-0.029648000
1	4.029462000	-2.395954000	-0.407812000
1	2.295270000	-2.013033000	-0.468294000
1	3.184301000	-1.850156000	1.052087000
6	3.729350000	-0.147332000	-1.925654000
1	3.941283000	0.883894000	-2.216436000
1	2.812064000	-0.471990000	-2.416071000
1	4.549620000	-0.774222000	-2.278892000
6	4.942389000	0.114472000	0.263999000
1	5.733071000	-0.554507000	-0.078823000
1	4.869787000	0.041765000	1.349255000
1	5.217945000	1.138767000	0.009342000

E(M06-2X) = -1638.0144734

Transition state for 27 → 28, optimized geometry (M06-2X/6-311++G(2df,p), polarizable continuum model, benzene)

1	3.443838000	-4.297069000	-0.421368000
6	3.069981000	-3.303664000	-0.208661000
7	2.121902000	-0.838056000	0.328189000
6	1.864035000	-2.913089000	-0.713031000
6	3.829530000	-2.426916000	0.591861000
6	3.324629000	-1.191877000	0.839984000
6	1.328126000	-1.621158000	-0.467887000
1	1.265865000	-3.573535000	-1.323862000
1	4.785325000	-2.708908000	1.006172000
1	3.804978000	-0.432475000	1.439209000
16	-0.139841000	-1.072730000	-1.073585000
8	1.691435000	0.421685000	0.640298000
6	1.997614000	1.361129000	-0.352798000
8	2.694045000	1.070985000	-1.269807000
16	-1.299771000	-0.401261000	1.393027000
6	-2.867490000	-0.332454000	0.613853000
6	-5.310265000	-0.190784000	-0.605167000
6	-3.550844000	-1.516272000	0.306701000
7	-3.371579000	0.873200000	0.320326000
6	-4.563206000	0.929311000	-0.264765000
6	-4.784348000	-1.440699000	-0.312954000
1	-3.101152000	-2.466808000	0.558772000
1	-4.941320000	1.923949000	-0.479262000
1	-5.329056000	-2.343339000	-0.561680000
1	-6.272553000	-0.079619000	-1.086763000
6	1.328161000	2.686294000	-0.066334000
6	-0.050134000	2.635359000	-0.750352000
1	-0.528124000	3.609131000	-0.625903000
1	-0.687891000	1.875284000	-0.298061000
1	0.051352000	2.428844000	-1.817057000
6	1.149370000	2.921332000	1.435727000
1	2.105048000	2.891400000	1.963405000
1	0.476914000	2.183432000	1.872639000
1	0.712832000	3.910840000	1.580426000
6	2.188404000	3.784139000	-0.693399000
1	1.697704000	4.746850000	-0.543967000
1	2.315861000	3.618736000	-1.762769000
1	3.176696000	3.825855000	-0.231227000

E(M06-2X) = -1638.0071047

Radical 28, optimized geometry (M06-2X/6-311++G(2df,p), polarizable continuum model, benzene)

1	2.797781000	2.950628000	-1.145941000
6	1.914694000	2.420950000	-0.812257000
7	-0.262210000	1.070074000	0.037894000
6	1.500377000	1.305087000	-1.481370000

6	1.205141000	2.880228000	0.315976000
6	0.113759000	2.177838000	0.716989000
6	0.356068000	0.569808000	-1.082600000
1	2.037724000	0.925403000	-2.338764000
1	1.504883000	3.760784000	0.863819000
1	-0.503179000	2.421700000	1.569606000
16	-0.172518000	-0.833779000	-1.838579000
8	-1.322655000	0.385721000	0.560146000
6	-2.530690000	0.656076000	-0.092863000
8	-2.611741000	1.519866000	-0.902237000
16	0.747528000	-2.450817000	0.087814000
6	2.129208000	-1.420481000	0.398489000
6	4.267380000	0.228644000	0.855871000
6	2.129818000	-0.587283000	1.526321000
7	3.148596000	-1.427931000	-0.471345000
6	4.179286000	-0.622848000	-0.238653000
6	3.214499000	0.238761000	1.758929000
1	1.280173000	-0.606561000	2.196763000
1	4.983571000	-0.659175000	-0.967249000
1	3.235144000	0.884799000	2.628689000
1	5.138160000	0.856308000	0.991749000
6	-3.608513000	-0.270696000	0.422908000
6	-3.250972000	-1.708077000	0.015875000
1	-4.022109000	-2.377803000	0.401472000
1	-2.284167000	-2.007080000	0.422341000
1	-3.212186000	-1.808660000	-1.069339000
6	-3.678737000	-0.161862000	1.953001000
1	-3.869557000	0.865811000	2.269793000
1	-2.758067000	-0.510970000	2.419744000
1	-4.501343000	-0.784018000	2.308919000
6	-4.933664000	0.151893000	-0.205219000
1	-5.721511000	-0.519182000	0.139871000
1	-4.883568000	0.101236000	-1.292862000
1	-5.197371000	1.172392000	0.076120000

E(M06-2X): -1638.0119376

Transition state for 28 → 6 + 9, optimized geometry (M06-2X/6-311++G(2df,p), polarizable continuum model, benzene)

1	-0.330382000	4.564171000	-0.642448000
6	-0.399270000	3.564770000	-0.237416000
7	-0.585939000	0.990343000	0.792786000
6	0.024789000	2.468790000	-0.980232000
6	-0.892356000	3.342450000	1.053096000
6	-0.975768000	2.070346000	1.543755000
6	-0.096170000	1.195960000	-0.467604000
1	0.463219000	2.592604000	-1.962809000
1	-1.192101000	4.166589000	1.686589000
1	-1.334830000	1.830963000	2.535009000
16	0.327528000	-0.202766000	-1.458270000
8	-1.645427000	-0.172520000	0.882903000
6	-2.712672000	-0.004170000	0.083019000
8	-2.925375000	0.992395000	-0.552691000
16	1.239177000	-1.483775000	-0.148693000
6	2.919739000	-0.896427000	-0.011419000
6	5.520519000	-0.261005000	0.411681000
6	3.406807000	0.275548000	-0.579193000
7	3.651483000	-1.715748000	0.730831000
6	4.928138000	-1.399203000	0.935334000
6	4.737641000	0.587169000	-0.357984000
1	2.770957000	0.916673000	-1.172341000
1	5.498134000	-2.091416000	1.545445000
1	5.158250000	1.490002000	-0.783493000
1	6.562768000	-0.047845000	0.605231000
6	-3.584922000	-1.260586000	0.076032000
6	-2.774876000	-2.389074000	-0.576985000
1	-3.384499000	-3.294567000	-0.611113000

1	-1.868238000	-2.601242000	-0.008798000
1	-2.491313000	-2.127319000	-1.598281000
6	-3.952526000	-1.643506000	1.513944000
1	-4.491581000	-0.833720000	2.010451000
1	-3.065005000	-1.880501000	2.099957000
1	-4.601361000	-2.521457000	1.495697000
6	-4.844126000	-0.974010000	-0.736141000
1	-5.469711000	-1.868509000	-0.758690000
1	-4.594853000	-0.694962000	-1.759910000
1	-5.418795000	-0.158286000	-0.295441000

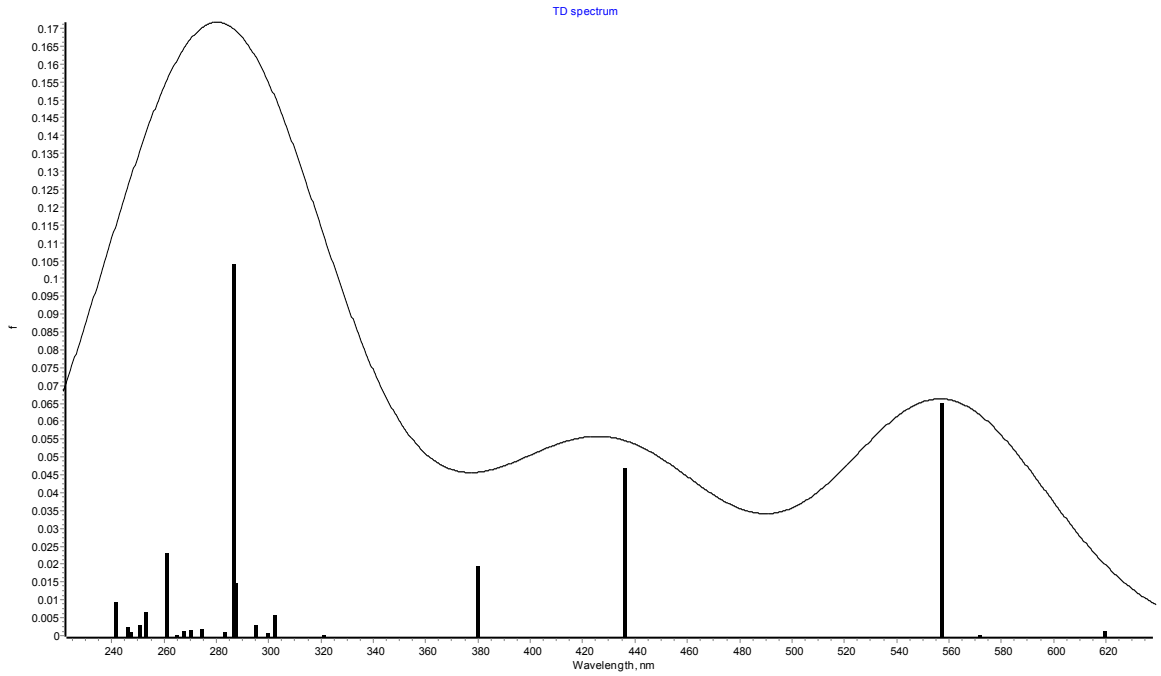
E(M06-2X): -1638.0032196

Di-2-pyridyldisulfide 9, optimized geometry (M06-2X/6-311++G(2df,p), polarizable continuum model, benzene)

1	2.408658000	2.201034000	1.967447000
6	2.571417000	1.476309000	1.179114000
7	2.976072000	-0.374407000	-0.841303000
6	1.584864000	0.555329000	0.874082000
6	3.760903000	1.467292000	0.463535000
6	3.911033000	0.524949000	-0.540693000
6	1.849015000	-0.352789000	-0.144466000
1	0.642187000	0.542985000	1.401541000
1	4.552212000	2.173540000	0.674170000
1	4.819856000	0.482010000	-1.131059000
16	0.720126000	-1.613515000	-0.708209000
16	-0.775854000	-1.653185000	0.665087000
6	-1.880842000	-0.343012000	0.149413000
6	-3.583903000	1.650354000	-0.529000000
7	-1.430817000	0.611573000	-0.642022000
6	-3.178743000	-0.382848000	0.658679000
6	-4.038896000	0.641076000	0.310754000
6	-2.276392000	1.586921000	-0.979458000
1	-3.496761000	-1.198431000	1.295534000
1	-5.056341000	0.646676000	0.681563000
1	-1.878808000	2.351820000	-1.637528000
1	-4.226877000	2.465909000	-0.830194000

E(M06-2X): -1291.7153796

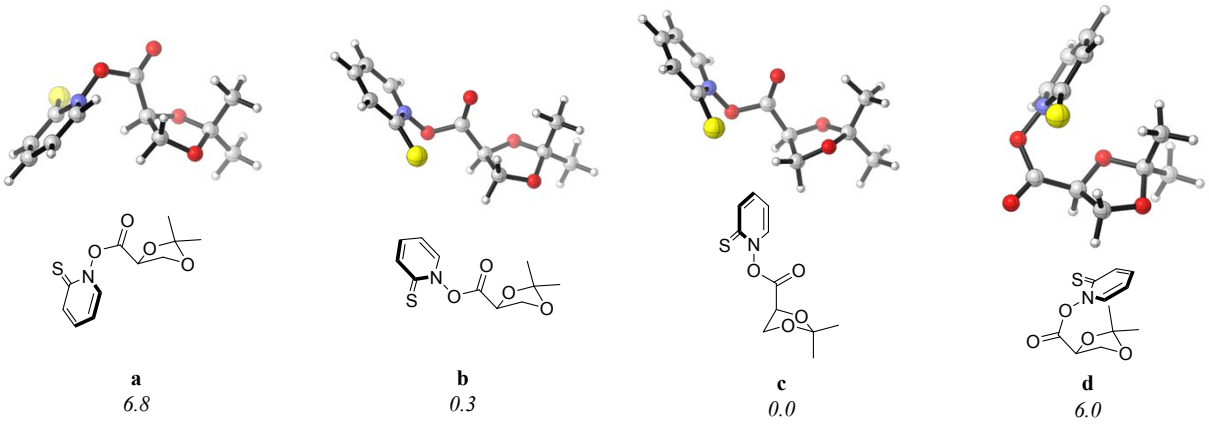
Calculated UV/Vis spectrum of 5 × benzene (TD-B3LYP/6-311++G(2df,p)//M06-2X/cc-pVTZ, polarizable continuum model, benzene):



Trajectory computations

Before performing Born-Oppenheimer molecular dynamics (BOMD) simulations, the conformational space of **4** was investigated. Four conformers were identified, namely **a**, **b**, **c** and **d**. All conformers were optimized at B3LYP-D3(BJ)/6-31G* level of theory.

Chart S1. Four possible ground state conformers of the Barton ester **4**. Numerical values are for relative free energies at 25 °C.



Quasiclassical trajectories (QCTs) were initialized from normal mode sampling of **c** in T1 state, taking the ground state geometry, to approximate a quantum mechanical Boltzmann distribution of the vibrational levels at 298 K. Total 100 trajectories, at UB3LYP-D3(BJ)/6-31G(d) level, were initiated from the sampled structures. Because there are several possibilities of fragmentation, no stopping criteria was used. Trajectories were ran for maximum of 3000 steps (MaxPoints=3000, iop(1/8=2500)). All the computations were done utilizing the Gaussian 09 program package.

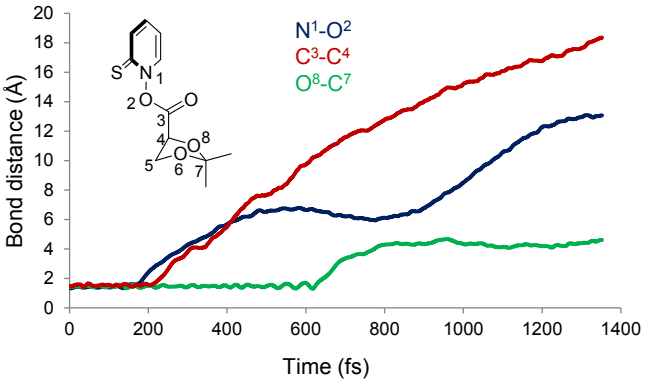
Table S1. Time of the breaking of N-O and C-CO_2 bonds.

Trajectory Number	time (fs) of N-O bond breaking as defined by the bond distance of 1.60 Å	C-CO_2 bond breaking time (fs) as defined by the bond distance of 1.90 Å
1	137	180
2	168	227
3	33	118
4	154	225
5	55	126
6	78	157
7	164	219
8	417	1121
9	23	104
10	249	298
11	336	594
12	141	190
13	92	175
14	227	281
15	225	276
16	110	182
17	226	271
18	286	358
19	143	187

20	217	273
21	275	312
22	370	422
23	217	274
24	172	233
25	164	222
26	175	231
27	787	832
28	236	291
29	139	193
30	50	102
31	281	338
32	228	279
33	214	266
34	64	140
35	263	324
36	233	287
37	168	221
38	142	183
39	140	210
40	25	78
41	150	200
42	459	500
43	91	157
44	42	116
46	151	234
47	221	274
48	159	214
49	93	164
50	205	258
51	41	116
52	218	251
53	212	259
54	132	200
55	284	628
56	281	415
57	162	200
58	145	735
59	230	274
60	175	698
61	129	187
62	171	229
63	182	245
64	201	258
65	565	621
66	171	227
67	213	275
68	175	229
69	102	149
70	335	385
71	217	254
72	150	192
73	227	274
74	185	232
75	197	265
76	258	322
78	141	188
79	118	180
80	351	419
81	72	134
82	147	195
83	143	204
84	333	379
85	184	233
86	266	328
87	119	171
88	223	282
89	390	443
90	148	202

91	406	459
92	218	280
93	190	237
94	119	163
95	89	245
96	111	172
97	224	272
98	217	264
99	181	222
100	90	162

Data for the productive trajectory:



Time (fs)	N^1-O^2 (Å)	C^3-C^4 (Å)	O^6-C^7 (Å)
0.00000	1.354413915	1.495538943	1.431063559
0.501956	1.349482037	1.484812104	1.427115299
1.00485	1.344933864	1.47509568	1.423714673
1.513749	1.340834313	1.466497972	1.420881372
2.031863	1.337273424	1.459175546	1.418652007
2.556776	1.334382716	1.453365107	1.417082543
3.078108	1.332293326	1.4492965	1.416205272
3.583326	1.331060793	1.447027646	1.415986733
4.067642	1.330635306	1.446409194	1.416333971
4.535826	1.330936452	1.447235402	1.417154114
4.997733	1.331916627	1.449363318	1.418393987
5.464399	1.333575192	1.452740944	1.420037673
5.945468	1.33596074	1.457370612	1.422095824
5.945468	1.339132842	1.463233452	1.424574367
6.96885	1.343118687	1.470191617	1.427447192
7.508303	1.347890382	1.477955433	1.430652504
8.059312	1.353356789	1.486129461	1.434089408
8.614641	1.359371458	1.49430062	1.437641572
9.16695	1.365752253	1.502128837	1.441185023
9.711456	1.372331996	1.509419107	1.444619726
10.247224	1.378989392	1.516105045	1.44788696
10.776434	1.385661747	1.522213978	1.45095279
11.302843	1.39231279	1.527806361	1.453803858
11.83023	1.398922143	1.532953159	1.456425637
12.361024	1.405453873	1.537722621	1.458795101
12.89519	1.411847238	1.542170623	1.460881315
12.89519	1.418003977	1.546343297	1.462644558
13.95411	1.423785981	1.550260302	1.464047155
14.460002	1.429066642	1.553926899	1.46507464
14.94179	1.433800239	1.557369481	1.465747557
15.402997	1.438035565	1.560651565	1.46610676
15.852566	1.441862802	1.563850975	1.466184387
16.301656	1.445370332	1.567048193	1.465992331
16.762092	1.448617802	1.570310481	1.465515568
17.244908	1.45162537	1.573688241	1.464713375
17.756695	1.454347261	1.57717266	1.463535232
18.294535	1.456670011	1.580676434	1.461947165
18.846806	1.458462227	1.584052792	1.459969824
19.401114	1.459641339	1.587183557	1.457672659
19.401114	1.460185248	1.590013489	1.455143923

20.487366	1.460111501	1.592531106	1.452472423
21.015759	1.459448239	1.594740185	1.449737
21.537178	1.458226904	1.596653639	1.446995448
22.055853	1.456460029	1.598265814	1.444295415
22.575838	1.454156385	1.599555119	1.441685663
23.099725	1.451323898	1.600479561	1.439216838
23.627877	1.447986642	1.600976775	1.436950562
24.157643	1.444202828	1.60097673	1.434949315
24.682086	1.440079559	1.600415109	1.433273895
25.191563	1.435770214	1.599261447	1.431961273
25.679921	1.43141315	1.597516064	1.431005823
26.148421	1.427075794	1.59518188	1.430370217
26.148421	1.422749927	1.592214383	1.430015867
27.056975	1.418394044	1.588516133	1.429913476
27.518143	1.413942881	1.583904762	1.430060569
27.998491	1.409335042	1.578117299	1.430474548
28.505154	1.404561148	1.570850227	1.431187259
29.035615	1.399717109	1.561906923	1.432224243
29.576613	1.395003112	1.551377479	1.433572381
30.113476	1.390607379	1.539616001	1.435181091
30.638318	1.386638537	1.527047375	1.436997679
31.150122	1.383125221	1.514056622	1.438980965
31.652079	1.380061188	1.500964519	1.441114938
32.149548	1.377430518	1.48802661	1.443397193
32.648729	1.375224073	1.475484219	1.445842229
32.648729	1.373446033	1.463599101	1.448471751
33.675632	1.372120423	1.452704083	1.451307289
34.21204	1.371281866	1.443213536	1.454364122
34.766039	1.370972379	1.435629975	1.457636236
35.33148	1.371212575	1.430506739	1.461071303
35.891613	1.37196711	1.428234087	1.464535965
36.429459	1.373127354	1.428766135	1.467882385
36.940947	1.37457931	1.431737782	1.471047416
37.433059	1.376248263	1.436793415	1.474040081
37.916918	1.378103193	1.443745071	1.476900258
38.404248	1.38014095	1.452560291	1.479661278
38.905765	1.382369143	1.463309655	1.482340833
39.428284	1.38478808	1.476041845	1.484919625
39.428284	1.387348701	1.490523787	1.487313361
40.512587	1.389947984	1.506081452	1.489401697
41.042935	1.392477582	1.521877652	1.491093085
41.553634	1.394890071	1.537378347	1.492372831
42.04716	1.397186694	1.552375985	1.493266705
42.529058	1.399390207	1.566811535	1.493804042
43.004926	1.401521917	1.580653088	1.494002265
43.479476	1.403600867	1.593847141	1.493870894
43.956535	1.40563688	1.606305931	1.493412171
44.439585	1.407641664	1.617913581	1.492619794
44.932332	1.409618403	1.628538894	1.491481113
45.438033	1.411567246	1.638014213	1.489978787
45.956302	1.413472951	1.646093893	1.488104243
45.956302	1.415287854	1.652488391	1.485886183
46.995773	1.416955327	1.657018314	1.483390711
47.498119	1.418444028	1.659724333	1.480688733
47.988151	1.419751263	1.660776039	1.477808695
48.472909	1.420884365	1.660323171	1.474737909
48.961577	1.421851292	1.658427746	1.471433588
49.46405	1.422642728	1.655050887	1.467839008
49.989576	1.423238121	1.650067622	1.463886985
50.542023	1.423600012	1.64334733	1.459554663
51.111075	1.423687378	1.634981747	1.454940584
51.674224	1.423501021	1.625432952	1.450266043
52.216423	1.42308604	1.615245203	1.445711627
52.737523	1.422495	1.604738864	1.441331604
52.737523	1.421769444	1.594058545	1.437112597
53.743235	1.420943362	1.583294346	1.433039704
54.239828	1.420044678	1.572544872	1.429116903
54.737456	1.419100875	1.561924899	1.425363542
55.239686	1.418133698	1.551539939	1.421808561

55.750666	1.417164442	1.541492712	1.418486941
56.272635	1.416211122	1.531931627	1.415458838
56.800924	1.415296698	1.523124453	1.412824622
57.323636	1.414447514	1.51539117	1.410696211
57.830702	1.41366763	1.508901501	1.409131755
58.320707	1.412943176	1.503622575	1.408115422
58.798781	1.412245267	1.499416558	1.407617875
59.272366	1.411540039	1.496142694	1.407620081
59.272366	1.410793416	1.493681965	1.408124434
60.234796	1.409966005	1.491935219	1.409162842
60.735282	1.40901479	1.490801055	1.410776748
61.253786	1.407894941	1.490164468	1.413019189
61.790581	1.406562619	1.489893954	1.41592823
62.339114	1.404991486	1.489841535	1.419485722
62.885229	1.403200547	1.489867967	1.423576472
63.416895	1.40123067	1.489863996	1.428038155
63.932417	1.399111301	1.489764403	1.432769297
64.43669	1.396851175	1.489535057	1.437737327
64.934973	1.394456766	1.489156035	1.442932872
65.430829	1.391946307	1.488625892	1.448336022
65.927437	1.389342981	1.487960168	1.453935406
65.927437	1.386667299	1.487190662	1.459726502
66.938463	1.383955059	1.486368081	1.465698427
67.454754	1.381273306	1.485568968	1.471778019
67.969859	1.378726741	1.484889745	1.477809978
68.47476	1.376416426	1.484419142	1.483625565
68.965639	1.374405825	1.484216388	1.489126796
69.444519	1.37271923	1.484308973	1.494285174
69.916678	1.371366373	1.484720526	1.499114772
70.388451	1.370364646	1.485472849	1.503631073
70.865946	1.369742044	1.486588619	1.50783152
71.35422	1.369544879	1.488095407	1.511689823
71.85675	1.369833741	1.490011107	1.515148491
72.375047	1.370673412	1.492337508	1.518125921
72.375047	1.372116413	1.495044122	1.520522135
73.444305	1.374170284	1.498050687	1.522238922
73.971656	1.376753654	1.501233015	1.523230262
74.479294	1.379744948	1.504499055	1.523534504
74.967936	1.383061364	1.507837312	1.523240857
75.443885	1.386666044	1.511291704	1.522419505
75.913501	1.390543367	1.514916544	1.521114169
76.381627	1.394680307	1.518763183	1.519350562
76.852494	1.399065123	1.522875944	1.517142527
77.330392	1.403685963	1.527295065	1.514486811
77.818416	1.408521921	1.532046205	1.511379898
78.316112	1.413505037	1.537100446	1.507835244
78.819173	1.418520387	1.542364738	1.503903358
78.819173	1.423441987	1.547713124	1.49964833
79.823369	1.428165157	1.55301752	1.495124813
80.321465	1.432621955	1.558164708	1.490367421
80.818475	1.436764206	1.563050699	1.485382427
81.317581	1.440555794	1.567563601	1.480158023
81.82268	1.443966606	1.571574312	1.474669089
82.33733	1.446954624	1.574905259	1.468888662
82.86399	1.44946781	1.577335168	1.462810586
83.403793	1.451446601	1.578607457	1.456445829
83.955882	1.452834525	1.578489754	1.449844695
84.515457	1.453589473	1.576876741	1.443128104
85.073048	1.453706078	1.573901964	1.436484367
85.619219	1.453236142	1.56992788	1.430111973
85.619219	1.452260109	1.565368043	1.424131855
86.669258	1.450852988	1.56056886	1.418595963
87.179038	1.449071689	1.555774811	1.413531341
87.683886	1.446959373	1.551162088	1.408970299
88.187373	1.444546058	1.546865226	1.404957652
88.691149	1.441864064	1.542998434	1.401555075
89.194054	1.43895388	1.539672546	1.398842058
89.693947	1.43586705	1.536973412	1.39688432
90.190054	1.432641266	1.534951694	1.395720138

90.682893	1.429311956	1.533630487	1.395368438
91.172716	1.425906473	1.533018946	1.395833376
91.658863	1.422459719	1.533111726	1.397104065
92.140553	1.419010675	1.53387979	1.39914252
92.140553	1.415586765	1.535275218	1.401902411
93.09144	1.412211445	1.537241278	1.405327057
93.563408	1.408900321	1.53970948	1.409357902
94.036287	1.405661033	1.542611503	1.413945888
94.51348	1.40249791	1.545876246	1.419048867
94.998655	1.399420969	1.549423259	1.424623011
95.49445	1.396445949	1.55315127	1.430609065
96.000832	1.393611418	1.556915734	1.436896825
96.514779	1.390966761	1.560527298	1.443316466
97.032433	1.388562207	1.56378896	1.449677301
97.551263	1.38642871	1.566516294	1.455805613
98.07022	1.384583338	1.568546875	1.46155388
98.589519	1.383029788	1.569744568	1.46680243
98.589519	1.381770829	1.569989846	1.471453692
99.632678	1.380807087	1.569190053	1.475417908
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100.682165	1.37975745	1.56427215	1.480981733
101.210627	1.379658826	1.560172402	1.482492584
101.742614	1.379836613	1.55506783	1.483122371
102.274899	1.380282497	1.549130118	1.48286807
102.801206	1.38097568	1.542623423	1.481778042
103.316597	1.381892823	1.535838247	1.479951762
103.820213	1.383012501	1.529001079	1.47749584
104.314597	1.384324822	1.522263077	1.474503653
104.804134	1.385832509	1.515712663	1.47104491
105.294074	1.387553638	1.509396915	1.46716034
105.294074	1.389510639	1.503340028	1.462883631
106.295773	1.39174013	1.497581797	1.45824829
106.813571	1.394268847	1.492195539	1.453321625
107.341377	1.397106257	1.487315449	1.448219529
107.875181	1.400246797	1.483141349	1.443092052
108.41083	1.403669014	1.479887222	1.438096562
108.944418	1.407344387	1.477763072	1.433382517
109.473119	1.411237211	1.476920024	1.42907327
109.996191	1.415323939	1.477435949	1.425255569
110.514478	1.419582768	1.479328631	1.421986413
111.030131	1.424006968	1.48256928	1.419307494
111.5471	1.428596927	1.487119145	1.417248168
112.070673	1.433372484	1.492940668	1.415841202
112.070673	1.438332869	1.499969237	1.415141125
113.147595	1.44342274	1.508028443	1.415208649
113.690717	1.448510461	1.516752547	1.416066045
114.224314	1.453454342	1.525690955	1.417674709
114.74431	1.458172863	1.534460168	1.419958258
115.252718	1.462640893	1.542809838	1.422851681
115.755003	1.466871913	1.550564583	1.426325604
116.258061	1.470880554	1.557570583	1.43038818
116.768949	1.474670725	1.56365283	1.435076178
117.293335	1.478219289	1.568576468	1.440434328
117.833463	1.481455639	1.572054625	1.446483862
118.387071	1.484277133	1.573807806	1.453189007
118.948186	1.48656551	1.573649684	1.460445017
118.948186	1.488221441	1.571568002	1.468086375
120.058253	1.489187862	1.56773901	1.475915226
120.592992	1.489462594	1.56245003	1.483774409
121.111283	1.489077276	1.556012728	1.491566497
121.615237	1.488067838	1.548696385	1.499253178
122.109411	1.486462377	1.540698978	1.506842367
122.600154	1.484261126	1.532151949	1.514378543
123.094431	1.481439662	1.523147614	1.521912876
123.597672	1.477952635	1.513798339	1.529467463
124.110294	1.473778462	1.504331176	1.536976824
124.625325	1.468980749	1.495126479	1.544265544
125.132399	1.463692108	1.486599649	1.551120434
125.625367	1.458047499	1.479028037	1.557413335

125.625367	1.452120235	1.472524966	1.563114012
126.573879	1.445930176	1.467117125	1.568244907
127.038773	1.439465458	1.462810544	1.572826003
127.50455	1.432700951	1.459630921	1.576861086
127.976359	1.425605988	1.457631364	1.580327094
128.458966	1.418155542	1.456896854	1.583165188
128.956134	1.410344769	1.457545205	1.585283161
129.468909	1.40222794	1.459709552	1.586545966
129.993257	1.393957509	1.46347213	1.586812139
130.520303	1.385777077	1.468791848	1.585978034
131.041304	1.377924448	1.475494226	1.584023812
131.551878	1.370553909	1.483355563	1.58098838
132.05169	1.363742309	1.492165642	1.576929254
132.05169	1.357524827	1.501740122	1.57188877
133.028718	1.351911504	1.511940568	1.565887564
133.514732	1.346910649	1.522663498	1.55890614
134.007049	1.342537406	1.533849121	1.550874075
134.512586	1.338838715	1.545436144	1.541680937
135.036703	1.335914254	1.557299993	1.531213421
135.578607	1.333927214	1.569130292	1.519492352
136.128052	1.333033169	1.580399028	1.506791442
136.671468	1.333296303	1.590586462	1.493553136
137.201957	1.334670594	1.599417436	1.480114566
137.720512	1.33708005	1.606851672	1.466618701
138.231688	1.340474128	1.612935309	1.453097999
138.740488	1.344828281	1.617731752	1.439562017
138.740488	1.350138717	1.621303714	1.426034201
139.768174	1.356409528	1.623707753	1.412574045
140.292546	1.363627136	1.625005576	1.399300473
140.822814	1.37171675	1.625267692	1.386456808
141.353174	1.380509036	1.624591286	1.37437665
141.877741	1.389796053	1.62310316	1.363369623
142.394211	1.399417981	1.620924365	1.353618201
142.903159	1.409273492	1.618147194	1.345224395
143.405778	1.419284978	1.61483805	1.338259979
143.903103	1.429385196	1.611047953	1.332787327
144.396608	1.439532744	1.60681082	1.328848319
144.888603	1.449710811	1.602145396	1.326470545
145.381745	1.459921672	1.597059419	1.325682187
145.381745	1.470160263	1.591562664	1.326514495
146.377345	1.48038463	1.585681077	1.328976262
146.877745	1.490511509	1.579470215	1.333027015
147.375249	1.500430009	1.573016347	1.338545546
147.866144	1.510036872	1.566402702	1.345341859
148.348508	1.519269122	1.559685374	1.353206567
148.822533	1.528111062	1.552887925	1.36195596
149.290086	1.536574076	1.545997779	1.371443826
149.754334	1.544690721	1.538979256	1.381577858
150.21951	1.552502648	1.531775659	1.392308695
150.690448	1.560049421	1.524328529	1.40363003
151.171547	1.567344263	1.516586249	1.415535105
151.665326	1.574361121	1.508540317	1.427971454
151.665326	1.581029615	1.500240951	1.440810757
152.689264	1.587265643	1.491777128	1.453886258
153.21679	1.592999103	1.483244246	1.467025794
153.753433	1.598173802	1.474752442	1.480065766
154.296573	1.602726354	1.466454532	1.492805436
154.841515	1.606605219	1.458553714	1.505009993
155.384277	1.609788782	1.451243561	1.516487748
155.923812	1.612293898	1.444682059	1.527137475
156.46121	1.614154905	1.438998297	1.536921714
156.997441	1.615402824	1.434323502	1.545799077
157.531558	1.616075052	1.430779795	1.553717242
158.060603	1.616210637	1.428451927	1.560609907
158.581494	1.615866737	1.427354344	1.56644497
158.581494	1.615108626	1.427433249	1.571238554
159.596159	1.613994183	1.428603266	1.575035625
160.09298	1.612574252	1.430778474	1.577886524
160.586353	1.610889579	1.433898151	1.579832451

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161.574328	1.606856869	1.442881112	1.581088529
162.071915	1.604577517	1.448720208	1.580401735
162.570103	1.60218927	1.455382736	1.578843449
163.06635	1.599751128	1.462759839	1.576445331
163.560737	1.597314303	1.470742796	1.573234117
164.05711	1.594909415	1.479278387	1.569214078
164.561122	1.592560879	1.488343632	1.564345284
165.076027	1.590313287	1.497868414	1.558595729
165.076027	1.588243816	1.507649785	1.552007344
166.120073	1.586440408	1.517379993	1.544728572
166.633665	1.584970617	1.526781508	1.536937526
167.137528	1.583866512	1.535704965	1.5287526
167.633569	1.583145462	1.544088183	1.520232492
168.12478	1.58282049	1.551890328	1.511406571
168.613745	1.5829141	1.559059866	1.50230461
169.102038	1.58344807	1.565520461	1.492965811
169.590172	1.584445762	1.571172815	1.483454994
170.077977	1.585926202	1.575902217	1.473847672
170.565277	1.587903622	1.579593829	1.464223573
171.052576	1.590394376	1.582144684	1.454646866
171.541179	1.59341522	1.583466314	1.445172013
171.541179	1.596991069	1.583494878	1.435851576
172.525377	1.601134622	1.582209998	1.426774343
173.017413	1.605832872	1.579669683	1.418069298
173.50412	1.611049087	1.576034949	1.40987026
173.983239	1.616753147	1.571514401	1.402260839
174.456405	1.622961845	1.566306965	1.395249838
174.928939	1.629753726	1.560558507	1.388794992
175.408768	1.637277438	1.554359238	1.382842387
175.904907	1.645743212	1.547788642	1.37736485
176.423921	1.655366704	1.540978876	1.372408206
176.962914	1.666207309	1.534231618	1.368125109
177.506635	1.678022241	1.528008852	1.36471359
178.039104	1.690444687	1.522700858	1.362255463
178.039104	1.70326026	1.518463339	1.360697077
179.055314	1.716428162	1.515312129	1.359938247
179.545884	1.729988515	1.513217878	1.359887804
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180.509321	1.758379847	1.512043702	1.361672557
180.985175	1.773187246	1.512852044	1.363409919
181.458519	1.788375686	1.514491536	1.365659353
181.931249	1.803961739	1.516880438	1.368387271
182.405574	1.819976741	1.519957598	1.371575966
182.882297	1.836408048	1.523674866	1.375199374
183.359005	1.853134673	1.52798479	1.379204694
183.83033	1.86991821	1.532813795	1.383503555
184.291095	1.886522294	1.538075473	1.387993177
184.291095	1.902827135	1.543697852	1.392598663
185.177191	1.918852695	1.549642774	1.397286132
185.608564	1.934712705	1.555902034	1.402055126
186.038783	1.950565413	1.562484256	1.406926307
186.473383	1.96658451	1.569406825	1.411930435
186.917566	1.982928814	1.576679056	1.417091665
187.374957	1.999699603	1.584267465	1.422420032
187.845452	2.016854956	1.592058939	1.427869356
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188.801954	2.051326969	1.607310767	1.438683848
189.274323	2.068111183	1.614280566	1.443816545
189.73969	2.084474259	1.620619498	1.448693862
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192.026928	2.162444788	1.640601971	1.469412417
192.484295	2.177600773	1.641816632	1.472833302
192.944632	2.192732096	1.641982397	1.476025817
193.409847	2.207911687	1.641063729	1.479003915
193.87946	2.223128683	1.639050653	1.481763565

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195.706878	2.281414097	1.622304718	1.490366464
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197.431338	2.334916237	1.598502651	1.495951049
197.872654	2.348314647	1.592001397	1.497085295
198.3233	2.361848217	1.58540449	1.498146473
198.781603	2.375450472	1.578845287	1.499140042
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199.699641	2.4021547	1.566570005	1.500918968
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203.654415	2.508340099	1.540236727	1.505711481
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205.523557	2.554229902	1.545047946	1.504460568
205.992382	2.565449895	1.547671422	1.503437562
206.45457	2.576424498	1.550786749	1.502079215
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207.366297	2.597866116	1.558442651	1.498257409
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208.76188	2.630313186	1.573629513	1.489138609
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209.741085	2.652912972	1.586126488	1.480260854
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211.172309	2.685808176	1.60575521	1.463800224
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223.169095	2.929061057	1.838341266	1.3815689
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224.023702	2.942214587	1.8611603	1.392110141
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343.266121	4.805865662	4.116266688	1.494710931
343.673249	4.809842728	4.12284721	1.493963253
344.077585	4.813754886	4.130371064	1.492990788
344.481905	4.81764334	4.13887209	1.491794371
344.889042	4.821552326	4.148394095	1.490373842
345.301894	4.82552912	4.158979249	1.48872207
345.723407	4.82962818	4.170673227	1.486831596
346.156309	4.83390986	4.183504945	1.484693597
346.602324	4.838434952	4.19745644	1.482304873
347.060837	4.843252569	4.212404448	1.479687347
347.527749	4.848379105	4.228069311	1.476894814
347.527749	4.853796667	4.244042832	1.474012817
348.458827	4.859463267	4.259906292	1.471140743
348.911203	4.865342137	4.275356538	1.468364041
349.351614	4.871409746	4.290242167	1.465742311
349.780795	4.877658252	4.304537899	1.463313018
350.201015	4.884095666	4.318304935	1.461096426
350.615489	4.890738967	4.331655799	1.459105122
351.027988	4.897619148	4.344735807	1.457345427
351.442461	4.904767434	4.357705407	1.455829013
351.86241	4.912211354	4.370714141	1.454569717
352.289821	4.919949844	4.383880619	1.453587328
352.723882	4.927925411	4.39724317	1.452908809
353.160703	4.936015202	4.410756399	1.452551958
353.160703	4.944079369	4.424333108	1.452515511
354.024007	4.952009104	4.437925702	1.452781863
354.446635	4.959757895	4.45155628	1.453324761
354.864945	4.967334512	4.46530731	1.454120481
355.282135	4.974771178	4.479295	1.455147907
355.70206	4.982118532	4.493651364	1.456402023
356.128971	4.989430165	4.508517292	1.457880195
356.567387	4.996766187	4.524039928	1.459586789
357.021665	5.004178352	4.540347763	1.461531797
357.494468	5.011691868	4.557495452	1.463717705
357.983462	5.019260649	4.575327089	1.466118437
358.478642	5.026738049	4.593376971	1.46866365
358.966237	5.033948726	4.611027392	1.471249808
358.966237	5.040804961	4.627839013	1.473793464
359.888785	5.047329669	4.643664489	1.476255242
360.323935	5.053603982	4.658534126	1.478621239
360.746276	5.059731038	4.672547021	1.480892742
361.160033	5.06581072	4.68581644	1.483075492
361.569511	5.071950777	4.698449524	1.485174851
361.979003	5.078258238	4.710545519	1.487196793
362.3925	5.08485024	4.722178735	1.489137503
362.812928	5.09182973	4.733372097	1.490987425
363.240865	5.099274468	4.744071854	1.492719085
363.673497	5.107199382	4.754136608	1.494288544
364.105423	5.115553607	4.763390759	1.495652677
364.531567	5.124262259	4.771699887	1.496774526
364.531567	5.133275833	4.779030316	1.497636816
365.360159	5.142589856	4.78542912	1.498235845
365.765667	5.152235072	4.790978362	1.498566431
366.169253	5.162257431	4.79577687	1.498625594
366.574299	5.172714992	4.799924226	1.498398839
366.984303	5.183676314	4.803527868	1.497867123
367.402965	5.195209404	4.806706389	1.497001603
367.834285	5.207398748	4.809602404	1.495758625
368.282302	5.220322424	4.812387845	1.494087402
368.74967	5.23401139	4.815278411	1.491928409
369.234288	5.248343366	4.818519528	1.489242099
369.726173	5.262939532	4.822330009	1.486061417
370.211128	5.27729528	4.826844361	1.482489975
370.211128	5.291053794	4.832107499	1.478650357
371.12951	5.30411101	4.838120326	1.474626282
371.563714	5.316516946	4.84488127	1.470455664
371.986545	5.328383647	4.852394091	1.46615164
372.402831	5.339832636	4.860666629	1.461709754
372.817519	5.350991239	4.86972553	1.457117673

373.235539	5.361975593	4.879601554	1.452356692
373.661362	5.372892171	4.890317569	1.447414633
374.097856	5.383795346	4.901841577	1.442298657
374.544433	5.394659298	4.914019035	1.43706923
374.99604	5.40535546	4.926531269	1.431846303
375.445528	5.415725984	4.938985883	1.426780087
375.88811	5.425678847	4.951074031	1.421984381
375.88811	5.435225057	4.962644977	1.417518877
376.753396	5.444426507	4.973665594	1.413408029
377.182145	5.453358315	4.984155075	1.409670277
377.612856	5.462078025	4.994154104	1.406332109
378.048392	5.470615514	5.003697282	1.403436409
378.49101	5.478973073	5.012824079	1.401040972
378.942456	5.487130867	5.021584811	1.399212019
379.403876	5.495042208	5.030037097	1.398027143
379.87503	5.502629825	5.038243737	1.397567954
380.352559	5.509768544	5.046247529	1.397900343
380.828902	5.51629516	5.054052714	1.399046795
381.294979	5.522070569	5.061654435	1.400955395
381.745239	5.52705598	5.069094741	1.403525222
381.745239	5.531295929	5.076472471	1.406659635
382.600895	5.534872124	5.08392329	1.410289463
383.014185	5.537867304	5.091591479	1.414382041
383.424172	5.540343444	5.099623312	1.418924567
383.835472	5.542347887	5.108160885	1.423921077
384.252138	5.543906125	5.11734494	1.42938317
384.67697	5.54503328	5.127292157	1.435312384
385.110313	5.545736139	5.138058396	1.441674197
385.548979	5.54603142	5.14959241	1.448367678
385.987075	5.545956865	5.161731935	1.455237319
386.419181	5.545577947	5.174278729	1.462124971
386.843019	5.544967325	5.187092044	1.468922761
387.259488	5.544196301	5.200115905	1.475581117
387.259488	5.543329949	5.213345471	1.482088461
388.081126	5.542425208	5.226793483	1.488438438
388.49213	5.54154592	5.240460961	1.494622624
388.906417	5.5407542	5.254325379	1.5006229
389.325691	5.540125182	5.268330673	1.506408262
389.751174	5.539739656	5.282391289	1.51193582
390.183661	5.539689077	5.296385395	1.517149868
390.623415	5.540068142	5.31015852	1.521985171
391.069662	5.540975718	5.323516111	1.526364802
391.519783	5.542492667	5.336216398	1.530199206
391.968994	5.544664837	5.348001416	1.533396244
392.411721	5.547485104	5.358660634	1.535895521
392.844074	5.550910599	5.36811793	1.537681045
392.844074	5.55488104	5.37642546	1.538773465
393.676819	5.559349873	5.383724846	1.539206548
394.08198	5.564289022	5.390191302	1.539009418
394.484334	5.569684474	5.396015488	1.538195351
394.887551	5.57553513	5.401393985	1.536759585
395.29491	5.581843544	5.406535091	1.534683879
395.708617	5.588599962	5.411656289	1.531943552
396.128829	5.595758173	5.4169785	1.528523581
396.553038	5.603225981	5.42270912	1.524445377
396.976982	5.610868666	5.429014471	1.51976861
397.396991	5.618562511	5.436026377	1.514581919
397.811777	5.626233503	5.443851162	1.508955507
398.222385	5.633856247	5.452584196	1.502937693
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399.040527	5.649010006	5.473142828	1.489804166
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399.870421	5.664172735	5.498261808	1.475292256
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401.162351	5.687131516	5.544585623	1.451479586
401.606676	5.694841662	5.562002164	1.443253972
402.055608	5.702549025	5.580077828	1.435062494
402.505326	5.710205168	5.59847314	1.427069272

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403.811753	5.732253464	5.651670549	1.405858151
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404.634149	5.746141748	5.683350919	1.394734908
405.038603	5.753005172	5.698031049	1.390075661
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406.704335	5.781491286	5.751007296	1.3776713
407.143004	5.788991595	5.763145848	1.37641734
407.584899	5.796503022	5.774832602	1.376053612
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408.45172	5.810992513	5.796784149	1.377991641
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409.283265	5.824392339	5.817543903	1.383085209
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410.100398	5.836868466	5.838606158	1.390980641
410.512428	5.842834665	5.849738292	1.395953193
410.930616	5.84863515	5.861520862	1.401611501
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412.239331	5.864909502	5.902498136	1.422650776
412.6939	5.869832588	5.91845711	1.430878521
413.153073	5.874400649	5.935563219	1.439523869
413.610722	5.878543659	5.953592769	1.448386453
414.060388	5.882215926	5.97220694	1.457242968
414.49795	5.885420135	5.99108053	1.465925619
414.922788	5.888194596	6.009990146	1.474341529
414.922788	5.890604157	6.02883009	1.482472714
415.744346	5.892713959	6.047575915	1.49033295
416.148709	5.894591069	6.066246545	1.497954416
416.554353	5.896296868	6.084873644	1.505364134
416.96537	5.897895004	6.1034967	1.512581018
417.385499	5.899455702	6.122131431	1.51960406
417.817294	5.901053637	6.140723923	1.526396473
418.260426	5.902771031	6.15908468	1.532867202
418.710168	5.904681434	6.176845768	1.538866985
419.158902	5.90683719	6.193585267	1.544235172
419.600679	5.909270383	6.209026249	1.54887679
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420.460541	5.915062052	6.236029471	1.555953764
420.460541	5.918455857	6.24789344	1.558435399
421.306166	5.92219338	6.258924767	1.560229059
421.730965	5.926272138	6.269312358	1.561326279
422.159919	5.930677281	6.279263408	1.561706362
422.594375	5.935382059	6.288986989	1.561339523
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423.480609	5.945525684	6.308578826	1.558236221
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424.375086	5.956173241	6.329384163	1.551950247
424.813748	5.961452683	6.340349786	1.547744089
425.241092	5.966603811	6.351622362	1.542966346
425.656132	5.971599807	6.363150995	1.537709527
426.060338	5.976455709	6.374920469	1.532034434
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426.848161	5.985890472	6.399264879	1.519527283
427.238603	5.990560623	6.411939575	1.512692052
427.631413	5.995262732	6.425050236	1.505443971
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428.856007	6.010043905	6.467885437	1.480973545
429.283658	6.015292177	6.483407124	1.471970399
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430.144681	6.026082121	6.515187742	1.453571433
430.56709	6.031517854	6.530882001	1.444569034
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433.07841	6.066580405	6.620196313	1.396202735
433.527125	6.073401556	6.63457082	1.389233353
433.992415	6.080635938	6.64872463	1.382759103
434.475179	6.088289811	6.66252298	1.376931099
434.97272	6.096295734	6.675728422	1.371953878
435.476044	6.104456863	6.6879889	1.36804907
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436.900816	6.127291093	6.716787803	1.363599829
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438.570455	6.151609933	6.742916558	1.371190714
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443.677157	6.189589576	6.876922718	1.460516938
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459.900833	6.22363581	7.326672526	1.49695688
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473.364181	6.497771336	7.572890594	1.46428248
473.827477	6.508300684	7.58231394	1.466875605
474.285709	6.518579976	7.590692862	1.469299042
474.730596	6.528410703	7.597793502	1.471481484
475.160372	6.537741115	7.603596197	1.473397594
475.577357	6.546605399	7.608182663	1.475049845
475.985209	6.555062262	7.611662255	1.476443156
476.387613	6.563159017	7.614127438	1.477582288
476.787956	6.570930044	7.615655822	1.478466257
476.787956	6.578392444	7.616304421	1.479084045
477.595106	6.585550457	7.616111854	1.479421274
478.008195	6.592397471	7.61510094	1.479457866
478.431813	6.598906876	7.613275542	1.479162989
478.868298	6.605024477	7.610640905	1.478503361
479.317398	6.610648309	7.607235499	1.477447427
479.773843	6.615628314	7.603196156	1.475987636
480.227737	6.619811783	7.598791045	1.474159825
480.670126	6.623127564	7.594350129	1.472034759
481.097918	6.625608606	7.590151466	1.469679568
481.513366	6.627325501	7.58638915	1.467129586
481.921332	6.628351982	7.583195615	1.464399578
482.327476	6.628726012	7.580683998	1.461486233
482.327476	6.628461169	7.578967971	1.458373193
483.157193	6.62753552	7.578179105	1.45504097
483.590774	6.625905713	7.5784735	1.451476207
484.039806	6.62353022	7.580002285	1.447689711
484.500336	6.62040656	7.582856974	1.443746541
484.963234	6.616615347	7.586972283	1.439760472
485.419101	6.612299326	7.592131027	1.435850531
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486.294947	6.602616158	7.604506372	1.428505658
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487.13319	6.59202919	7.618160506	1.421847614
487.546379	6.586484204	7.62501754	1.418758153
487.960351	6.580796644	7.631660518	1.415818262
487.960351	6.574977579	7.637895472	1.413032487
488.804797	6.569038544	7.643489737	1.410409451
489.241434	6.563007148	7.648175436	1.407973343
489.689851	6.556936908	7.651646207	1.405771192
490.148245	6.550924844	7.653621342	1.403865441
490.610412	6.545122402	7.653933752	1.402332338
491.066759	6.539697579	7.65263858	1.401235652
491.509059	6.534770503	7.650008909	1.400596144
491.934618	6.530373128	7.646406055	1.400396988

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494.792048	6.511313644	7.614642428	1.410563294
495.230311	6.510191252	7.611663898	1.413891831
495.67541	6.509560627	7.60984463	1.417710807
496.12081	6.509435154	7.609382862	1.421943691
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496.990967	6.510592672	7.61266276	1.431263661
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603.445506	6.647830382	9.794268529	1.63863053
603.87912	6.649956513	9.803121074	1.629694193
604.300616	6.65224701	9.811909324	1.620391564
604.714022	6.65469087	9.820702443	1.610692961
605.123346	6.657284919	9.829568449	1.600543363
605.531588	6.660029469	9.838556365	1.589897039
605.940254	6.662916374	9.8476735	1.578737139
606.349322	6.665929372	9.856892798	1.567090361
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607.164114	6.672223437	9.875487758	1.542593012
607.567778	6.675445569	9.884857132	1.52988399
607.96899	6.67868623	9.89436533	1.516929583
608.36913	6.681928665	9.90415601	1.503730426
608.770429	6.685169107	9.914412947	1.49026193
609.175511	6.688397621	9.925340248	1.476482227
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615.699251	6.705801376	10.15443839	1.295312857
616.143019	6.702975087	10.16674252	1.291512548
616.590628	6.699587965	10.17794804	1.289480234
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738.93829	6.100867895	12.0377001	3.656429467
738.93829	6.102250204	12.03996013	3.655221618
739.832283	6.10319146	12.04205046	3.653859659
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740.711972	6.103516395	12.04565208	3.650866613
741.143142	6.102850903	12.04716177	3.649325223
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741.99621	6.099860422	12.0496251	3.646331011
742.423217	6.097551548	12.05058301	3.644948448
742.854831	6.094711975	12.05134978	3.64368859
743.295079	6.091346978	12.05191282	3.642594842
743.74797	6.087465289	12.05224659	3.641722844
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746.097242	6.064046161	12.0497757	3.643055724
746.535112	6.059739818	12.0485643	3.644643264
746.961219	6.055752986	12.04718559	3.64664034
747.380865	6.052081131	12.04564723	3.649052136
747.799397	6.048720572	12.04395169	3.651897734
748.221808	6.045676854	12.04209383	3.655211484
748.652579	6.042967364	12.04006643	3.659039597
749.09523	6.040624794	12.0378727	3.663429586
749.551185	6.038694989	12.03552903	3.668412816
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752.742651	6.036865186	12.02103942	3.713401161
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758.399851	6.017396183	12.05303602	3.799720737
758.828518	6.013193808	12.05964715	3.805176443
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762.391769	5.979862762	12.13160865	3.849637716
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763.698833	5.976315218	12.14691398	3.858431395
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764.522438	5.974209859	12.16100406	3.866913288
764.928954	5.973572067	12.16775698	3.871159768

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769.777242	5.968685024	12.24991332	3.929848509
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873.82209	6.564704094	13.56534722	4.281426763
874.277399	6.562235915	13.57468186	4.282950004
874.72751	6.559722582	13.58341335	4.284794198
875.172902	6.557255468	13.59148301	4.286946192
875.614261	6.554910983	13.59888758	4.289391389
876.052455	6.55274763	13.60566908	4.292115341
876.488629	6.550808795	13.61191037	4.29510821
876.924119	6.549125419	13.61772298	4.29835625
877.360107	6.547713372	13.62324023	4.301849417
877.79708	6.546579521	13.62859664	4.305568317
878.234298	6.545714832	13.63392594	4.309485987
878.669707	6.545097979	13.63934622	4.313555983
878.669707	6.544692326	13.64495932	4.317722432
879.526336	6.544450412	13.65086038	4.32194146
879.946868	6.54432277	13.65714831	4.326186512
880.364838	6.544264428	13.66393176	4.330451317
880.783481	6.544244738	13.6713175	4.334736912
881.206005	6.544240818	13.67940895	4.339046115
881.634989	6.544240598	13.68828313	4.343371788
882.072007	6.544250812	13.69798231	4.347690369
882.517403	6.544290218	13.70848865	4.351961732
882.970212	6.544396468	13.71971757	4.356130503
883.42826	6.544621199	13.73151376	4.360125988
883.8886	6.545024289	13.7436708	4.363875031
884.348341	6.545668908	13.75596488	4.367309826
884.348341	6.54661243	13.76819748	4.37038057
885.259444	6.547907669	13.78021664	4.373052163
885.71091	6.549602953	13.79192097	4.375304483
886.161537	6.551746963	13.8032502	4.377122681
886.613675	6.554392987	13.81416438	4.378492545
887.070137	6.55760122	13.8246396	4.379398765
887.53383	6.56144043	13.83464903	4.379820954
888.007048	6.565983168	13.84414812	4.379735519
888.490414	6.571289634	13.85305996	4.379121838

888.981801	6.577379002	13.86127744	4.37797545
889.475866	6.584206674	13.86868237	4.376328831
889.965399	6.591653142	13.8751982	4.374248068
890.444742	6.599580337	13.88083824	4.371829022
890.444742	6.607888581	13.88571064	4.369152929
891.371118	6.616540826	13.88996752	4.366276103
891.824938	6.625539304	13.89378071	4.363229717
892.27834	6.634900161	13.89731232	4.360035518
892.734848	6.644619313	13.9007172	4.356715411
893.196611	6.654650907	13.90415153	4.35329922
893.66414	6.664900993	13.90776694	4.349828334
894.136311	6.675215626	13.91171187	4.346359072
894.610894	6.685408644	13.91612054	4.342954161
895.085512	6.6952854	13.92110549	4.339675644
895.558409	6.704681899	13.92674981	4.33657248
896.028553	6.713477619	13.93310941	4.333684724
896.495257	6.721597006	13.94019836	4.331045227
896.495257	6.72900773	13.94798425	4.328677396
897.415959	6.735725084	13.95639134	4.326599352
897.869362	6.741807211	13.96531085	4.324822571
898.318286	6.74735141	13.97460537	4.323352505
898.762817	6.752469379	13.98411364	4.322192305
899.20277	6.75727803	13.99365286	4.321342264
899.637981	6.761901659	14.00303962	4.320797348
900.068637	6.766454788	14.01210808	4.320549821
900.49523	6.771042838	14.02071183	4.320592135
900.918295	6.775758841	14.02872864	4.320911792
901.338358	6.780679891	14.03606559	4.321495846
901.756223	6.785867754	14.04266205	4.322335368
902.173324	6.79138236	14.04849617	4.323422769
902.173324	6.797278782	14.05358435	4.324749647
903.014284	6.803618973	14.05796709	4.326319543
903.443454	6.810454614	14.06170606	4.328137397
903.881496	6.817827522	14.06488432	4.330208466
904.329492	6.825752956	14.06760818	4.332532219
904.787064	6.834200569	14.07001223	4.335102314
905.252584	6.843095582	14.07224898	4.337891635
905.72398	6.852336199	14.07449324	4.340869351
906.199625	6.86180557	14.07691831	4.343995742
906.67871	6.871396751	14.07968753	4.34723585
907.161001	6.881006757	14.08294501	4.350549895
907.646265	6.890535898	14.08681383	4.353897201
908.133805	6.899883547	14.09138917	4.35723587
908.133805	6.908955252	14.09672252	4.360518704
909.110322	6.91766745	14.10282771	4.363704514
909.5952	6.925955526	14.10966309	4.366752151
910.073988	6.933774901	14.11713413	4.369633311
910.54398	6.941112106	14.12510491	4.372329615
911.003755	6.948000301	14.13343868	4.374842306
911.453134	6.954498174	14.14200674	4.377187079
911.892595	6.960680007	14.15069485	4.379388046
912.323042	6.966620715	14.1594085	4.381470635
912.74596	6.972403214	14.16807148	4.383463158
913.163488	6.978113167	14.17663248	4.385397434
913.578197	6.983839372	14.18506171	4.387304507
913.992691	6.989665191	14.19333307	4.389209827
913.992691	6.99567408	14.20141659	4.391143382
914.8291	7.001936802	14.20926735	4.393122611
915.252835	7.008506817	14.21682454	4.395166046
915.679691	7.015424277	14.22401258	4.397282325
916.108233	7.022706038	14.23075367	4.399476335
916.536825	7.030356663	14.23698047	4.401747719
916.96407	7.038372422	14.24264564	4.404096013
917.389018	7.046748165	14.24772246	4.406520817
917.811235	7.055474011	14.25220238	4.409024093
918.230889	7.064542566	14.25610162	4.411609049
918.648815	7.073956325	14.25945455	4.414281777
919.066363	7.08371719	14.26231338	4.417053546
919.484934	7.093824864	14.26474151	4.419939134

919.484934	7.104253968	14.26682137	4.422947838
920.327155	7.114939149	14.2686461	4.426081373
920.749192	7.125776196	14.2703267	4.429337601
921.170106	7.136643304	14.27198836	4.432709815
921.589601	7.14744194	14.27376569	4.436201297
922.008653	7.158095974	14.27579923	4.439823123
922.428876	7.16854842	14.27823019	4.443595256
922.851572	7.178732358	14.28119157	4.447536995
923.277215	7.188562465	14.28480047	4.451657109
923.7057	7.197958725	14.28915078	4.455959239
924.137038	7.206860484	14.29430377	4.460447016
924.571794	7.215245282	14.30029799	4.465127347
925.011024	7.223123269	14.30714564	4.47001119
925.011024	7.230530057	14.31483167	4.475110321
925.907775	7.237523697	14.32331325	4.480437731
926.367344	7.244172476	14.33250725	4.485996309
926.834953	7.250553422	14.34229214	4.491781152
927.309925	7.256741733	14.35249883	4.497772328
927.790461	7.262804007	14.36290978	4.503929104
928.273878	7.268792463	14.37327338	4.510192544
928.757185	7.274746692	14.38333968	4.516492007
929.237893	7.28069705	14.39288747	4.522763228
929.714952	7.286674605	14.40176169	4.528953448
930.189408	7.292722201	14.40988691	4.53503614
930.664312	7.298896034	14.41725589	4.541009001
931.143672	7.305260363	14.42389774	4.546876745
931.143672	7.311857611	14.42985233	4.55262638
932.123067	7.318674884	14.4351504	4.558192142
932.615946	7.325618195	14.43983562	4.563473
933.101802	7.332569204	14.44400003	4.568371624
933.576497	7.339443487	14.44779235	4.572850697
934.03933	7.34620376	14.45138734	4.576922931
934.491604	7.35284746	14.45495201	4.580623781
934.935628	7.359387171	14.45864596	4.583997979
935.374171	7.365849329	14.46261376	4.58709173
935.810001	7.372262075	14.46699513	4.589948004
936.245576	7.378656939	14.47192502	4.592605429
936.682962	7.385065642	14.47753583	4.595094502
937.123825	7.391520262	14.48395828	4.597443943
937.123825	7.398058793	14.49131479	4.599673995
938.019979	7.404719687	14.49971418	4.601803694
938.475086	7.411539786	14.50922771	4.603841068
938.93292	7.418551045	14.51986762	4.605790257
939.390905	7.425779325	14.53158011	4.607650235
939.84631	7.433248476	14.54424226	4.609417868
940.296885	7.440985362	14.55768125	4.611088534
940.741268	7.449019214	14.57170814	4.612663852
941.17926	7.457383452	14.5861345	4.61414334
941.611948	7.466124909	14.60080975	4.615534116
942.041629	7.47531247	14.61562454	4.616844518
942.471487	7.485030985	14.63049994	4.618082731
942.905163	7.495381078	14.64538011	4.619259986
942.905163	7.506470398	14.66019235	4.620382875
943.797623	7.518390198	14.67482747	4.621459802
944.260661	7.5311918	14.68911353	4.622495175
944.734316	7.54484663	14.70280136	4.623495297
945.214362	7.55920133	14.71558907	4.624467462
945.693976	7.573989157	14.72719488	4.625418037
946.166581	7.588913625	14.73746001	4.626362532
946.628886	7.60376239	14.74640374	4.627319333
947.081423	7.618440247	14.75418346	4.628316225
947.52718	7.632937173	14.76101473	4.629379711
947.970182	7.647277431	14.76712526	4.630541791
948.4147	7.661488229	14.7727475	4.6318305
948.864916	7.675578486	14.77811017	4.633281333
948.864916	7.689525631	14.78345716	4.634924312
949.7972	7.703258098	14.78903821	4.636792306
950.283799	7.71662932	14.79511463	4.638906951
950.782735	7.729399814	14.80190595	4.641270189

951.287559	7.741253118	14.8095293	4.64384352
951.787985	7.751881167	14.81793421	4.64654888
952.274344	7.761118166	14.8269358	4.649290331
952.74225	7.76900863	14.83632266	4.651994116
953.193168	7.775729558	14.84595426	4.65462225
953.63214	7.781500236	14.85576201	4.657162823
954.06576	7.78651876	14.86573175	4.6596183
954.50123	7.790952749	14.87587958	4.661992953
954.945908	7.794932437	14.88622401	4.664281975
954.945908	7.798561333	14.89674245	4.666470438
955.885869	7.801904989	14.90730532	4.668511041
956.379998	7.804989229	14.91758949	4.670321142
956.876376	7.807824538	14.92713374	4.671801976
957.362948	7.810439104	14.93558309	4.672897468
957.835382	7.812910388	14.94282283	4.673599163
958.295895	7.815328452	14.94890069	4.673924636
958.749202	7.817787884	14.95389837	4.673886321
959.20012	7.820372014	14.95789114	4.67349117
959.652782	7.823165196	14.96093146	4.672730639
960.110531	7.826245921	14.96305735	4.671594119
960.575909	7.829696062	14.96430782	4.670062507
961.050439	7.833594787	14.96473017	4.668117031
961.050439	7.838003388	14.96439334	4.665749762
962.024268	7.842952015	14.96340529	4.662967406
962.515593	7.848413858	14.96192228	4.659811847
963.000574	7.854297892	14.96013306	4.656359359
963.472677	7.860480003	14.95822221	4.652700178
963.929139	7.866860134	14.95633314	4.648909494
964.371312	7.873382968	14.95455913	4.645027469
964.803181	7.880041632	14.95294757	4.64106239
965.229876	7.886859443	14.95152789	4.63700075
965.656805	7.893883497	14.95031623	4.632819957
966.089134	7.901162446	14.94932732	4.628492595
966.531014	7.908742657	14.94857407	4.623994629
966.983968	7.916630918	14.94806655	4.619330816
966.983968	7.924756122	14.94779724	4.614550628
967.904789	7.932962086	14.94772936	4.609756598
968.35535	7.941084784	14.9477888	4.605058191
968.791929	7.949040528	14.94788953	4.600506546
969.215253	7.956843824	14.94794757	4.596097508
969.628846	7.964560986	14.94788113	4.591796442
970.037017	7.972273779	14.94761668	4.587554846
970.44396	7.980066815	14.94707959	4.583325175
970.853555	7.988016055	14.94618696	4.579063419
971.269447	7.996196489	14.94485196	4.57472082
971.69513	8.004679172	14.94298109	4.570254569
972.133793	8.013524314	14.94048019	4.565618205
972.587613	8.022769877	14.93726328	4.5607727
972.587613	8.032389078	14.93329668	4.55570902
973.534639	8.042250131	14.92864546	4.550459237
974.013996	8.052126713	14.92349876	4.545111427
974.48537	8.06178234	14.91813157	4.539756267
974.944426	8.071079447	14.91279823	4.534446833
975.391848	8.079984945	14.90768994	4.52917657
975.831291	8.088528971	14.90294505	4.523911217
976.267567	8.096761548	14.89868008	4.518596499
976.705773	8.104729019	14.89500981	4.513175698
977.150983	8.112464197	14.89206631	4.507586544
977.607994	8.119983802	14.89000944	4.501775996
978.080537	8.127271244	14.88903482	4.495703349
978.56928	8.134261023	14.88935624	4.489373409
978.56928	8.140825014	14.89113764	4.482878582
979.568091	8.146815103	14.89439126	4.476401305
980.055562	8.152160317	14.89894471	4.470122566
980.52661	8.156915806	14.90455162	4.46413953
980.982715	8.161211128	14.9109958	4.458460693
981.428136	8.165193745	14.91812478	4.453058956
981.867614	8.168999039	14.92581777	4.447901887
982.305561	8.172753823	14.93397919	4.44296263

982.745848	8.176575643	14.9425124	4.438225551
983.191521	8.18057521	14.95130864	4.433691291
983.644077	8.184849779	14.9602192	4.429376095
984.102379	8.189472173	14.96903201	4.425321132
984.562173	8.194470739	14.97748089	4.421584862
984.562173	8.199829286	14.9853051	4.418216378
985.464112	8.205513211	14.99232187	4.415234536
985.900314	8.211501459	14.99845532	4.412618658
986.327524	8.217794297	15.00371003	4.410331727
986.748418	8.224410298	15.00812776	4.408325045
987.165846	8.231376418	15.01176264	4.406559863
987.582151	8.238713196	15.01466914	4.404996265
987.998882	8.246428033	15.01690783	4.403606395
988.416859	8.254515631	15.01854837	4.402358711
988.836543	8.262959421	15.01967845	4.401222548
989.258522	8.271742725	15.02040358	4.400166832
989.683798	8.280852058	15.02084663	4.399156479
990.113641	8.290276598	15.02114836	4.398154141

Coordinate of **a**, optimized geometry (B3LYP-D3(BJ)/6-31G*)

C	-3.021404000	-1.508607000	-1.176415000
C	-2.079958000	-1.580023000	-0.194134000
C	-3.344909000	0.829733000	-0.630552000
C	-3.663651000	-0.259359000	-1.395692000
H	-3.268274000	-2.391157000	-1.753084000
H	-1.541860000	-2.474788000	0.089139000
H	-3.836917000	1.783890000	-0.774026000
H	-4.421337000	-0.173109000	-2.168497000
C	-2.357186000	0.793202000	0.412338000
S	-1.924267000	2.089364000	1.370430000
N	-1.749898000	-0.463418000	0.521830000
O	-0.893233000	-0.704450000	1.593447000
C	0.440502000	-0.260810000	1.452938000
C	0.856718000	0.292967000	0.091257000
C	0.990643000	-0.839443000	-0.975874000
H	0.157553000	1.074148000	-0.213285000
C	3.059103000	0.037540000	-0.568181000
H	0.225495000	-0.775883000	-1.752587000
H	0.942926000	-1.837187000	-0.514692000
O	1.147354000	-0.436523000	2.396756000
O	2.142629000	0.856183000	0.174892000
O	2.251726000	-0.599986000	-1.559330000
C	3.724452000	-0.987546000	0.347867000
H	4.412329000	-1.613606000	-0.228602000
H	4.280213000	-0.473945000	1.136777000
H	2.982239000	-1.626933000	0.831520000
C	4.047006000	0.948575000	-1.270845000
H	4.628140000	1.508282000	-0.533027000
H	4.731443000	0.357752000	-1.886165000
H	3.504004000	1.650590000	-1.907862000

G = -1180.630109, E = -1180.819258

Coordinate of **b**, optimized geometry (B3LYP-D3(BJ)/6-31G*)

C	4.022907000	-1.670357000	0.074014000
C	2.767050000	-1.623237000	-0.456548000
C	3.860557000	0.701873000	0.548825000
C	4.575834000	-0.466493000	0.583838000
H	4.563459000	-2.608032000	0.100325000
H	2.234350000	-2.464584000	-0.878794000
H	4.267552000	1.625349000	0.941657000
H	5.574640000	-0.473070000	1.009689000
C	2.534174000	0.782861000	0.011288000
S	1.585784000	2.163006000	-0.020007000
N	2.095453000	-0.440136000	-0.492027000
O	0.850478000	-0.469659000	-1.096917000
C	-0.196422000	-0.545966000	-0.158793000
C	-1.482157000	-0.132976000	-0.843460000
C	-1.929117000	1.277360000	-0.356979000
H	-1.344443000	-0.162084000	-1.928934000

C	-3.547832000	-0.218881000	0.215775000
H	-1.734501000	2.058301000	-1.092142000
H	-1.438782000	1.544536000	0.585307000
O	-0.032221000	-0.888419000	0.974434000
O	-2.535487000	-0.993906000	-0.468806000
O	-3.328322000	1.118159000	-0.207962000
C	-3.374484000	-0.373957000	1.725214000
H	-4.105889000	0.246936000	2.251677000
H	-3.524106000	-1.419401000	2.010438000
H	-2.367097000	-0.086084000	2.034081000
C	-4.909356000	-0.663834000	-0.284957000
H	-5.067728000	-1.720531000	-0.052422000
H	-5.696575000	-0.075252000	0.194953000
H	-4.964101000	-0.520980000	-1.366817000

G = -1180.640372, E = -1180.829956

Coordinate of **c**, optimized geometry (B3LYP-D3(BJ)/6-31G*)

C	1.542305000	-0.249859000	-1.036899000
C	1.974396000	1.202326000	-0.744232000
C	3.411630000	-0.209330000	0.346887000
H	1.143302000	1.877959000	-0.536273000
H	2.571495000	1.583382000	-1.584977000
O	2.611729000	-1.022848000	-0.553383000
O	2.746457000	1.045266000	0.430660000
C	4.798383000	-0.059370000	-0.270542000
H	5.440928000	0.532629000	0.387981000
H	5.253413000	-1.042994000	-0.419855000
H	4.732117000	0.440914000	-1.241377000
C	3.420881000	-0.838089000	1.728907000
H	3.900648000	-1.820615000	1.690971000
H	3.975284000	-0.201234000	2.424844000
H	2.393129000	-0.950932000	2.078240000
H	1.395686000	-0.433652000	-2.105449000
C	0.258044000	-0.588469000	-0.295595000
O	0.113111000	-1.011502000	0.811439000
O	-0.818020000	-0.324260000	-1.165063000
C	-2.494404000	0.807482000	0.089594000
C	-2.690179000	-1.560097000	-0.554949000
C	-3.794821000	0.645936000	0.674460000
C	-3.920792000	-1.683713000	0.018493000
H	-2.157505000	-2.351769000	-1.064256000
C	-4.480142000	-0.539392000	0.646414000
H	-4.205764000	1.525119000	1.155057000
H	-4.437402000	-2.634723000	-0.010474000
H	-5.459226000	-0.606586000	1.111050000
N	-2.045593000	-0.360280000	-0.522316000
S	-1.600312000	2.221666000	0.122892000

G = -1180.640908, E = -1180.830137

Coordinate of **c**, optimized geometry (B3LYP-D3(BJ)/6-31G*)

C	-2.554640000	-1.537841000	1.330946000
C	-1.925153000	-0.360320000	1.615044000
C	-2.335714000	-1.024619000	-1.025139000
C	-2.765267000	-1.866542000	-0.031589000
H	-2.877412000	-2.185472000	2.136274000
H	-1.710035000	0.008510000	2.608555000
H	-2.484053000	-1.262648000	-2.071164000
H	-3.270720000	-2.792099000	-0.290453000
C	-1.652907000	0.203919000	-0.755290000
S	-1.027666000	1.238713000	-1.917498000
N	-1.519823000	0.450834000	0.604162000
O	-1.001529000	1.671825000	1.011077000
C	0.360955000	1.937413000	0.767149000
C	1.411144000	0.836504000	0.740992000
C	2.361534000	0.941483000	-0.459983000
H	1.978488000	0.994209000	1.672084000
C	1.900115000	-1.275878000	-0.090865000
H	3.164845000	1.663957000	-0.313486000
H	1.802526000	1.175607000	-1.372987000

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O         0.684165000      3.088964000      0.807301000
O         0.945732000     -0.494494000      0.678657000
O         2.918291000     -0.363987000     -0.489082000
C         1.178854000     -1.867525000     -1.294183000
H         1.870018000     -2.488660000     -1.871827000
H         0.339090000     -2.485129000     -0.962382000
H         0.790300000     -1.071160000     -1.933478000
C         2.529061000     -2.322118000      0.815090000
H         1.767002000     -3.023132000      1.167974000
H         3.295735000     -2.879610000      0.268913000
H         2.994474000     -1.834934000      1.676149000
G = -1180.631273, E = -1180.822190
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