Electronic Supplementary Information (ESI†)

A combined photobiological-photochemical route to C_{10} cycloalkane jet fuels from carbon dioxide via isoprene

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Table of Content

1. Details for cell culture and trapping of isoprene

1.1 Biological material, cultivation and isoprene production

Isoprene production in cyanobacteria was performed using an engineered *Synechocystis* sp. PCC 6803 strain, expressing an optimized version of isoprene synthase from *Eucalyptus globulus*, together with two other enzymes - DXS and IDI - previously shown to be bottlenecks in the biosynthetic pathway. [S1]

The seed cultures were prepared by inoculating cells from the cryo-stocks into 2 mL of BG11 medium containing 20 µg mL^{-1} chloramphenicol (>98%, Sigma) in 6-well plates and growing at 30 ºC with constant shaking and constant white light at an intensity of 50 µmol photons m^{-2} s^{-1}. These cultures were scaled-up into 20 mL of medium and grown for 2 days in Erlenmeyer flasks at 30 ºC and constant light supply.

The isoprene production experiments were carried out in closed vials with bicarbonate feedstock. The seed cultures were centrifuged at 4700 x *g* for 10 minutes and the cells were resuspended in BG11 medium supplemented with 20 µg mL^{-1} chloramphenicol, 50 mM $NaHCO_3$ and 50 mM TES buffer (pH = 8.0) and diluted to an optical density at 750 nm of 0.5. Then, 20 mL of culture were transferred to 60 mL glass tubes with teflon-coated silicon septum screw caps and grown at 30 ºC with constant light. Isoprene content in the headspace of the culture tubes was assessed by sampling the gas phase and analyzing it by gas chromatography (GC, Clarus 580 FID, Perkin Elmer), as described [S1]. Growth was monitored by measuring the optical density at 750 nm after the isoprene capture from the headspace of the culture tubes.

1.2 Isoprene extraction and trapping

The photosynthetically produced isoprene was extracted from the culture tube atmosphere and trapped in a cold solvent using a custom-made vacuum system. Fig. S1 exemplifies the trapping system. From all n-alkanes (C6 to C12) tested as solvents, heptane was the only one that did not show peaks close to isoprene in the GC runs and remained liquid at the temperatures used for the isoprene trapping. In brief, 20 mL of heptane were poured into a 60 mL glass tube (TraceClean® 60 mL vials, VWR) with a teflon-coated silicon septum screw cap (PP screw caps with septum, VWR), connected to a vacuum line. A 21 gauge needle (0.80 x 120 mm sterile needle, BRAUN) was submerged in the heptane and used as gas inlet. The vial (hereafter collector tube) was then cooled down to -40 ºC using a dry ice / acetonitrile slurry. To prevent

ice formation inside the needle when cooling down the collector tube, argon was flushed through the gas inlet and the vacuum line was kept open. A 20 gauge needle (0.90 x 50 mm sterile needle, BRAUN) was plugged in the culture tube (to serve as gas outlet) and connected to the gas inlet of the collector tube, once cold. All connections were made using T-valves (Discofix® sterile stopcock, BRAUN) and teflon tubing (3 mm inner diameter PTFE tubing, VWR), as other plastics were shown to absorb isoprene.

In order to capture the isoprene from the culture tubes, the collector tube was first cooled down. Then, vacuum was created inside the tube and the culture tube was connected. Subsequently, the vacuum line was closed and the culture tube outlet / collector tube inlet was opened to draw the atmosphere out and pass it through the cold heptane. To equilibrate the pressure inside the entire system and further push the isoprene towards the collector tube, a 27 gauge needle (0.40 x 20 mm sterile needle, Terumo) was plugged in the culture tube to let air go inside. Finally, the collector tube was removed from the slurry and stored at -20 ºC until used for chemical processing.

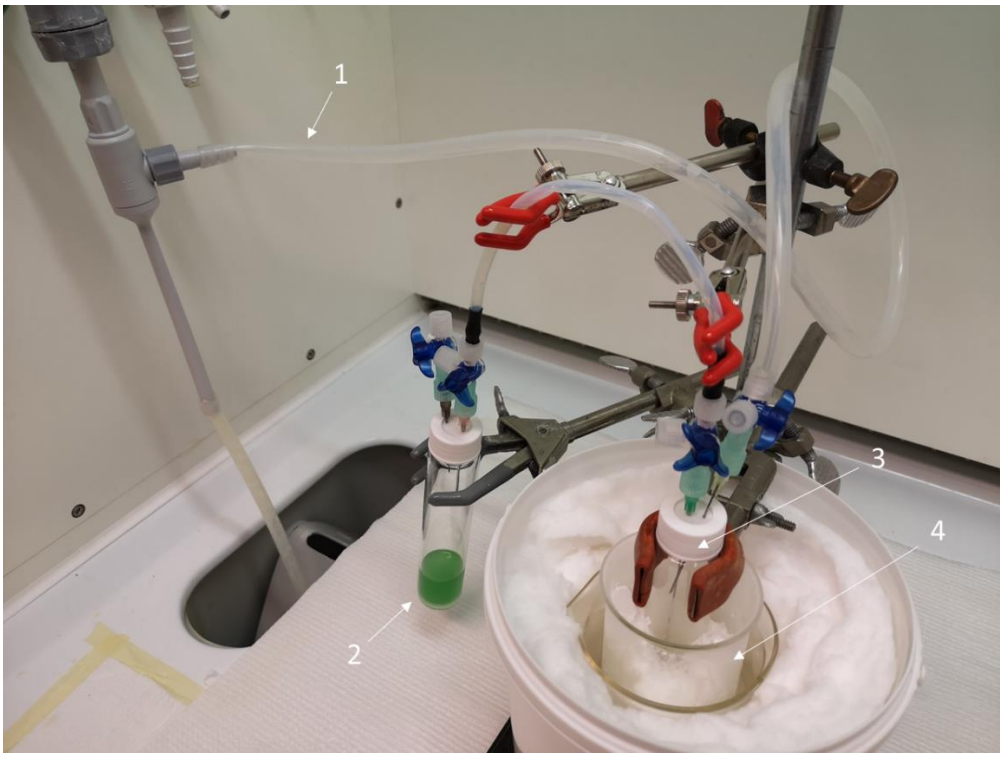


Fig. S1 Customized trapping system used to capture isoprene from the culture tubes (1 - vacuum line; 2 - culture tube; 3 - collector tube; 4 - acetonitrile / dry ice slurry at -40 ºC).

1.3 Isoprene quantification & capture efficiency

In order to quantify the amount of isoprene inside the culture tubes, a series of dilutions of isoprene standard (analytical standard grade, Sigma) in air were prepared in 60 mL glass tubes containing 20 mL of culture medium. The vials were left for 1 hour at 30 ºC and then isoprene was sampled from the headspace and analysed by gas chromatography, using the previously described method .[S1] Fig. S2 shows the correlation between the isoprene peak area (retention time at 1.75') and isoprene concentration, in µg L^{-1} culture.

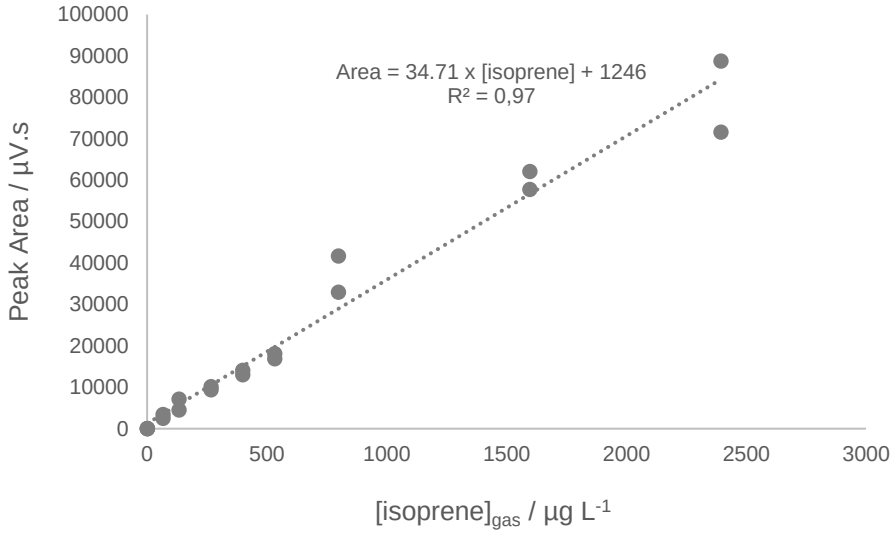


Fig. S2 Calibration with isoprene standard in 60 mL glass tubes containing 20 mL of culture medium.

The capture efficiency was estimated by measuring the isoprene content in the culture tube headspace by GC, before and after the vacuum abstraction. The highest amount of isoprene produced in this setup is described in Table S1. Note that, although the single trapping efficiencies were *ca.* 50% for the experiment described in Table S1, efficiencies of up to 89% were observed in this capture system.

Table S1 Example of isoprene production and capture. Two capturing cycles were performed, as there were still significant amounts of isoprene remaining in the culture vial after the first trapping.

Capture event	Isoprene peak area in the culture tube / µV.s		[Isoprene] / µg L^{-1}		Trapping efficiency / %
	Before trapping	After trapping	In culture tube	Trapped	
1st capture	56660.45	33711.78	1596	661	41.4
2nd capture	33711.78	16709.20	935	490	52.4

1.4 Generation of a new isoprene-producing strain by genome integration of isoprene biosynthesis genes

In order to overcome the genetic instability issues observed with the engineered strain, a second isoprene-producing strain was generated. The synthetic construct carrying the genes that encode EgIspS, DXS and IDI was integrated in the genome in the *slr0168* neutral site (NS1) together with a kanamycin resistance cassette, via homologous recombination. The resulting strain was cultivated in BG11 medium supplemented with 50 µg mL^{-1} of kanamycin over several passages to ensure the integration of the synthetic construct in all copies of the cyanobacterial genome. Full segregation was confirmed by genomic DNA extraction and PCR amplification. The new strain demonstrated higher genetic stability, as growing it for longer periods in standard conditions did not lead to loss of the ability to produce isoprene (data not shown).

1.5 Isoprene milking experiments

Seed cultures of the ΔNS1::2MEP-EgIspS engineered strain were prepared by inoculating cells from the cryo-stocks into 2 mL of BG11 medium containing 50 µg mL^{-1} kanamycin (>98%, Sigma) in 6-well plates and growing at 30 ºC with constant shaking and constant white light at an intensity of 50 µmol photons m^{-2} s^{-1}. These cultures were scaled-up into 20 mL of medium and grown for 2 days in Erlenmeyer flasks at 30 ºC and constant light supply.

The isoprene milking experiments were performed in closed vials with periodic venting of the culture atmosphere and periodic replacement of 10% of the culture with fresh medium (see Fig. S3A for a schematic representation of the procedure).

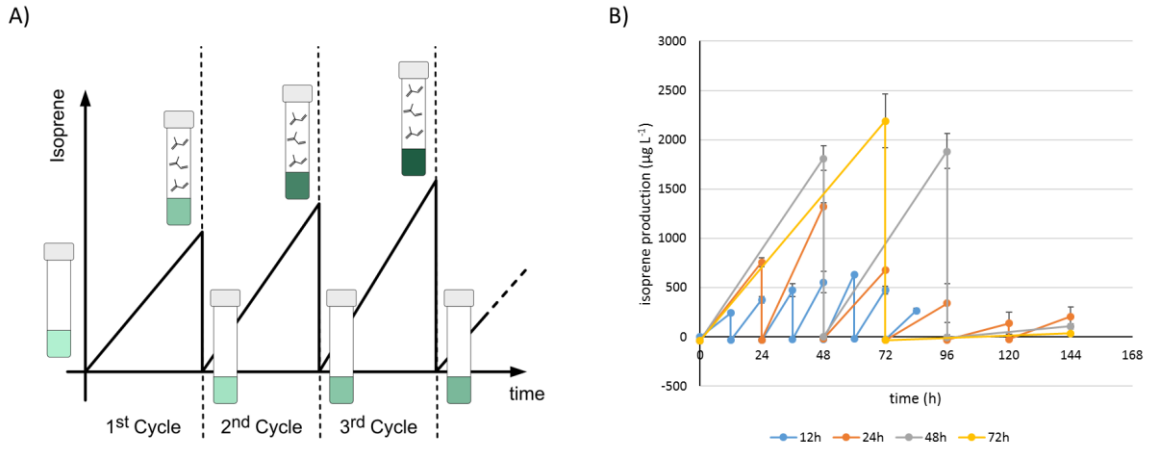


Fig. S3 Isoprene milking experiments on the engineered strain with the synthetic genetic construct for isoprene production integrated in the genome. A) Schematic representation of the cycles of isoprene production and removal in closed vials; the cultures were grown in closed vials and on every cycle isoprene was measured, the atmosphere of the vial was reset and 10% of culture was replaced with fresh medium while maintaining sterility. B) Isoprene measured in milking experiments with cycles of 12 (blue line), 24 (orange line), 48 (yellow line) and 72 hours (grey line) of isoprene production and removal. See also Fig. 3. Error bars correspond to standard deviation of two biological replicates.

The seed cultures were centrifuged at 4700 x *g* for 10 minutes and the cells were resuspended in BG11 medium supplemented with 50 µg mL^{-1} kanamycin, 50 mM $NaHCO_3$ and 50 mM TES buffer (pH = 8.0) and diluted to an optical density at 750 nm of 0.5. 20 mL of culture were then transferred to closed vials with Teflon-coated rubber septa and incubated at 30 ºC with constant shaking and constant white light at an intensity of 50 µmol photons m^{-2} s^{-1} for 6 days. At intervals of 12, 24, 48 or 72h, isoprene accumulated in the headspace of the culture tubes was measured by sampling the gas phase and analyzing it by gas chromatography (GC). The vials were then opened in a sterile way to remove all isoprene in the culture headspace, and 2 mL of culture were removed and replaced by fresh medium. After resetting the culture atmosphere, the isoprene content was measured again, to ensure that no isoprene was left inside of the closed vials, and the cultures were then placed back 30 ºC with constant shaking and constant white light for another cycle of production and isoprene accumulation. Growth was monitored by measuring the optical density at 750 nm at every cycle. The resulting cycles of isoprene production and venting with different periodicities (12, 24, 48 and 72h) can be observed in Fig. S3B and the cumulative productions and highest production rates are described in Table S2.

Table S2 Isoprene cumulative production over time and highest production rates observed when applied 12, 24, 48 or 72h cycles of isoprene accumulation and venting. See also Fig. 3.

Cycle period (h)	Cumulative production (mg L^{-1})		Highest production rate ($\mu g\ L^{-1}\ OD^{-1}\ h^{-1}$)
	3-4 days*	6 days	
12	2.9 ± 0.3	-	22 ± 2
24	3.2 ± 0.3	3.6 ± 0.5	16 ± 1
48	3.70 ± 0.06	3.81 ± 0.06	12.2 ± 0.6
72	2.2 ± 0.3	2.3 ± 0.3	8 ± 1

* - Cumulative production after 3 days for 12h and 72h cycles and 4 days for 24h and 48h cycles.

2. General experimental (chemistry) details

All common reagents used for synthesis of photo sensitizers were purchased from commercial suppliers and used as received without further purification. Isoprene (99%, contains < 1000 ppm *p-tert*-butylcatechol inhibitor as stabilizer) used for these studies, was purchased from Sigma Aldrich (Merck). Inhibitor was removed by passing isoprene through a pack of activated basic alumina and used immediately. Benzophenone (99%), xanthone (97%) and thioxanthone (97%) were purchased from Sigma Aldrich (Merck) and used for photoreaction without further purification.

The spectroscopic grade solvents used for UV-Vis measurement. The ^{1}H and ^{13}C NMR spectra were recorded on Agilent MR Spectrometer (^{1}H NMR at 399.97 MHz, ^{13}C NMR at 100.58 MHz). The residual solvent peak in NMR used as reference. The relative concentration method used for quantitative ^{1}H NMR measurement. HRMS data were obtained using a Bruker MicroTOF-Q II instrument operation at ambient temperature. UV-Vis absorption spectra were measured by a Varian Cary 5000 UV-Vis spectrophotometer. The emission spectrum of the 365 nm lamps used for photoirradiation in Rayonet photoreactor were recorded by the portable spectrometer FLAME-S-XR1.

Gas chromatography – mass spectrometry (GC-MS) (Agilent 7890A GC and 5975 MSD system) was for used for monitoring the photoreactions. Samples were introduced using split-injection (1μL injection volume; split ratio: 100:1; 250 ºC inlet temperature; Flow Rate: 120 mL/min). The starting temperature of the column oven was 70 ºC (0.5 min equilibration time)

and the ending temperature was 320 ºC. The temperature rate was set to 20 ºC/min resulting in a 12.5 min total run time. Helium was used as a carrier gas at a flow rate of 1.2 mL/min. The column used was an Agilent 19091S-433: 325 ºC: 30 m x 250 μm x 0.25 μm (front SS-inlet: He; out: vacuum). Mass spectrometer: Source temperature: 230 ºC, Quad-temperature 150 ºC.

RPR-100 and 200, Rayonet Photochemical Chamber Reactors were used for photoreaction. A set of 16 x 24W UV lamp at 365 nm (purchased from Southern New England Ultraviolet Company) were used for photo irradiation. Photoreactions were performed on two different set up (a) small-scale photoreactions: 18 mL quartz cylindrical tubes (RQV-7: Rayonet; Ø 13 mm) were used for batch reaction setup and solution was stirred during photoirradiation to homogenize the irradiation to the solution. The quartz tube above the solvent level covered with aluminum foil to avoid the complex photoreaction in vapor phase. The typical ambient temperature of Rayonet photo reactor was ~35-40 °C. (b) Large-scale photoreactions: Fluorinated ethylene propylene polymer (FEP) tube (O.D. × I.D.: 3.18 mm × 2.1 mm, loop volume ~120 mL) and FEP tube (O.D. × I.D.: 6.35 mm x 7.94 mm, loop volume: 400 mL) coiled around the water-cooled jacketed beaker (2 L, Ø:130 mm; height: 280 mm) were used. The distance between sample solutions and the lamps was 8.5 cm ≈ 3.3".

A SS-F5-3A solar simulator by Enlitech, with a 300 W Xe lamp, was used in the experiments with solar simulated light. The photoreaction in solar simulator (~10 mL loop volume) and solar irradiation (~50 mL loop volume) were carried out in home designed flat type cell. In this setup, FEP tube (O.D. × I.D.: 3.18 mm × 2.1 mm) was coiled spirally on a flat wooden surface and surface was covered with reflective aluminum foil to facilitate reflection of incident light. Parr hydrogenation apparatus was used for hydrogenation of unsaturated isoprene dimers.

The heat of combustions of hydrogenated isoprene dimers (**HIDs**) were measured by using ASTM D4809. It is determined by burning a weighed sample (~0.5 g) in an IKA C5003 oxygen-bomb calorimeter under controlled conditions. The temperature increase is measured by a temperature reading instrument which allows the precision of this test method to be met. The heat of combustion is calculated from temperature observations before, during, and after combustion, with proper allowance for thermochemical and heat-transfer corrections.

The viscosities and densities of **HIDs** were measured by using SS-EN 16896 and ASTM D4052-18a method, respectively. A test portion of a sample is introduced into the measuring cells, which are at closely controlled and known temperature. The measuring cells consist of a pair of rotating concentric cylinders and an oscillating U-tube. The dynamic viscosity is

determined from the equilibrium rotational speed of the inner cylinder under the influence of the shear stress of the test specimen and an eddy current brake in conjunction with adjustment data. The density is determined by the oscillation frequency of the U-tube in conjunction with adjustment data. The kinematic viscosity is calculated by dividing the dynamic viscosity by the density.

The flash points of the **HIDs** were measured as follows. In a typical measurement, 2 mL of **HIDs** were introduced into a stainless steel sample cup and allowed to reach equilibrium vapor pressure at the temperature specified. Then an external flame was introduced to check the flash point. The measurements were taken with the gradual increase of temperature of 0.5 °C.

3. General details on computational methods

Geometry optimizations are performed with Gaussian 16 [S2] at the (U)B3LYP/6-311+G(d,p), (U)B3LYP-D3/6-311+G(d,p) and (U)M06-2X/6-311+G(d,p) levels.[S3,S4,S5] Triplet states were calculated with the unrestricted Kohn-Sham formalism. Stationary points were characterized as minima or transition states through frequency calculations. The enthalpy corrected energies used for the calculation of the triplet energies of photosensitizers and isoprene at 298 K. The Gibbs free energies used in the mechanistic investigation were calculated at 298 K.

The enthalpies of combustion (ΔH_{comb}) are computed using the method provided by Major and co-workers[S6] at the M06-2X/6-31+G(d,p). The combustion reaction is described in Eq. 1 and the ΔH_{comb} is computed using Eq. 2. The enthalpies of vaporization (ΔH_{vap}) for hydrocarbons are obtained using the multilinear regression equation for terpenes obtained by Major and co-workers. For enthalpies of vaporization corrections, the SMD model[S7] using toluene as a solvent was employed.

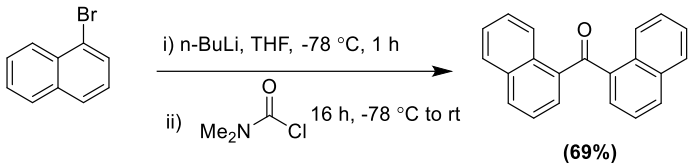
$$C_nH_m + \left(n + \frac{m}{4}\right) O_2 \rightarrow nCO_2 + \frac{m}{2} H_2O \qquad (1)$$

$$\begin{aligned} \Delta H_{\text{comb}} = n(\varepsilon_0 + \mathrm{H}^{\text{corr}})^{298K}_{CO_2(g)} + \frac{m}{2}\left[(\varepsilon_0 + \mathrm{H}^{\text{corr}})^{298K}_{H_2O(g)} - \Delta H_{\text{vap},\mathrm{H_2}O}\right] \\ - \left[(\varepsilon_0 + \mathrm{H}^{\text{corr}})^{298K}_{C_nH_m(g)} - \Delta H_{\text{vap},C_nH_m}\right. \\ \left. + (n + \frac{m}{4})(\varepsilon_0 + \mathrm{H}^{\text{corr}})^{298K}_{O_2(g)}\right] \end{aligned} \qquad (2)$$

The barriers for the closure of the radical intermediates (Fig. S46-S48) were also computed using coupled cluster with single and double substitutions and triple excitations (CCSD(T)) with single point calculations at the DFT (B3LYP and M06-2X) geometries ((U)CCSD(T)/6-311G(d,p)//(U)DFT/6-311G(d,p)).[S8-9]

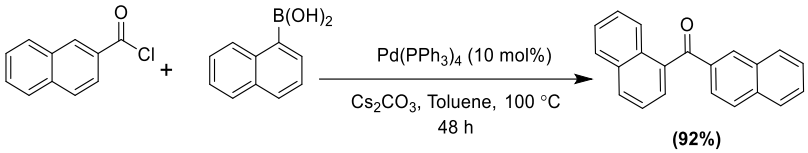
4. Detailed synthesis descriptions

4.1 Synthesis of di(naphthalen-1-yl)methanone (12)



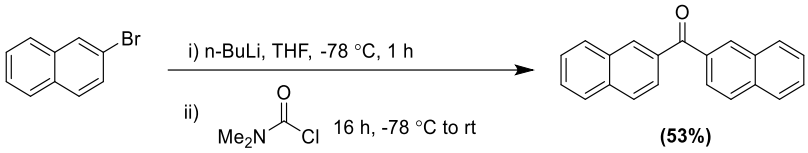
A solution of 1-bromonapthalene (24 mL, 171.5 mmol) in THF (160 mL) was placed on a dryice/ acetone bath under argon atmosphere. Then, n-BuLi (2.5 M in hexane) (75.6 mL, 188.7 mmol) was added slowly at -78 ºC and reaction mixture was allowed to stirred for 1 h. Dimethylcarbamoyl chloride (8.68 mL, 94.3 mmol) was added to the reaction mixture at -78 ºC and reaction mixture was allowed to warm up and stirred at room temperature overnight. The reaction mixture was quenched by addition of saturated ammonium chloride solution and allowed to stir for additional 10 min. Then THF was evaporated under reduced pressure and water layer was extracted thrice with DCM (~ 50 mL). The combined organic layer was dried over anhydrous sodium sulphate and evaporated to dryness under reduced pressure. The part of the crude reaction mixture crystallized by standing overnight. The mixture was washed with pentane and followed by MeOH to obtained pure **12** (15.2 g) as white crystalline solid. The pentane and MeOH washed fraction combined and evaporated under reduce pressure to obtained light yellow viscous oil. The crude reaction mixture was purified by silica gel column chromatography by using EtOAc and pentane (1:19) as eluent to yield additional pure product **12** (1.5 g, combined 16.7 g, 69% yield) as white crystalline solid. The all spectroscopic data were in good agreement with the data previously reported in literature.[S10] ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.55-8.58 (m, 2H), 8.03 (d, *J* = 8.4 Hz, 2H), 7.93-7.97 (m, 2H), 7.56-7.62 (m, 6H), 7.44 (t, *J* = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): 199.88, 137.25, 133.97, 132.62, 131.30, 130.57, 128.60, 127.97, 126.66, 126.00, 124.47.

4.2 Synthesis of naphthalen-1-yl(naphthalen-2-yl)methanone (13)



The synthesis of **13** carried out by following method reported earlier.[S11] A mixture of 2-napthoyl chloride (1.05 g, 5.51 mmol), 1-napthylboronic acid (600 mg, 3.50 mmol) and anhydrous cesium carbonate (2.3 g, 7.16 mmol) were taken under agron atmosphere. Toluene (105 mL) was added to the reaction mixture and the reaction mixture was degassed by using freeze-pump-thaw cycles. Then $Pd(PPh_3)_4$ (318 mg, 0.28 mmol) was added to the reaction mixture and allowed to stirred for 48 h at 100 ºC. After completion of the reaction, water (~100 mL) was added to the reaction mixture. The organic layer was collected and aqueous layer was washed with ethylacetate (~ 50 mL x 3). The combined organic layer was washed successively with water (~100 mL), saturated $NaHCO_3$ (~100 mL) and brine solution (~100 mL). The combined organic layer was dried over anhydrous Na_2SO_4 and evaporated under reduced pressure to dryness. The crude reaction mixture was purified by silica gel column chromatography by using EtOAc/pentane (1:4) to yield desired product **13** as white crystalline solid (910 mg, 92% yield). The all spectroscopic data were in good agreement with the data previously reported in literature.[S12] ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.25 (s, 1H), 8.04-8.12 (m, 3H), 7.90-7.97 (m, 3H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.48-7.66 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): 198.18, 136.73, 135.82, 135.76, 133.88, 133.07, 132.47, 131.35, 131.17, 129.80, 128.82, 128.58, 128.56, 127.95, 127.85, 127.42, 126.93, 126.64, 125.86, 125.50, 124.55.

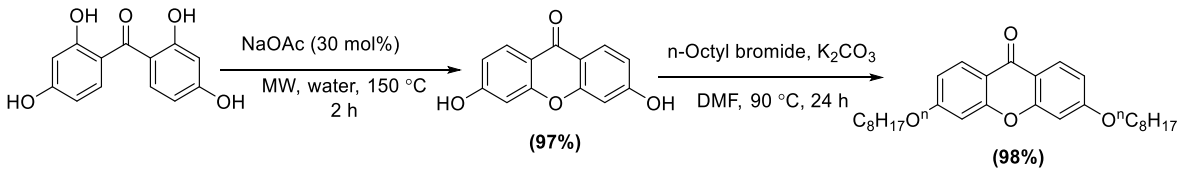
4.3 Synthesis of di(naphthalen-2-yl)methanone (14)



A solution of 2-bromonapthalene (2 g, 9.66 mmol) in THF (20 mL) was placed on a dryice/ acetone bath under argon atmosphere. Then, n-BuLi (2.5 M in hexane) (4.3 mL, 10.62 mmol) was added slowly at -78 ºC and reaction mixture was allowed to stirred for 2 h. Dimethylcarbamoyl chloride (0.5 mL, 5.43 mmol) was added to the reaction mixture at -78 ºC

and reaction mixture was allowed to warm up and stirred at room temperature overnight. The reaction mixture was quenched by addition of saturated ammonium chloride solution (~20 mL) and allowed to stir for additional 10 min. Then THF was evaporated under reduced pressure and water layer was extracted thrice with DCM (~ 20 mL). The combined organic layer was dried over anhydrous magnesium sulphate and evaporated to dryness under reduced pressure. The crude reaction mixture was purified by silica gel column chromatography by using EtOAc and pentane (1:4) as eluent to yield pure product **14** (800 mg, 53% yield) as white crystalline solid. The all spectroscopic data were in good agreement with the data previously reported in literature.[S13] ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.32 (s, 2H), 7.99 (m, 4H), 7.91-7.95 (m, 4H), 7.55-7.65 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): 196.95, 135.38, 135.27, 132.41, 131.96, 129.56, 128.49, 128.45, 127.98, 126.96, 126.01.

4.4 Synthesis of 3,6-bis(octyloxy)-9H-xanthen-9-one (15)



3,6-Dihydroxy xanthone was synthesized by the modification of procedure reported earlier.[S14] A mixture of bis(2,4-dihydroxyphenyl)methanone (1.25 g, 5.08 mmol) and NaOAc (125 mg, 1.52 mmol) in water (20 mL) was placed in microwave vial. The microwave vial was sealed and irradiated in microwave at 150 ºC for 2 h. The reaction mixture was allowed to cool down to the room temperature and the product precipitated as white fluffy solid. The precipitate was filtered, washed several time with water and dried under vacuum to obtained the desired product 3,6-dihydroxy xanthone (1.12 g, 97% yield) as white solid. The all spectroscopic data were in good agreement with the data previously reported in literature.[S14] ^{1}H NMR (400 MHz, DMSO-d_6), δ (ppm): 10.83 (brs, 2H), 7.98 (d, J = 8.8 Hz, 2H), 6.85-6.87 (dd, J = 8.8, 2.4 Hz, 2H), 6.82 (d, J = 2.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): 174.00, 163.43, 157.54, 127.83, 114.05, 113.71, 102.15.

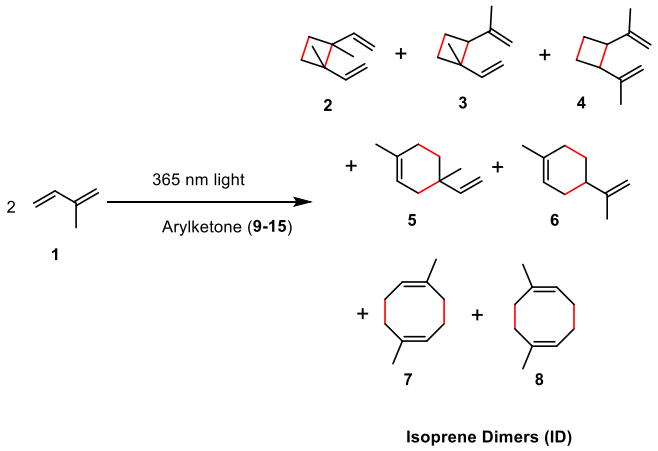
A solution of 3,6-dihydroxy xanthone (1 g, 4.38 mmol) and anhydrous K_2CO_3 (3.03 g, 21.90 mmol)in dry DMF (30 mL) was taken under argon atmosphere. Then n-octylbromide (1.55 mL, 8.98 mmol) was added to the reaction mixture and the reaction mixture was stirred at 90 °C for 24 h. The reaction mixture was quenched by addition water (~150 mL) which resulted the precipitation of the product. The precipitate was filtered and washed several time with water and dried under vacuum which resulted the desired product **15** (1.20 g, 98% yield) as white

powdery solid. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.23 (d, *J* = 8.8 Hz, 2H), 6.90-6.93 (m, 2H), 6.83 (d, *J* = 2.0 Hz, 2H), 4.06 (t, *J* = 6.6 Hz, 4H), 1.84 (q, *J* = 6.8 Hz, 4H), 1.49 (q, *J* = 6.8 Hz, 4H), 1.30-1.41 (m, 16H), 0.90 (t, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): 175.60, 164.29, 158.08, 128.10, 115.70, 113.29, 100.67, 68.73, 31.91, 29.43, 29.33, 29.11, 26.09, 22.76, 14.21; HRMS (ESI+): *m*/*z*: calculated for $C_{29}H_{40}NaO_4$ ($M+Na^+$): 475.2819; found: 475.2817.

4.5 General procedure for photochemical dimerization of isoprene

4.5.1 Rayonet reactor

A mixture of inhibitor free isoprene and photosensitizer was taken under argon and the solution was degassed by using freeze-pump-thaw cycles. Then the reaction mixture was placed in the



Rayonet reactor for photo irradiation at 365 nm for desired time. After completion of the reaction, the reaction mixture was passed through short silica gel column by using pentane as eluent to separate isoprene dimers from photosensitizer. Then pentane and unreacted isoprene was removed carefully under reduced pressure to yield desired isoprene dimers as colorless liquid. The isoprene dimers also separated from the reaction mixture by distillation under reduced pressure (65 ºC at ~0.1 mmHg). The remaining residue was passed through silica gel column by using ethylacetate and pentane mixture (1:9) as eluent to obtain the pure photosensitizer, which could be use again in the next photoreaction.

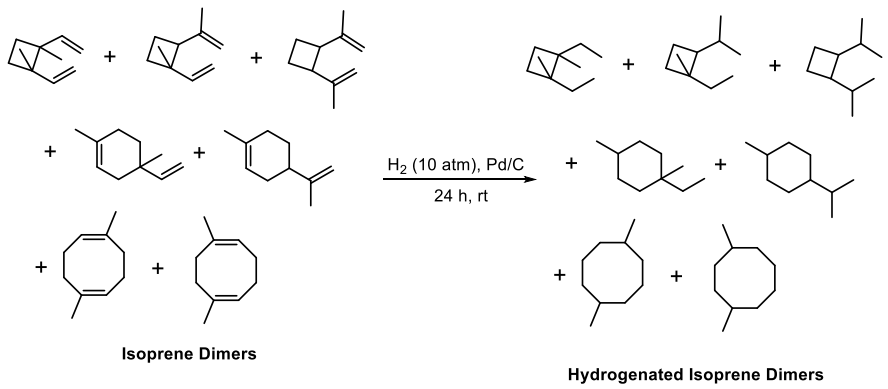
4.5.2 Solar Simulator

A mixture of inhibitor free isoprene and photosensitizer was taken under argon and the solution was degassed by using freeze-pump-thaw cycles. Then the reaction mixture (~3 mL) was transferred to the flat spiral coil and placed in the solar simulator for photo irradiation for desired time. Prior to the reaction, the distance between the sample and the lamp was adjusted to give a light intensity of one sun equivalent (AM 1.5 G) by measuring the photocurrent produced in a reference photovoltaic cell (47.6 mA). After completion of the reaction, the unreacted isoprene was removed carefully under reduced pressure.

4.5.3 Natural sunlight

A non-degassed mixture of inhibitor free isoprene and photosensitizer (~4 mL) was transferred to the flat spiral coil and placed outdoors (Uppsala, Sweden 59°51'09.5"N 17°39'19.9"E, approximately 30 m above sea level, see Fig. S14) for photo irradiation for desired time. After completion of the reaction, the unreacted isoprene was removed carefully under reduced pressure.

4.6 Hydrogenation of isoprene dimers (HID-1)



A mixture of isoprene dimers (30 g, 0.22 mol) and 10% Pd/C (2.37 g) was placed in Parr hydrogenation glass reaction vessel. The reaction mixture was stirred under 10 atm H_2 pressure for 24 h. In between, the pressure of the reaction vessel was checked several times and refilled with H_2 gas to 10 atm pressure until the pressure remains uniform to indicate the completion of the reaction. Then the reaction mixture was passed through a plug of celite and washed with

pentane. Then pentane was removed carefully under reduced pressure which leave desired hydrogenated isoprene dimers (29.8 g, 97% of yield) as colorless liquid.

4.7 General procedure for photochemical dimerization of bio-isoprene

A non-degassed mixture of bio-isoprene trapped in heptane and photosensitizer (~3 mL) was transferred to the flat spiral coil and placed in the solar simulator for photo irradiation for desired time. Prior to the reaction, the distance between the sample and the lamp was adjusted to give a light intensity of one sun equivalent (AM 1.5 G) by measuring the photocurrent produced in a reference photovoltaic cell (47.6 mA). After completion of the reaction, the reaction mixture was used for GCMS analysis.

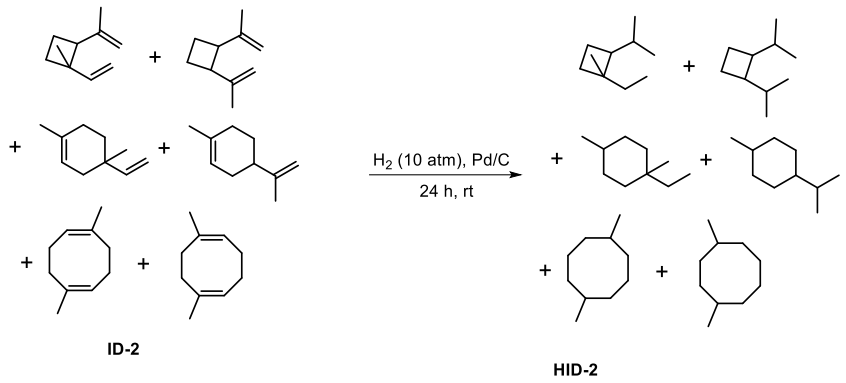
4.8 Modification of isoprene dimers at 135 °C (ID-2)

Isoprene dimers (**ID**) (20 g) was placed in a 50 mL schlenk bomb and degassed by carefully applying vacuum followed by charged with argon. This cycle was repeated for three time and flask was refilled with argon. Then the schlenk bomb was sealed under argon and placed on a heating oil bath with stirring. The isoprene dimers was heated at 135 °C for 1.5 h. Then the reaction flask was allowed to cool down to room temperature. The isoprene produced in this reaction was removed under reduced pressure to obtained desired **ID-2** (18.4 g, 92% of yield) as colorless liquid.

4.9 Modification of isoprene dimers at 160 °C (ID-3)

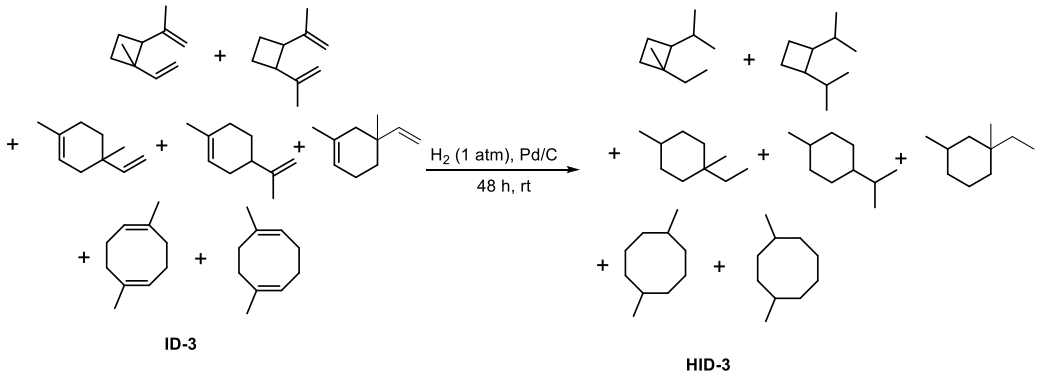
Isoprene dimers (**ID**) (20 g) was placed in a 50 mL schlenk bomb and degassed by carefully applying vacuum followed by charged with argon. This cycle was repeated for three time and flask was refilled with argon. Then the schlenk bomb was sealed under argon and placed on a heating oil bath with stirring. The isoprene dimers was heated at 160 °C for 4 h. Then the reaction flask was allowed to cool down to room temperature. The isoprene produced in this reaction was removed under reduced pressure to obtained desired **ID-3** (17.6 g, 88% of yield) as colorless liquid.

4.10 Hydrogenation of ID-2 (HID-2)



A mixture of modified isoprene dimers **(ID-2)** (27.3 g, 0.20 mol) and 10% Pd/C (2.13 g) was placed in Parr hydrogenation glass reaction vessel. The reaction mixture was stirred under 10 atm H_2 pressure for 24 h. In between, the pressure of the reaction vessel was checked several times and refilled with H_2 gas to 10 atm pressure until the pressure remains uniform to indicate the completion of the reaction. Then the reaction mixture was passed through a plug of celite and washed with pentane. Then pentane was removed carefully under reduced pressure, which leave desired **HID-2** (27.1 g, 96% of yield) as colorless liquid.

4.11 Hydrogenation ID-3 (HID-3)



A mixture of isoprene dimers (30.3 g, 0.22 mol) and 10% Pd/C (2.37 g) were placed in a round bottom flask. The reaction mixture was charged with hydrogen gas and stirred under 1 atm H_2 pressure (hydrogen balloon) for 48 h. In between, the reaction vessel was refilled with H_2 gas and progress of the reaction was monitored by ^{1}H NMR for the completion of the reaction. The reaction mixture was passed through celite and washed with pentane. Pentane was removed under reduced pressure, which leave desired hydrogenated isoprene dimers (30.1 g, 96% of yield) as colorless liquid.

5. Additional Figures

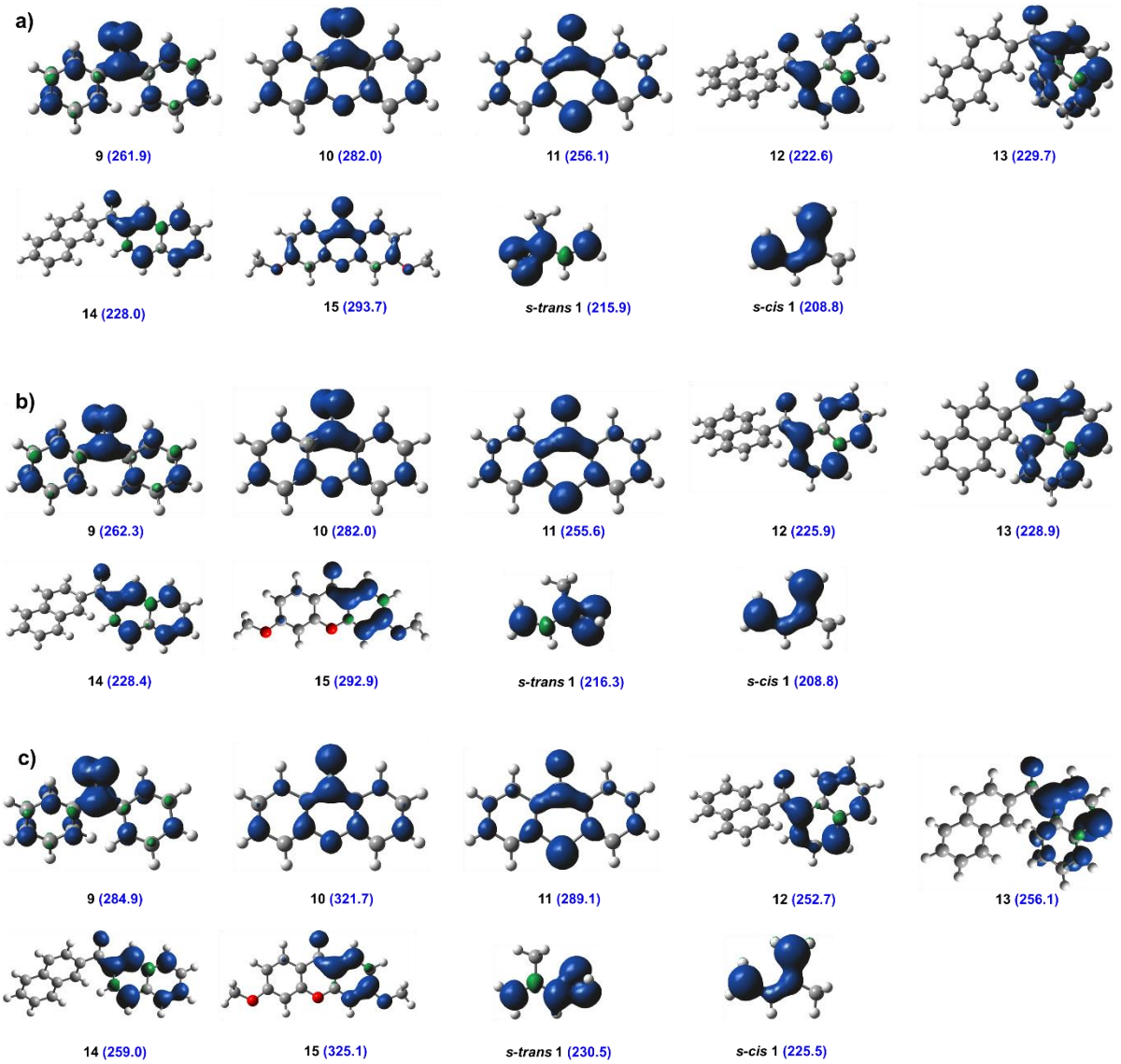


Fig. S4 The spin density (iso value: 0.004) of the triplet photosensitizers used in this studies and isoprene with their calculated adiabatic triplet energies (kJ/mol) at, a) B3LYP/6-311+G(d,p), b) B3LYP-D3/6-311+G(d,p) and c) M0-62X/6-311+G(d,p) level in parenthesis in blue color. Dioctyl groups of **15** was replaced with methyl group for ease of calculation.

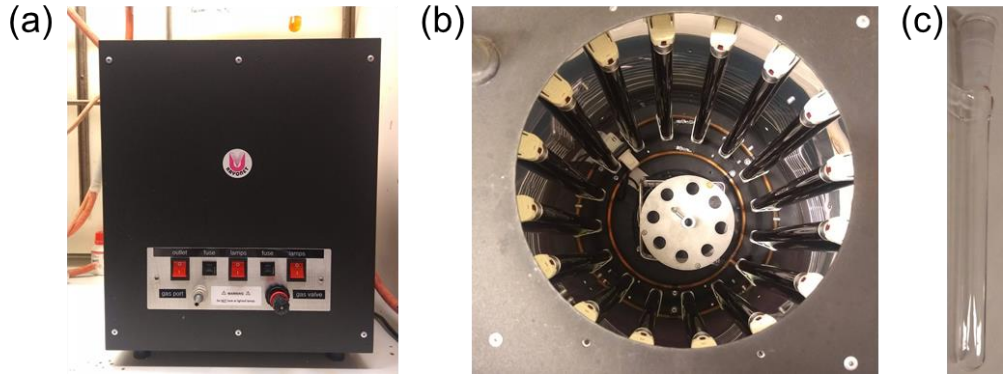


Fig. S5 (a) The Rayonet photoreactor (RPR-200) used for photo irradiation of isoprene (side view). (b) Top view of Rayonet photoreactor which showing the array of 16 lamp aligned vertically and sample place on the middle in a carosel. (c) The quartz tube (18 mL) used for photoirradiation of isoprene in batch setup.

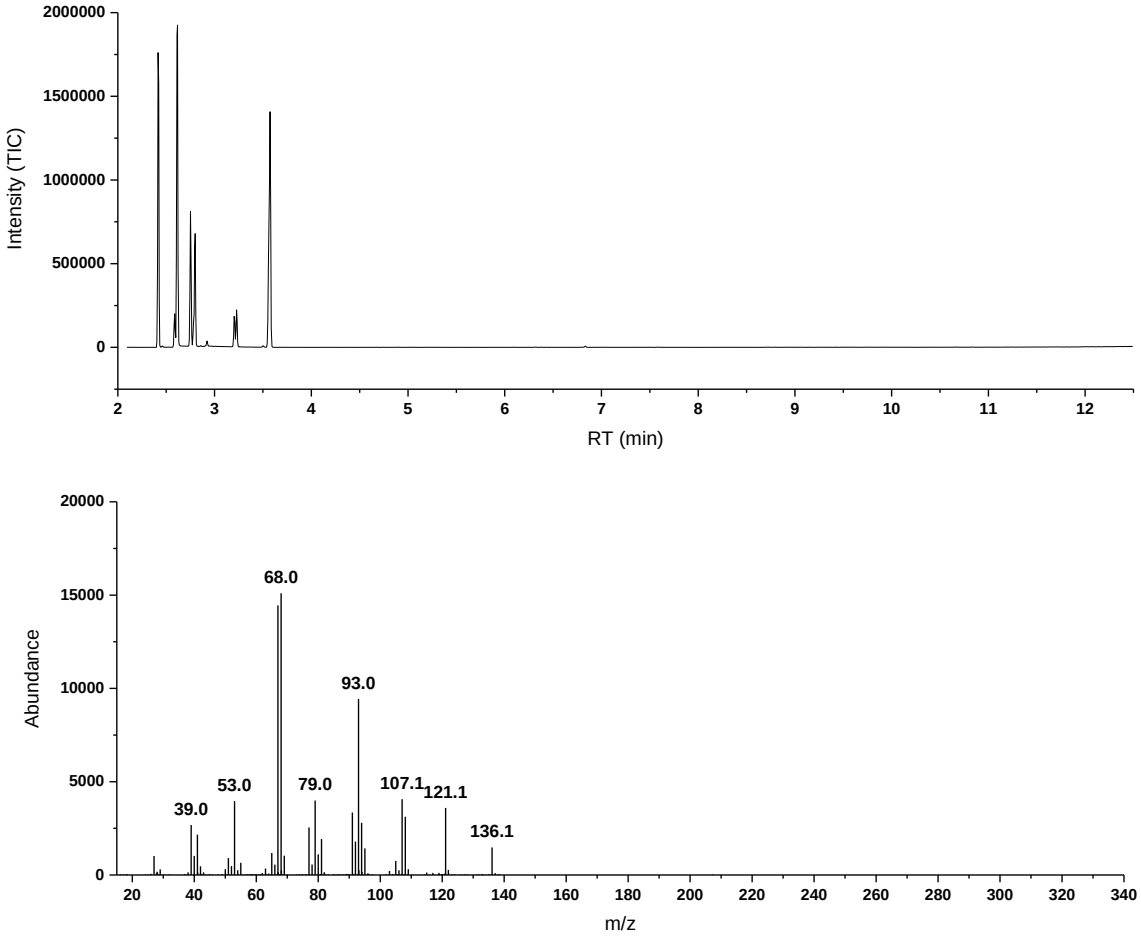


Fig. S6 Gas chromatogram showing dimers of isoprene (top) and the average mass spectrum (bottom) for the region RT = 2.367 to 3.617 min. The isoprene dimers were produced in the dimerization of isoprene photosensitized by benzophenone **9**. The sample was irradiated in the Rayonet photoreactor, 365 nm lamp, for 44 h.

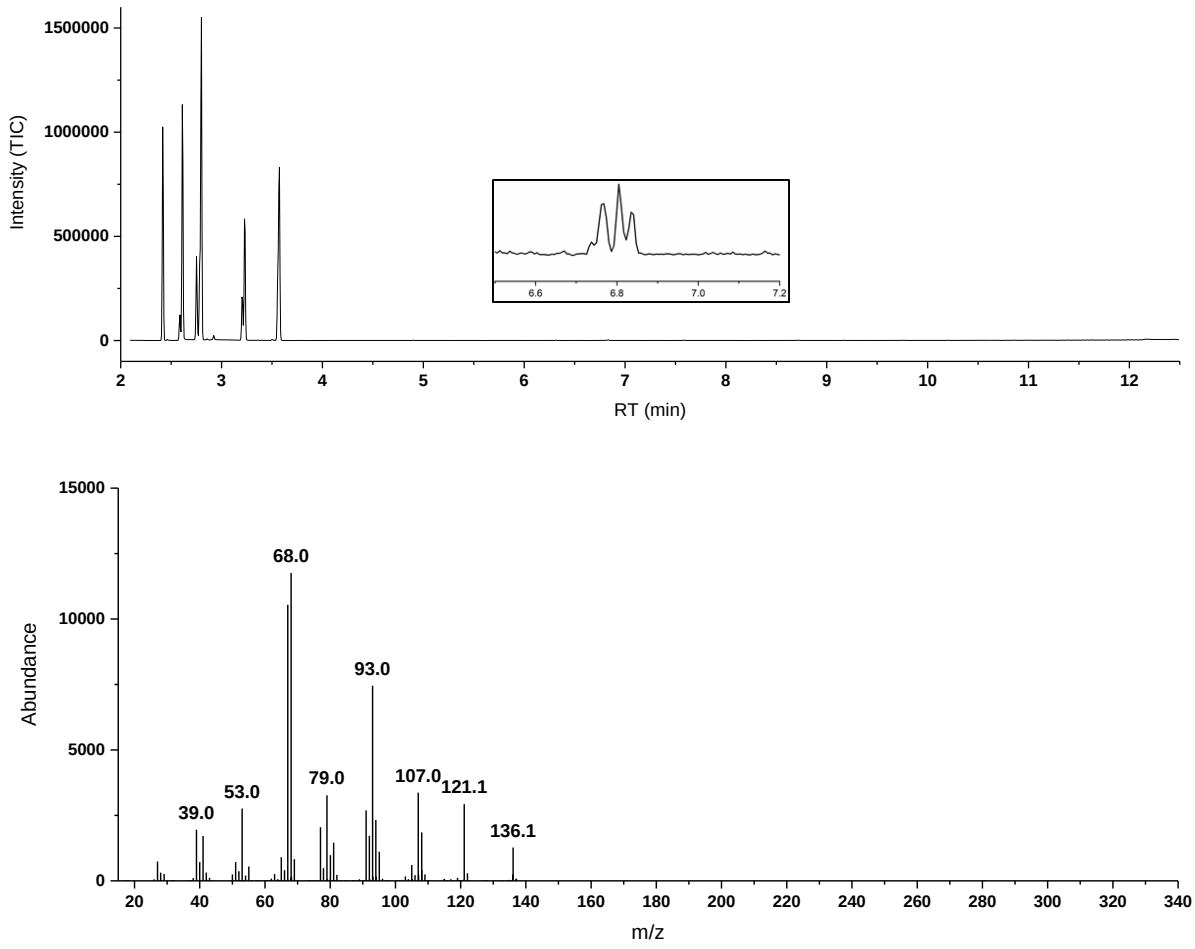


Fig. S7 Gas chromatogram (top) showing dimers of isoprene and the average mass spectrum (bottom) for the region RT = 2.361 to 3.605 min. The isoprene dimers were produced in the dimerization of isoprene photosensitized by **12**. The inset in the GC (top) showed the trace amount of isoprene trimers formed. The sample was irradiated in the Rayonet photoreactor, 365 nm lamp, for 44 h.

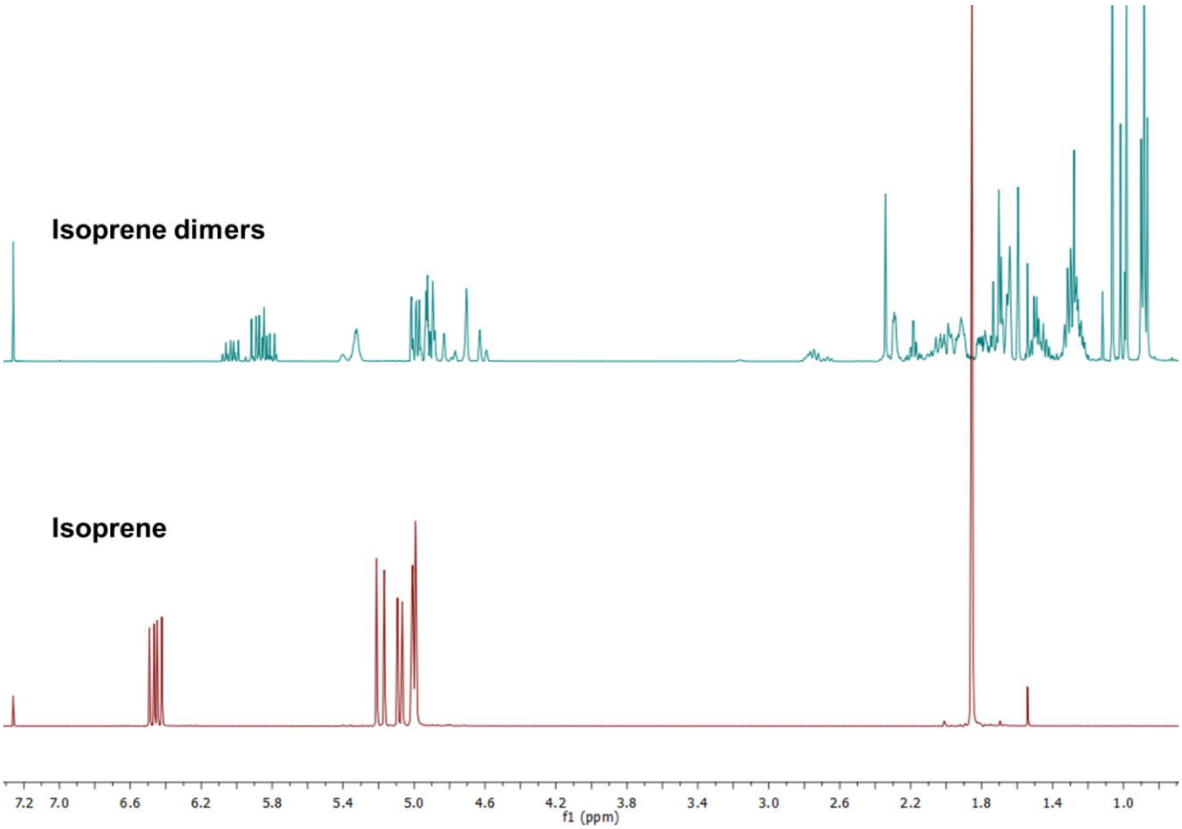


Fig. S8 The full scale ^{1}H NMR of isoprene and isoprene dimers.

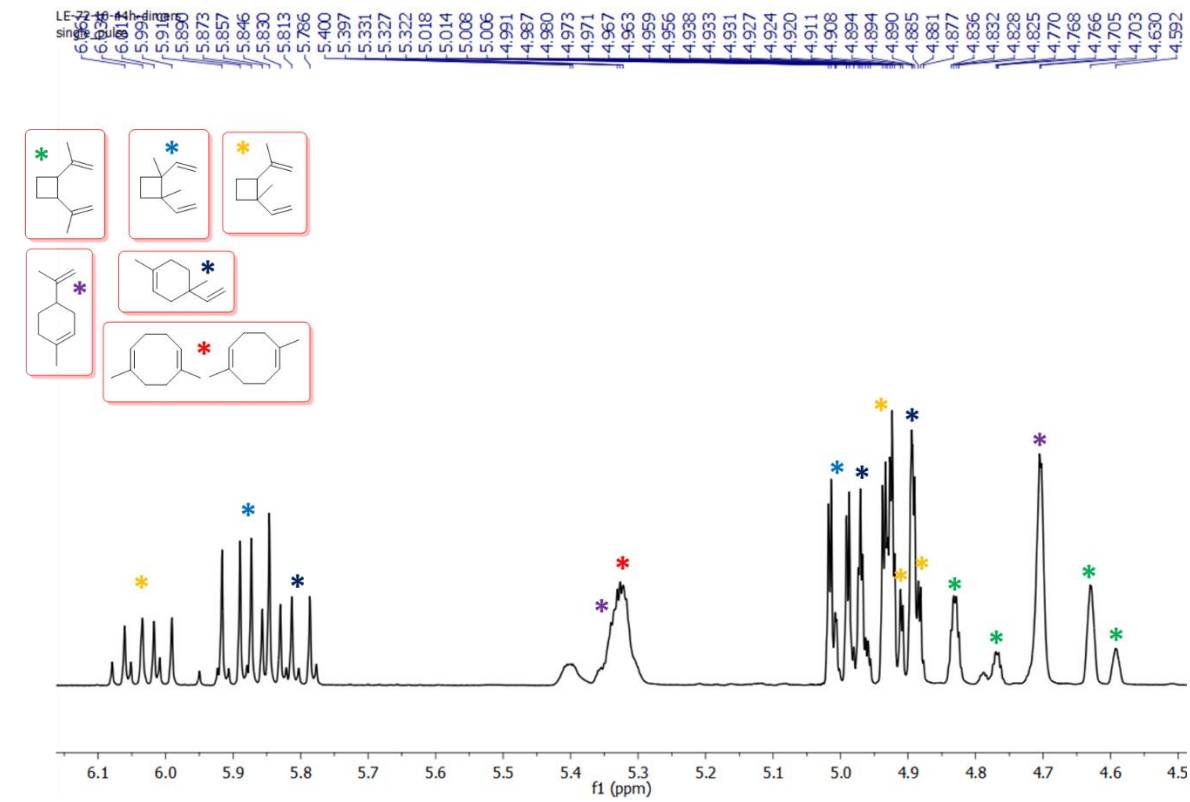


Fig. S9 The partial ^{1}H NMR of isoprene dimers (alkene part) and the corresponding assigned peaks for seven isomers.

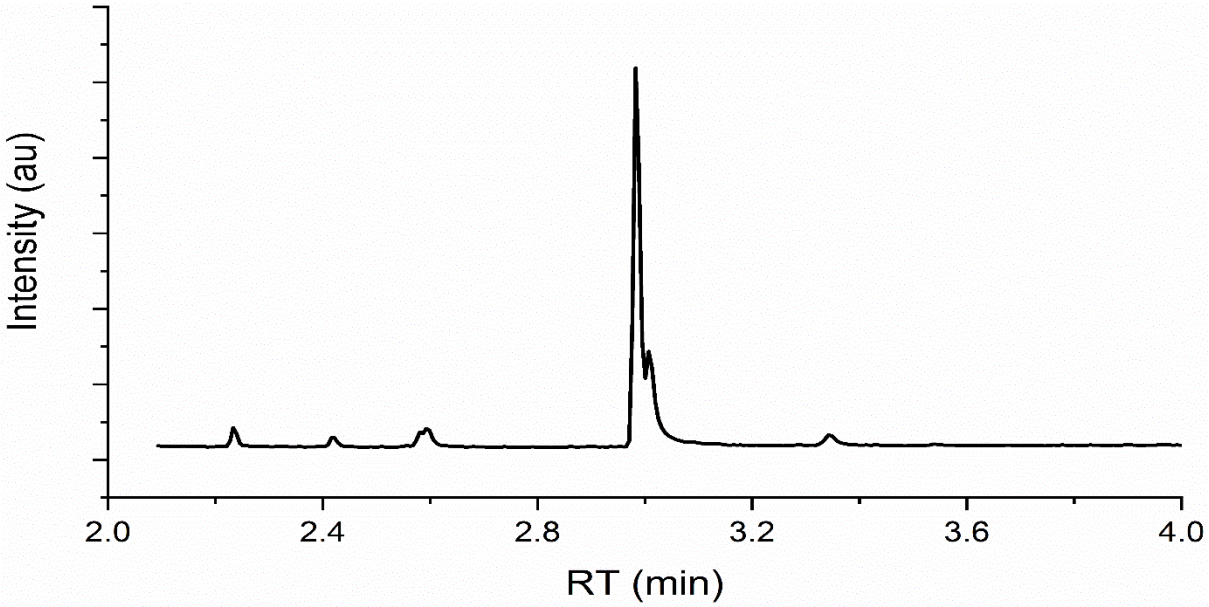


Fig. S10 Gas chromatogram of isoprene irradiated in absence of photosensitizers at 365 nm for 44 h.

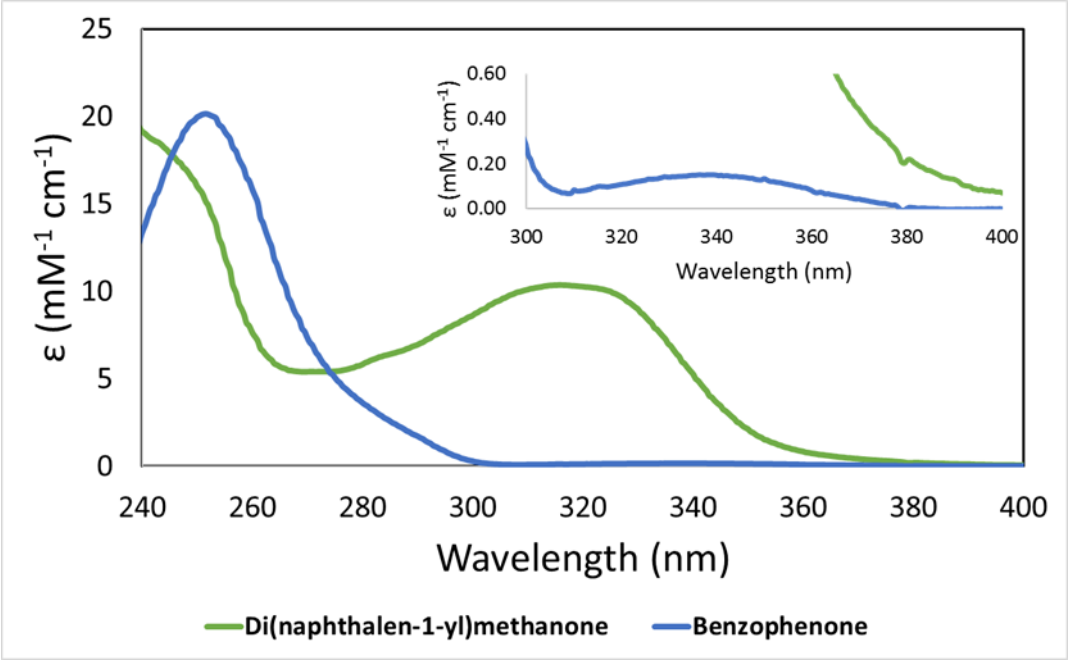


Fig. S11 UV-Vis absorption of benzophenone and di (naphthalene-1-yl)methanone in dichloromethane at room temperature (in inset: expanded part for 300 to 400 nm range).

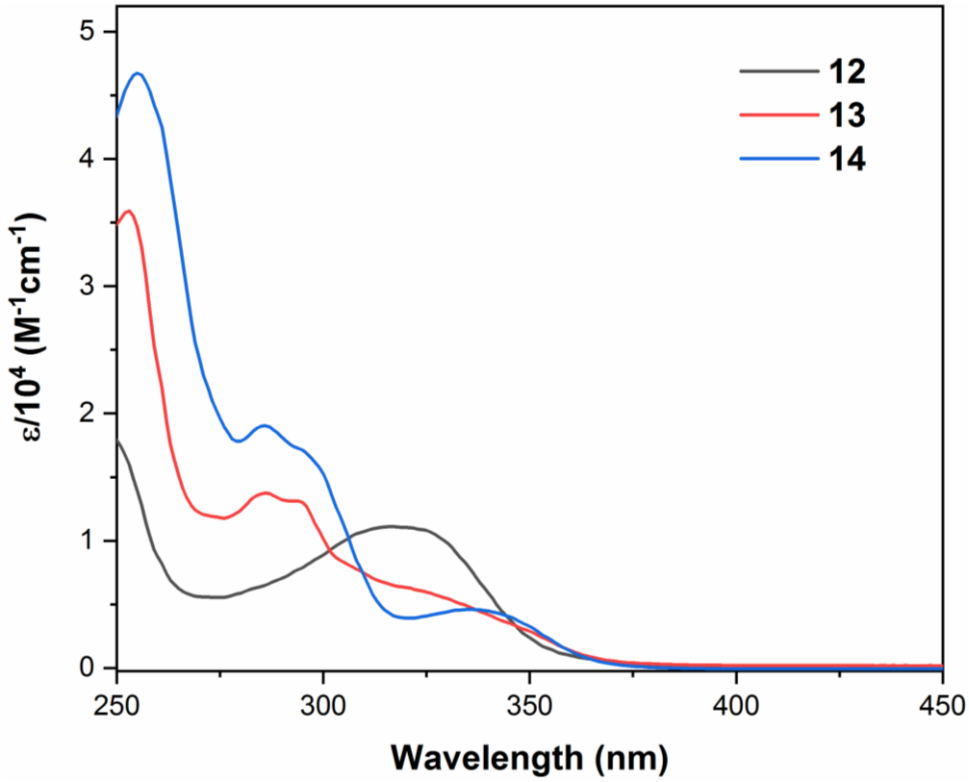


Fig. S12 UV-Vis absorption of di (naphthaleneyl)methanones in dichloromethane at room temperature (in inset: expanded part for 300 to 400 nm range).

Table S3 Screening of the loading of dinapthylmethanone **12** for isoprene photodimerization.

Entry	Loading of 12 (mol%)	Isolated yield (%)
1	0.50	41
2	0.20	40
3	0.10	41
4	0.05	31
5	0.025	31
6	0.01	21

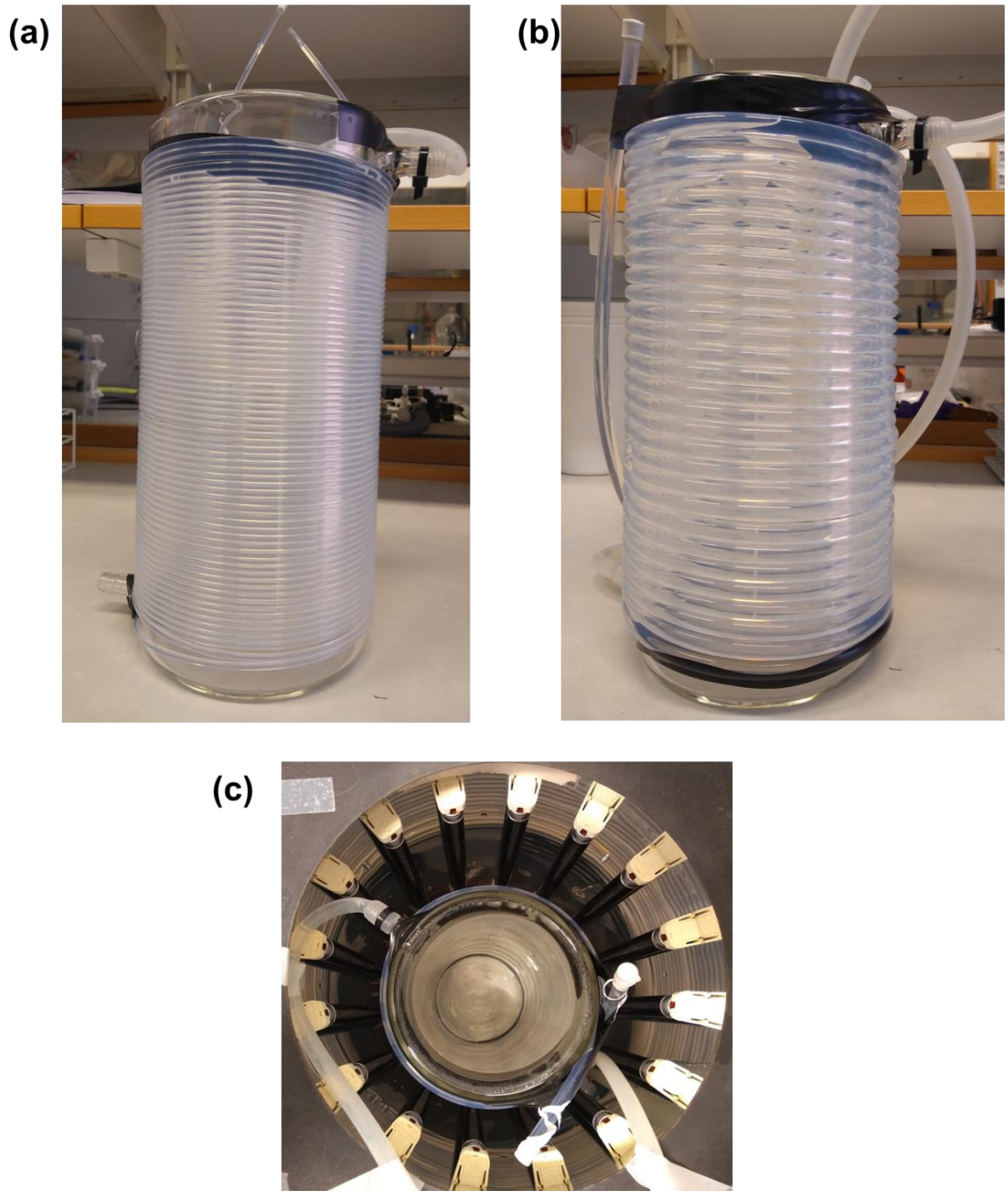
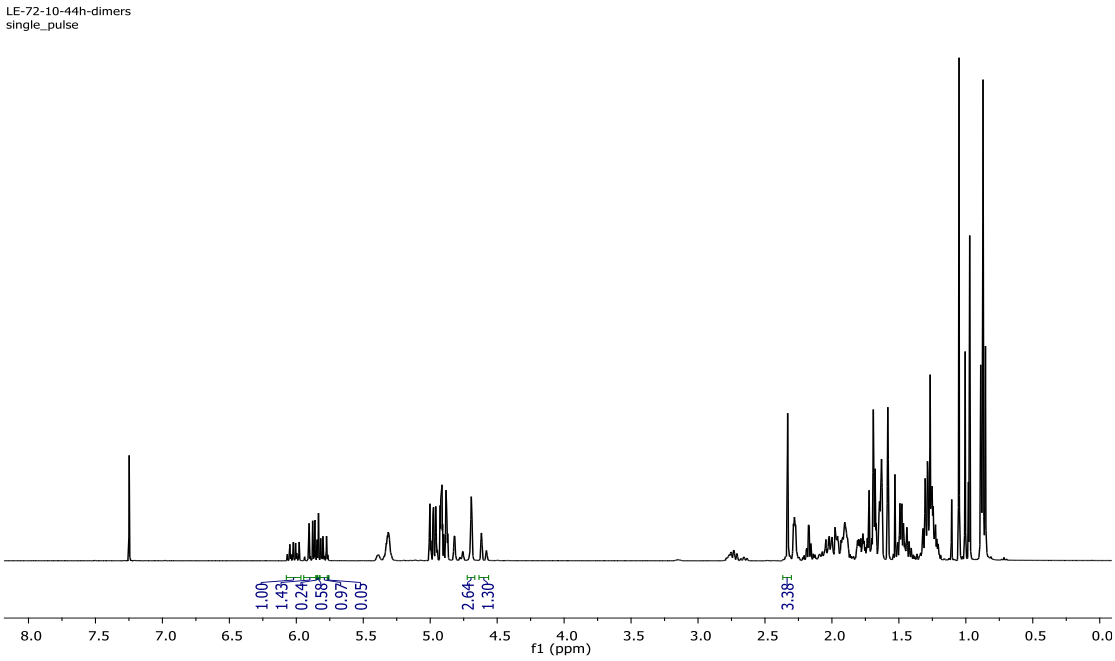


Fig. S13 The homemade FEP tube (a) (O.D. × I.D.: 3.18 mm × 2.1 mm; loop volume: 120 mL) and (b) (O.D. × I.D.: 6.35 mm x 7.94 mm, loop volume: 400 mL) coiled around the water-cooled jacketed beaker (2 L, Ø:130 mm; height: 280 mm) used for photoirradiation isoprene. The water condenser allows the reaction to run at ~10 °C. The isoprene and photosensitizers mixture inserted into to Teflon tube and sealed at both end using rubber septa. (c) Coiled FEP tubing on water cooled jacketed beaker placed inside Rayonet photoreactor for photoirradiation.



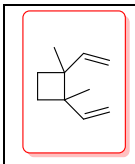
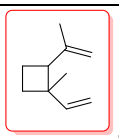
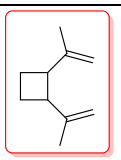
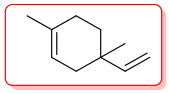
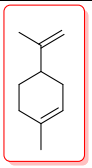
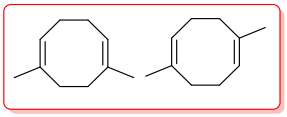
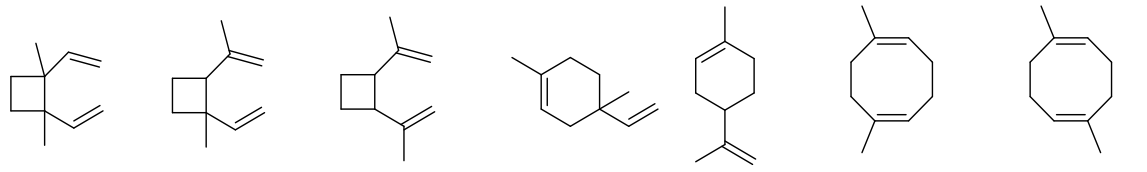
 **2** Relative integration = (1.96/2) = 0.98	 **3** Relative integration = (1/1) = 1	 **4** Relative integration = (1.30/2) = 0.65
 **5** Relative integration = (1.26/1) = 1.26	 **6** Relative integration = (2.64/2) = 1.32	 **7** and **8** Relative integration = (3.38/4) = 0.845
Total integration= 6.055		
% of isoprene dimers  **2** b.p. 135 °C (16.1%) **3** b.p. 153 °C (16.5%) **4** b.p. 155 °C (10.7%) **5** b.p. 162 °C (20.8%) **6** b.p. 177 °C (21.8%) **7** b.p. 184 °C **8** b.p. 182 °C (14.0%)		

Fig. S14 The % of isoprene dimers (boiling point mentioned) in the mixture of photodimers of isoprene obtained by quantitative ^{1}H NMR (the relative concentration method used) analysis.

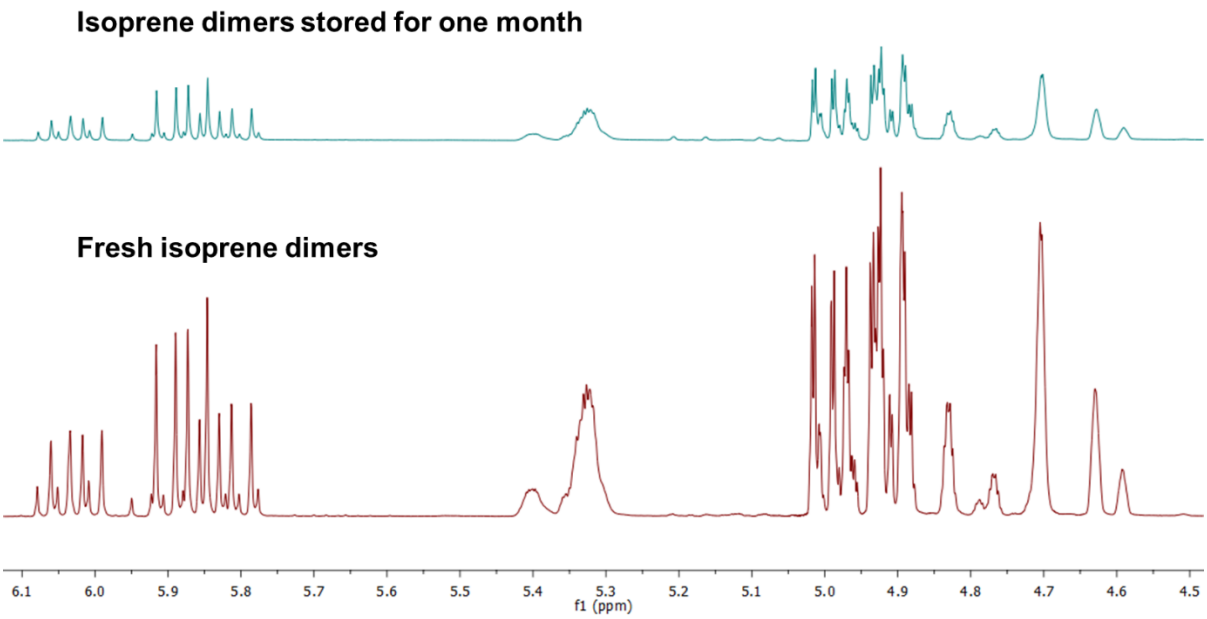


Fig. S15 Comparative ^{1}H NMR of fresh isoprene dimers and isoprene dimers stored at 4 ºC for one month. There is no noticeable changed is observed for isoprene dimers when stored at 4 ºC.

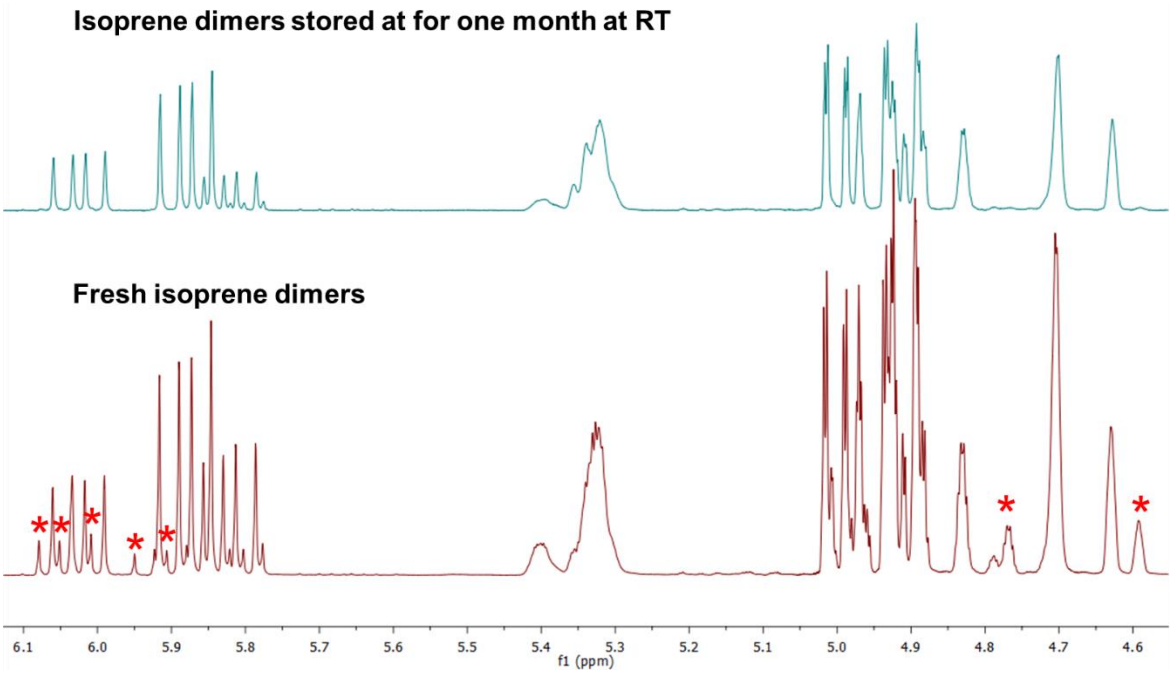


Fig. S16 Comparative ^{1}H NMR of fresh isoprene dimers and isoprene dimers stored at room temperature for one month. The peaks corresponding to the minor isomers of [2+2] photodimers significantly diminished.

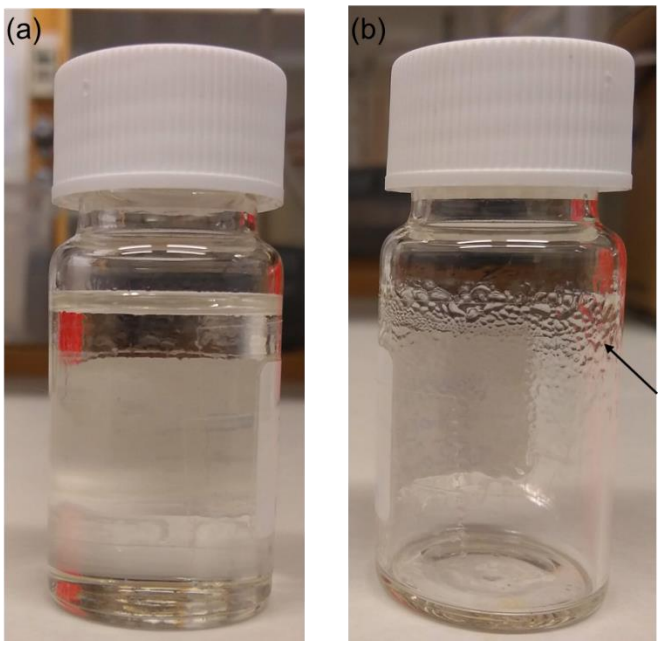


Fig. S17 (a) Isoprene dimers stored under ambient condition for more than one month in a sample vial. (b) Isoprene dimers were removed from the sample vial, which revealed the formation of insoluble colorless viscous oxidized dimers on the surface (marked with black arrow)

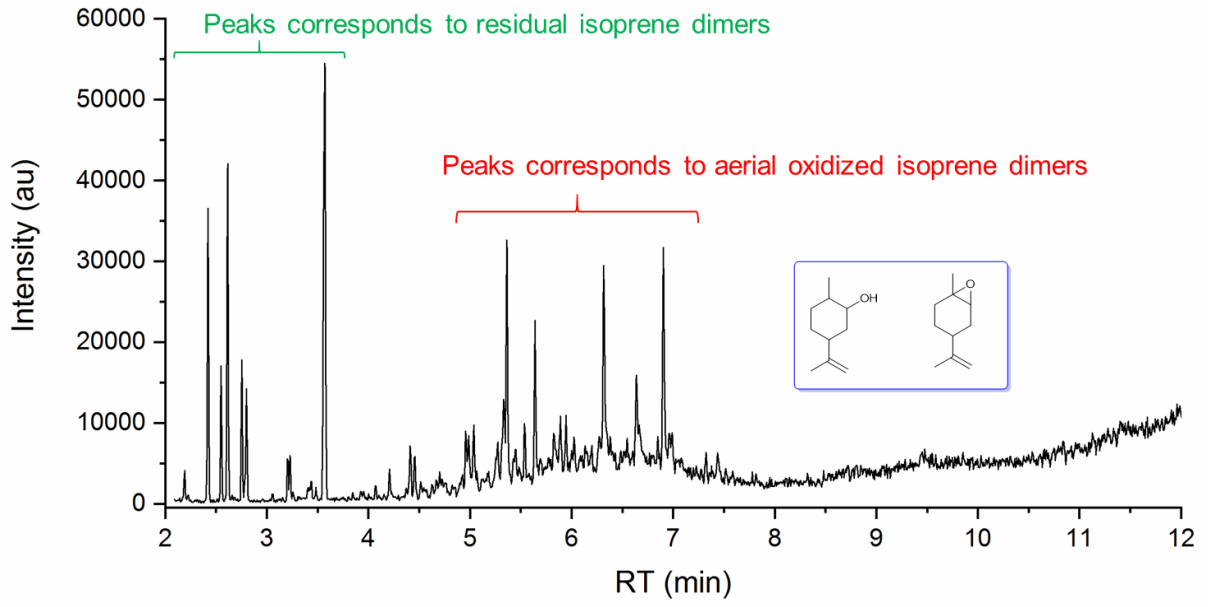


Fig. S18 Gas chromatogram (GC) of the oxidized isoprene dimers. The peaks corresponds to residual isoprene dimers was also seen in this GC. The two identified products of oxidized limonene by GCMS analysis, showed in the inset.

Quantum yield determination of the dimerization of isoprene photosensitized by α-dinaphthylketone and benzophenone under UV irradiation (365 nm, Rayonet photoreactor)

The quantum yield of the photosensitized isoprene dimerization was determined by ferrioxalate actinometry, following procedure from recent literature.[S15-17] A full spectra analysis was necessary since the light source was not monochromatic and both the actinometer and photosensitizers had different extinction coefficients of absorption in the multiple wavelengths available. Moreover, ferrioxalate photoreduction has wavelength-dependent quantum yields. All manipulation of ferrioxalate was performed under dark red-light conditions.

Three quartz test tubes containing ferrioxalate Solution A (c = 0.01 M, 3 mL) were irradiated for different times (30, 60 and 90 s) in the Rayonet photoreactor (365 nm lamp). In a 10 mL volumetric flask, 1 mL of each irradiated sample was complexed with 4 mL of 1,10-phenantrhroline solution (0.1 %) and 0.5 mL of $H_3CCOONa$ buffer was added. Then the flask was filled with deionized water up to the 10 mL mark. Samples were kept in the dark for 1 h for color development. The concentration of Fe^{2+} was determined by UV-Vis, recording the absorbance of each sample at 510 nm. The extinction coefficient ε_{510} = 11050 M^{-1} cm^{-1} was used to convert the absorbance to concentration of Fe^{2+} ions. The concentration of Fe^{2+} ions against reaction time is plotted in Fig. S19.

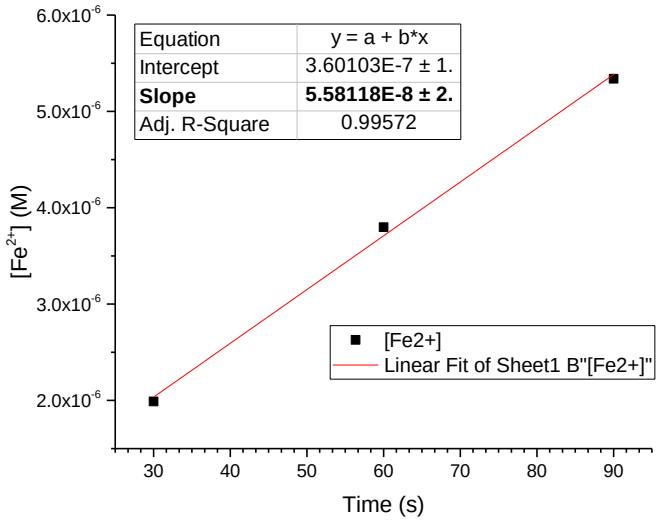


Fig. S19 Concentration of Fe^{2+} ions produced after ferrioxalate samples were irradiated for different times. Inset shows the linear correlation parameters calculated for this plot.

The slope from the plot on Fig. S18 is the rate constant for the production of Fe^{2+}, $k(Fe^{2+})$:

$$k(Fe^{2+}) = (5.58\ x\ 10^{-8})\ M.s^{-} \qquad \text{Eq. 1}$$

On the same conditions, 3 mL of a solution of α-dinaphthylketone in isoprene (0.5 $_{mol}$% or 0.05 M, Solution B) and 3 mL of a solution of benzophenone in isoprene (2.0 $_{mol}$% or 0.66 M, Solution C) were irradiated for 19h 43min and 24h 16min, respectively. The rate constants for the formation of dimers from the irradiation of solutions B and C were calculated as in Equations 2-3:

$$k_B(dimers) = \frac{0.00274\ mol}{70980\ s} = 3.86\ x\ 10^{-8}\ mol\ s^{-} \qquad \text{Eq. 2}$$

$$k_C(dimers) = \frac{0.00151\ mol}{87360\ s} = 1.73\ x\ 10^{-8}\ mol\ s^{-} \qquad \text{Eq. 3}$$

The emission spectrum of the 365 nm lamps from Rayonet photoreactor were recorded by the portable spectrometer FLAME-S-XR1 (Fig. S19).

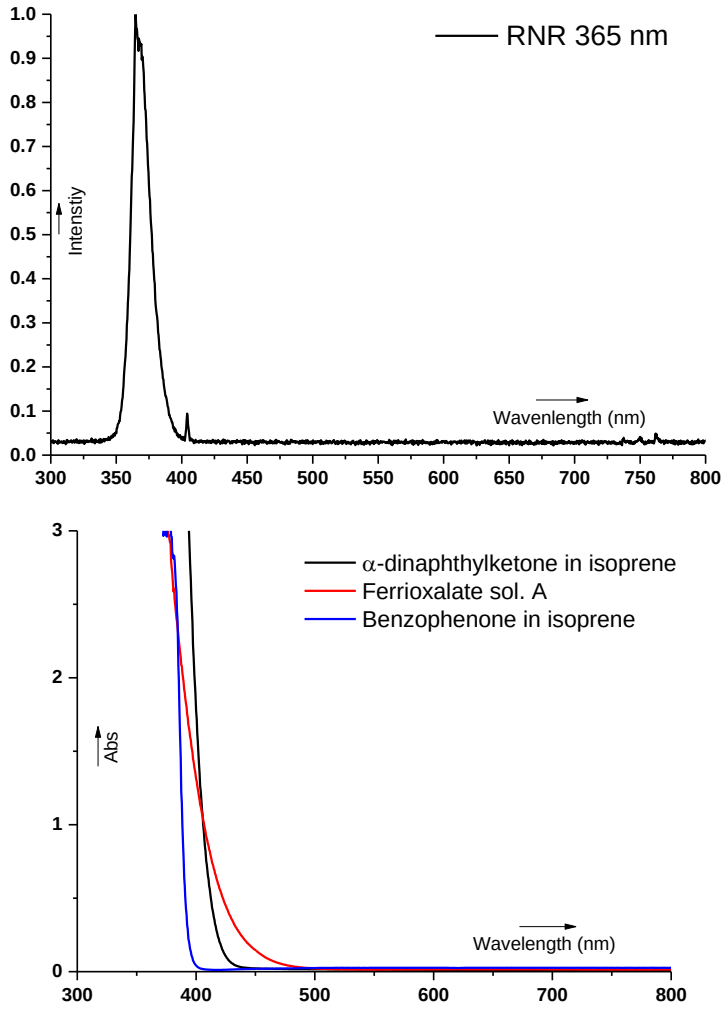


Fig. S20 Normalized emission spectrum of 365 nm lamp used in Rayonet photoreactor setup (top) and absorption spectra of the irradiated solutions (bottom).

Since ferrioxalate, benzophenone and α-dinaphthylketone absorb in multiple wavelengths present at the emission spectrum of the 365 nm lamps from Rayonet photoreactor, all solutions A, B and C had their spectra recorded, as also shown on Fig. S19. One can see that these solutions have a high absorption on the spectral region correspondent to 365 nm lamp emission.

The light intensity absorbed by the ferrioxalate solution A was calculated by multiplying the intensity of RNR 365 nm lamp at each wavelength by the transmittance of ferrioxalate (obtained from the absorption spectrum shown on Fig. S19) subtracted from unit, at each wavelength, as in Equation 4:

$$I(ferriox, \lambda) = I(RNR365)\ x\ [1 - T(ferriox, \lambda)] \qquad \text{Eq. 4}$$

Similarly, the light intensity absorbed by α-dinaphthylketone or benzophenone (PS) was calculated, as in Equation 5:

$$I(PS,\lambda) = I(RNR365)\ x\ [1 - T(sol.B\ or\ C,\lambda)] \qquad \text{Eq. 5}$$

The total light intensities absorbed by ferrioxalate and by α-dinaphthylketone or benzophenone (PS) were calculated by integration of their spectra in the region 300 – 450 nm:

$$I(ferriox,total) = \int_{300}^{450} I(ferriox,\lambda) \qquad \text{Eq. 6}$$

$$I(PS,total) = \int_{300}^{450} I(PS,\lambda) \qquad \text{Eq. 7}$$

The photon flux P was calculated by integration of $k(Fe^{2+})$, in mol . s^{-1} units, divided by the quantum yields of ferrioxalate in different wavelengths, obtained from literature,[S16] in the region between 300 – 450 nm, as shown in Equation 8:

$$P = \int_{300}^{450} \frac{k(Fe^{2+})}{\phi(\lambda)} \qquad \text{Eq. 8}$$

Table S4 Calculated values for quantum yield determination.

Entry	Value	Unit
$k(Fe^{2+})$	$5.58\ x\ 10^{-8}$	M s^{-}
$k(Fe^{2+})$	1.67 x 10^{-10}	mol s^{-}
$k_B(dimers)$ α-dinaphthylketone	$3.86\ x\ 10^{-8}$	mol s^{-}
$k_C(dimers)$ benzophenone	$1.73\ x\ 10^{-8}$	mol s^{-}
P	$2.14\ x\ 10^{-8}$	Einstein s^{-}
$I(ferriox,total)$	293716	a.u.
$I_B(PS,total)$ α-dinaphthylketone	289493	a.u.
$I_C(PS,total)$ benzophenone	275362	a.u.

Substituting the values summarized on Table 1 in the Equation 9, the quantum yields for the dimerization for both photosensitizers were determined:

$$\phi_{dimers} = \frac{k(dimers)}{P}\ x\ \frac{I(ferriox,total)}{I(PS,total)}\ x\ \frac{1}{2} \qquad \text{Eq. 9}$$

For the dimerization photosensitized by α-dinaphthylketone:

$$\phi_B = \frac{(3.86\ x\ 10^{-8})}{(2.14\ x\ 10^{-8})}\ x\ \frac{293716}{289493}\ x\ \frac{1}{2} = 0.91 \qquad \text{Eq. 10}$$

For the dimerization photosensitized by benzophenone:

$$\phi_C = \frac{(1.73\ x\ 10^{-8})}{(2.14\ x\ 10^{-8})}\ x\ \frac{293716}{275362}\ x\ \frac{1}{2} = 0.43 \qquad \text{Eq. 11}$$

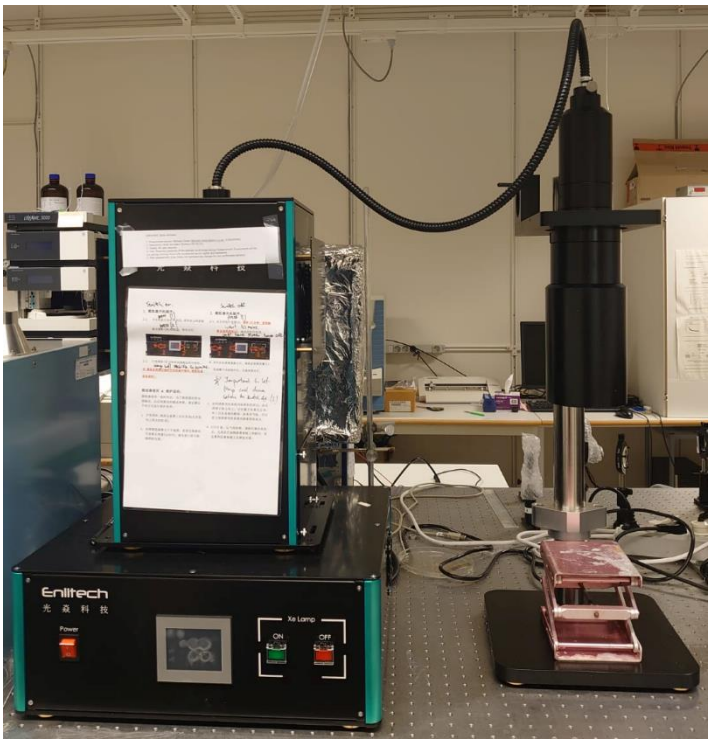


Fig. S21 SS-F5-3A solar simulator by Enlitech, with a 300 W Xe lamp, was used for photodimerization of isoprene by using solar simulated light.

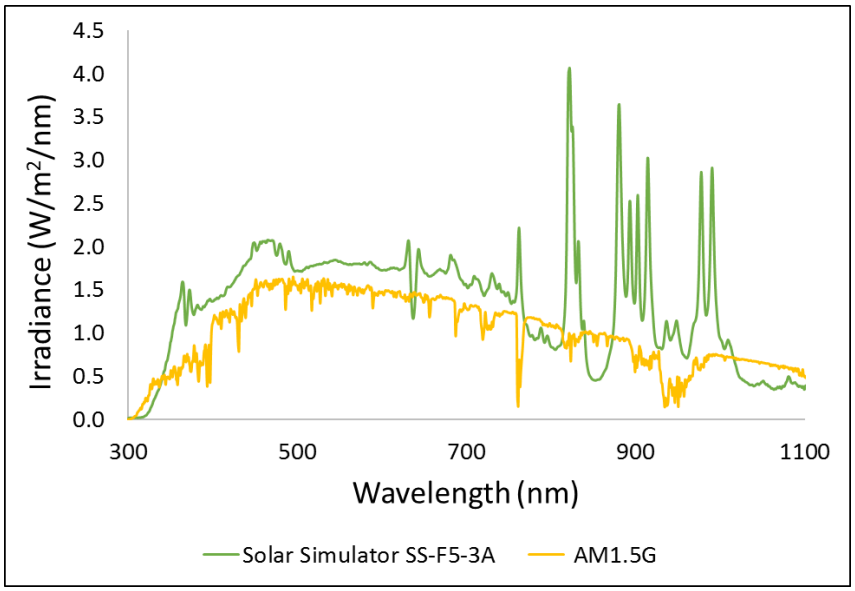


Fig. S22 The solar simulator spectrum (**AM1.5G** solar spectrum from the National Renewable Energy Laboratory (NREL), U.S. and **SS-F5-3A** simulated solar spectrum by Enlitech.

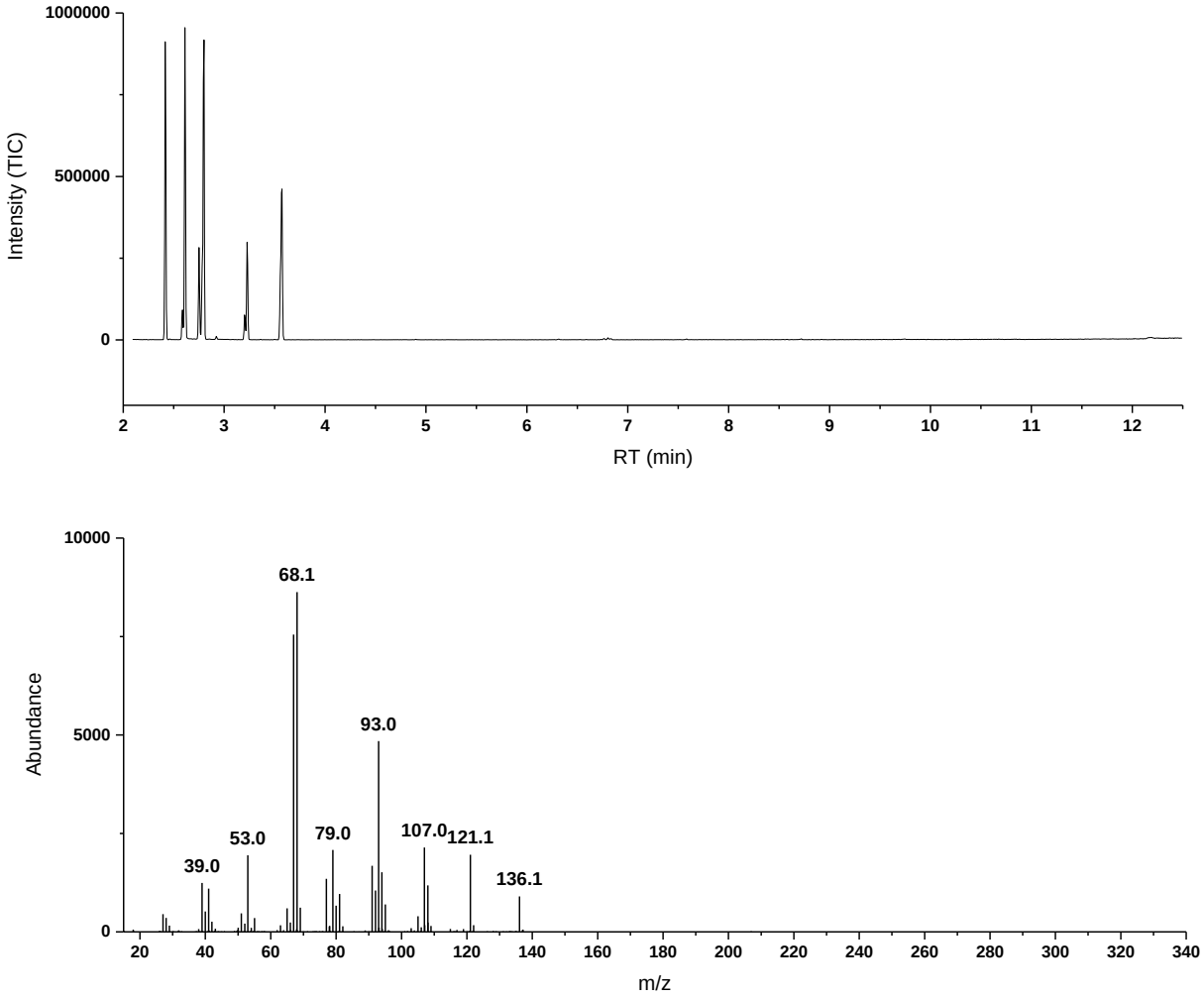


Fig. S23 Gas chromatogram (top) showing dimers of isoprene and the average mass spectrum (middle) for the region RT = 2.386 to 3.611 min. The isoprene dimers were produced in the dimerization of isoprene photosensitized by alpha-dinaphthylketone. The sample was irradiated under simulated sunlight, Xenon lamp, for 44 h.

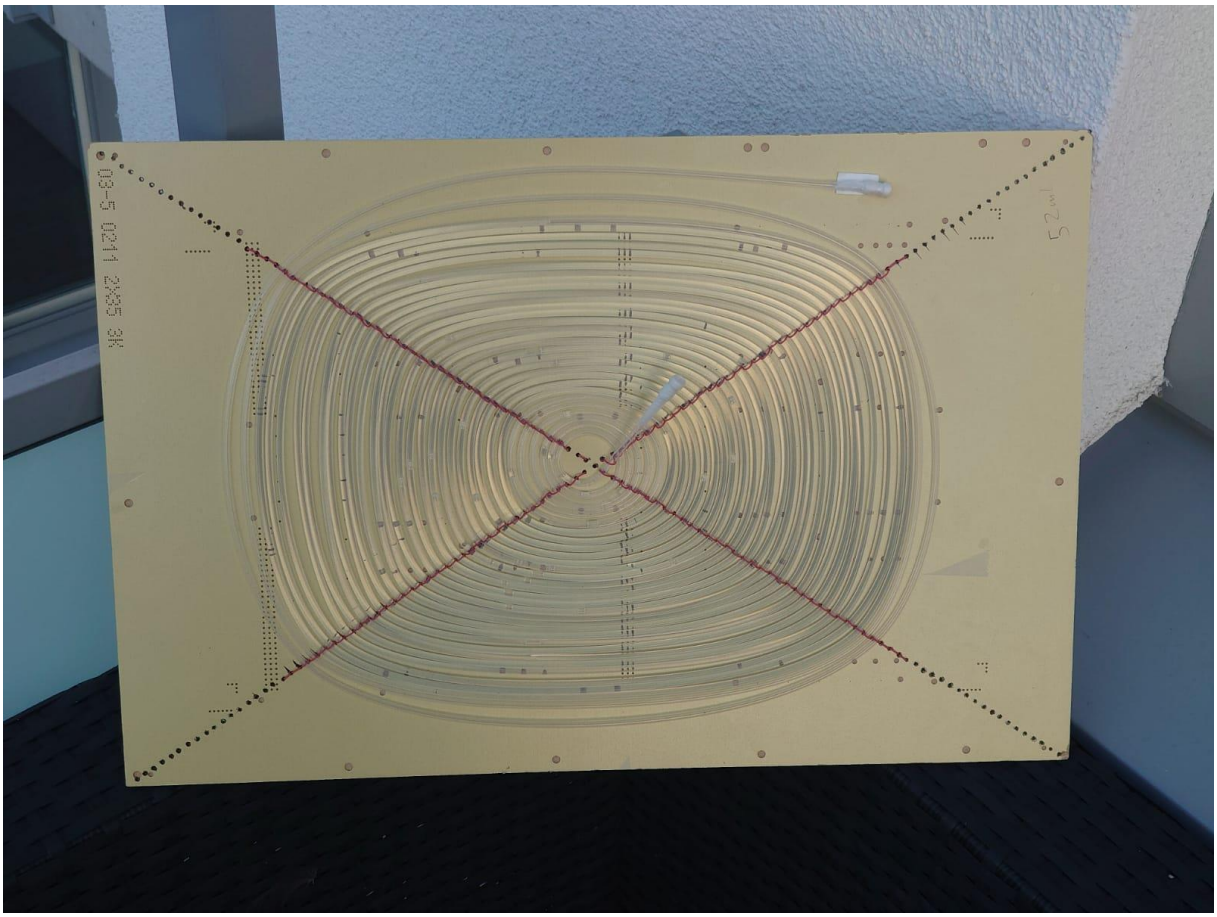


Fig. S24 The isoprene was photoirradiated in FEP coiled setup (O.D. × I.D.: 3.18 mm × 2.1 mm; loop volume: 50 mL) by solar light in Uppsala, Sweden.

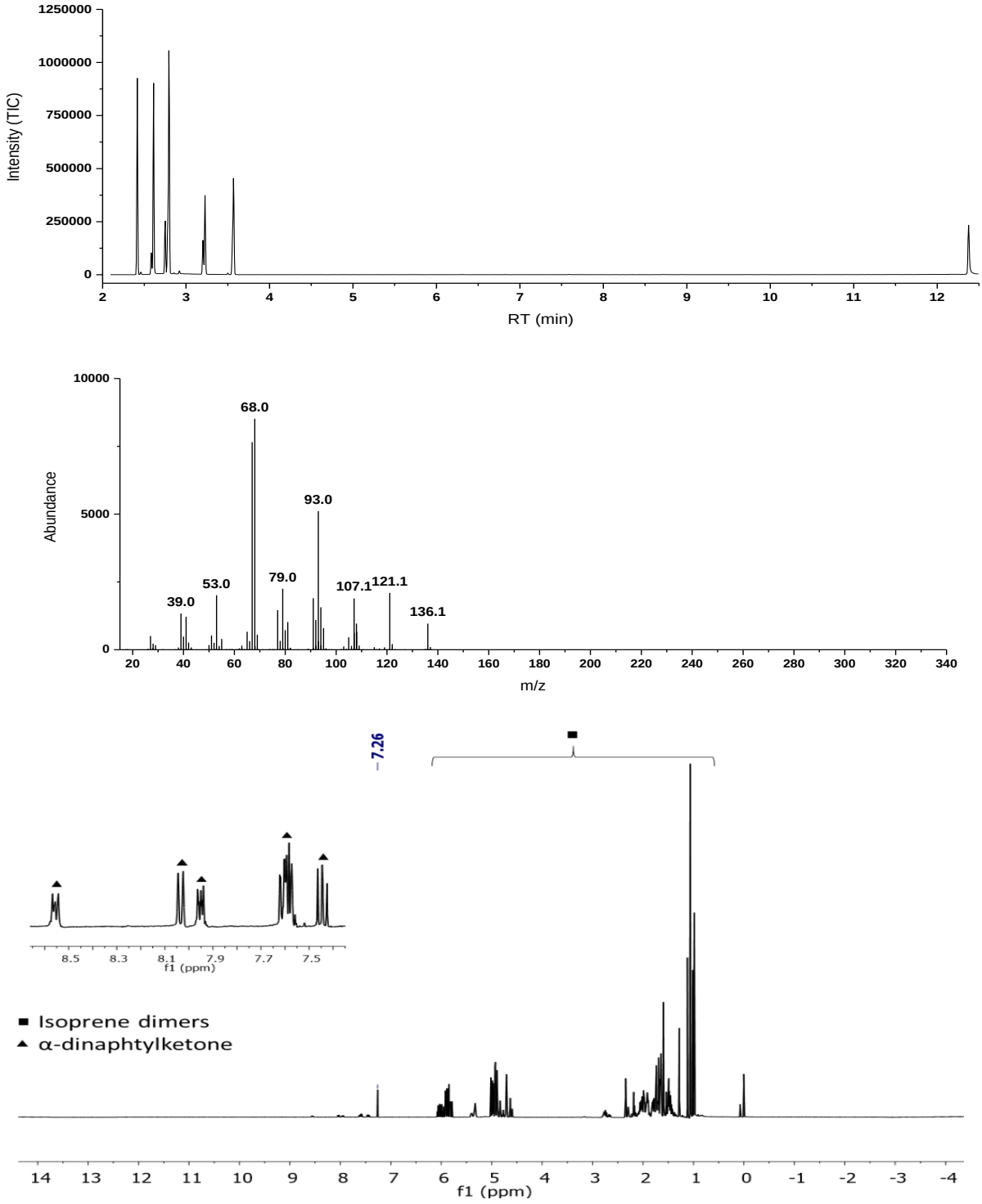


Fig. S25 Gas chromatogram (top) showing dimers of isoprene, the average mass spectrum (middle) for the region RT = 2.386 to 3.605 min, and the ^{1}H NMR spectrum (bottom, $CDCl_3$). The isoprene dimers were produced in the dimerization of isoprene photosensitized by alpha-dinaphthylketone. The sample was irradiated in natural sunlight, for 10 h, in Uppsala, Sweden. The dimers distribution is similar to the one observed in experiments with simulated sunlight (see **Fig. S22**). Note: the last peak in the chromatogram belongs to the photosensitizer which was not removed before GC and ^{1}H NMR analysis for this sample.

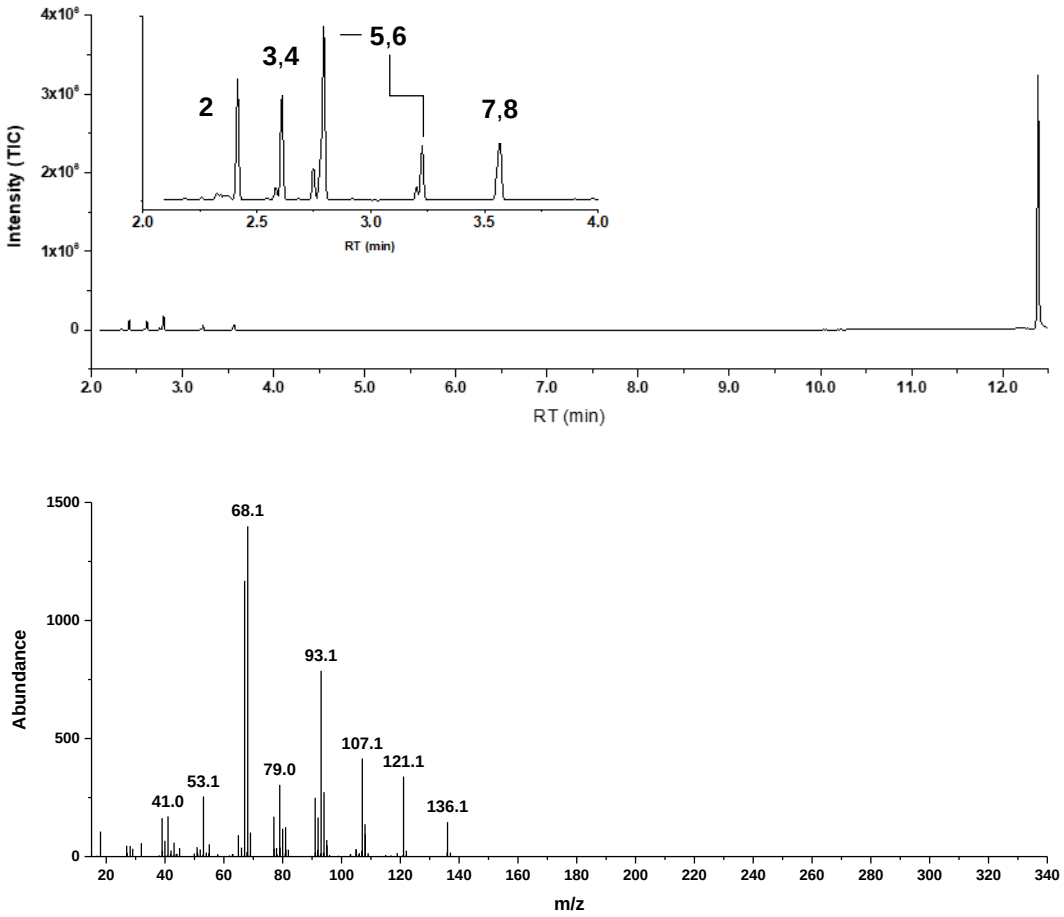


Fig. S26 Gas chromatogram (top) showing peaks of bio-isoprene dimers (inset: region of C10 hydrocarbons on the chromatogram, the isoprene dimers (**2**-**8**) were assigned by using NIST-2017 library as reference), and the average mass spectrum (bottom) is for the region RT = 2.392 to 3.623 min. Data for bio-isoprene solution in heptane. The reaction was photosensitized by dinaphthylmethanone **12** (0.02 M, heptane). The sample was irradiated under simulated sunlight, Xenon lamp (1 sun, AM 1.5 G, 24 h, flat spiral coil). Note: the last peak in the chromatogram (RT = 12.388 min) belongs to the photosensitizer, which was not removed before GC-MS analysis for this sample.

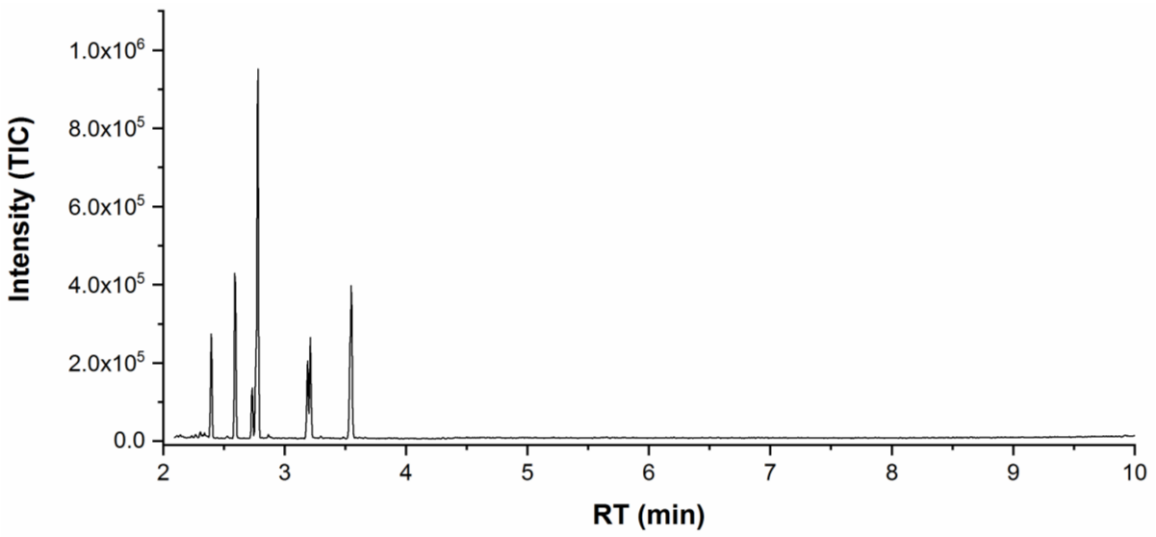


Fig. S27 The gas chromatogram (GC) of isoprene dimers produced by the photo-irradiation isoprene in heptane (0.05 M) in solar simulator under ambient condition for 24 h, **12** (0.1 mol%) was used as photosensitizers. The reaction mixture was diluted to 0.01 M isoprene equivalent for GCMS analysis. The GC pattern of these isoprene dimers are similar with the isoprene dimers obtained from the photo-irradiation of bio-isoprene.

Fig. S28 The hydrogenated isoprene dimers (**HID-1**, ~100 mL) used for testing of fuel properties.

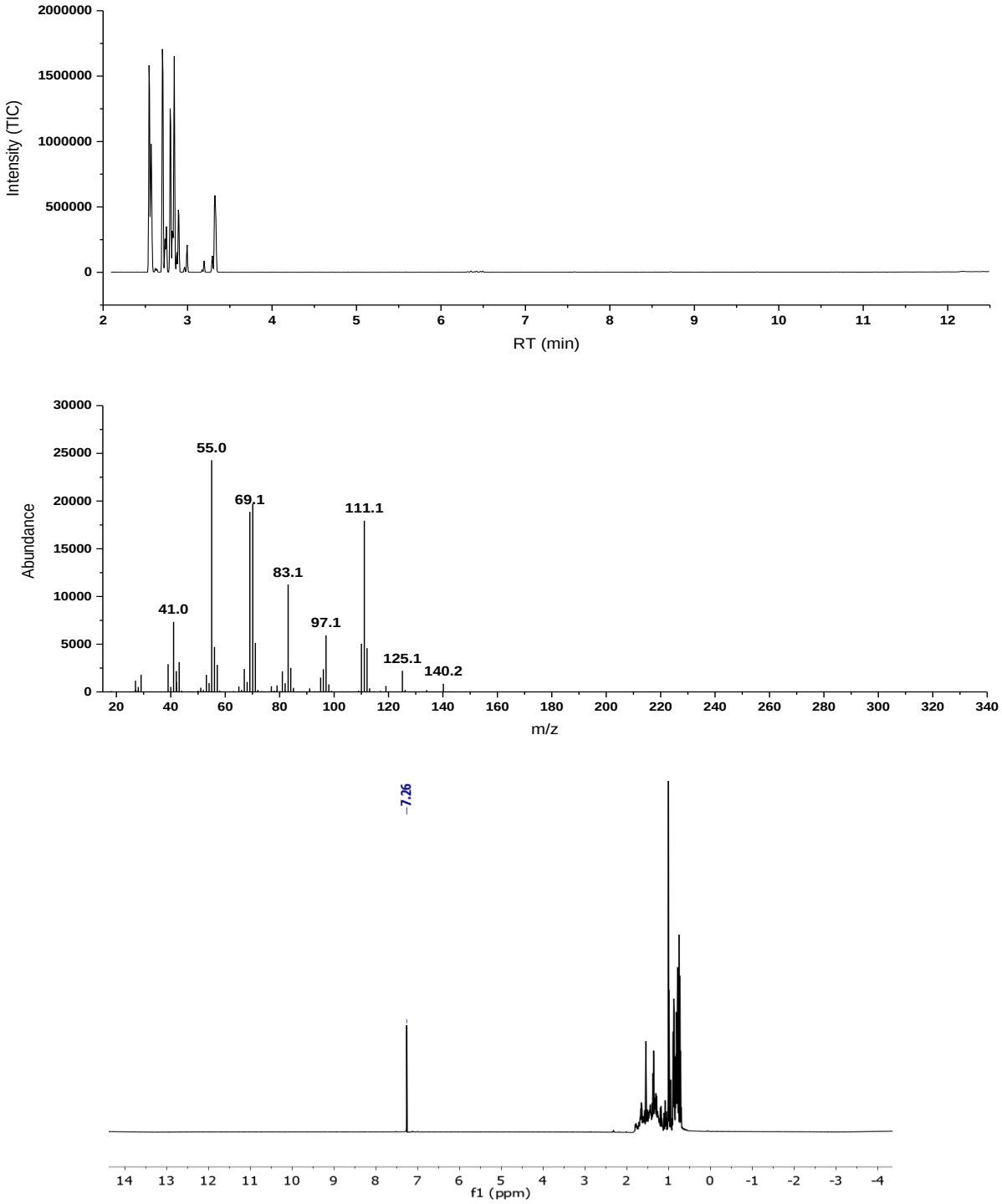


Fig. S29 Gas chromatogram (top) showing hydrogenated dimers of isoprene – our jet fuel surrogate - and the average mass spectrum (middle) for the region RT = 2.495 to 3.391 min. The observed m/z for molecular ion (140.2) and the absence of alkene proton on the ^{1}H NMR spectrum (bottom, solvent $CDCl_3$) points to the full hydrogenation catalyzed by PdC. The initial unsaturated dimers had been produced in the dimerization of isoprene photosensitized by α-dinaphthylketone, irradiated in the Rayonet photoreactor, 365 nm lamp, for 44 h.

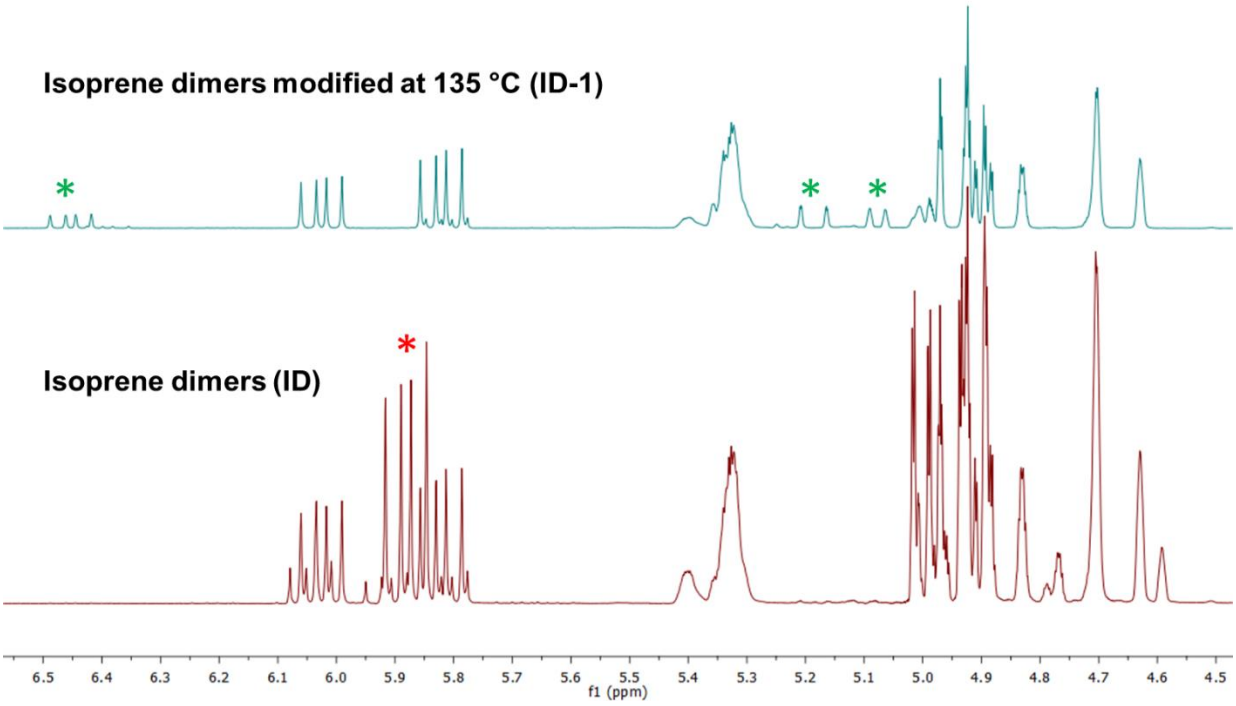


Fig. S30 The partial comparative ^{1}H NMR (alkene part) of isoprene dimers and isoprene dimers modified upon heating at 135 °C. The isoprene dimer **2** (indicated by * in isoprene dimers) completely converted to **5** and **8**. The isoprene is produced as byproduct (indicated by *).

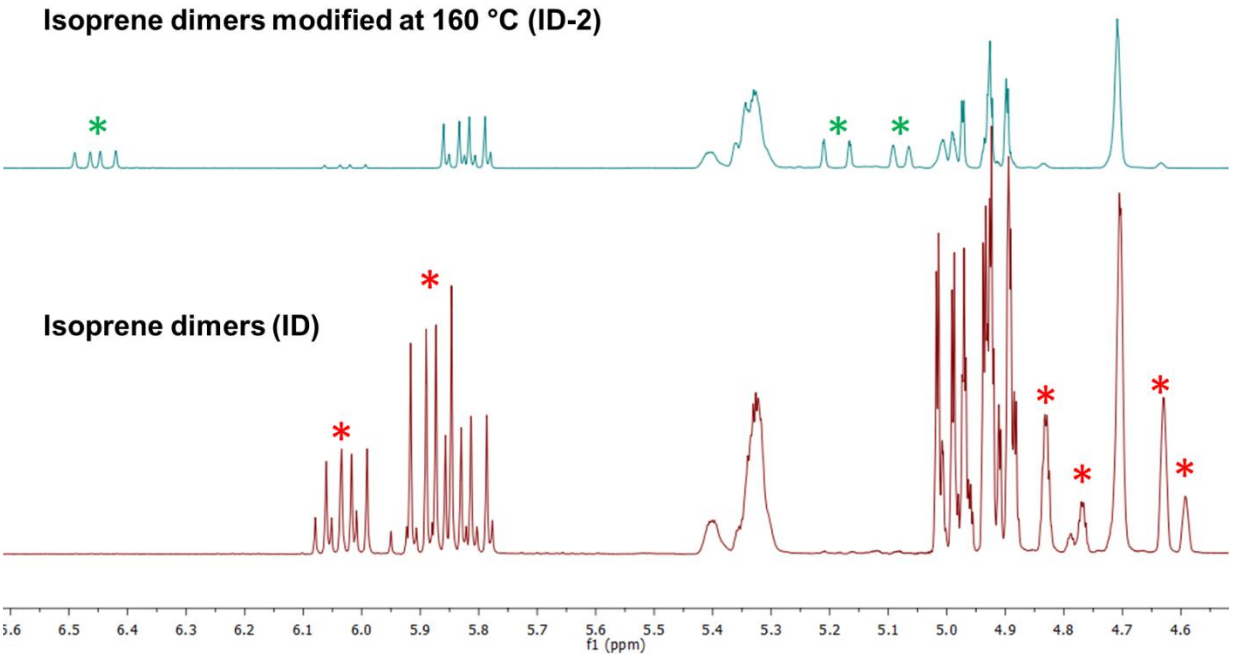


Fig. S31 The partial comparative ^{1}H NMR (alkene part) of isoprene dimers and isoprene dimers modified upon heating at 160 °C. The isoprene dimers **2, 3** and **4** (indicated by * in isoprene dimers) could be modified in this process. The isoprene is produced as byproduct (indicated by *).

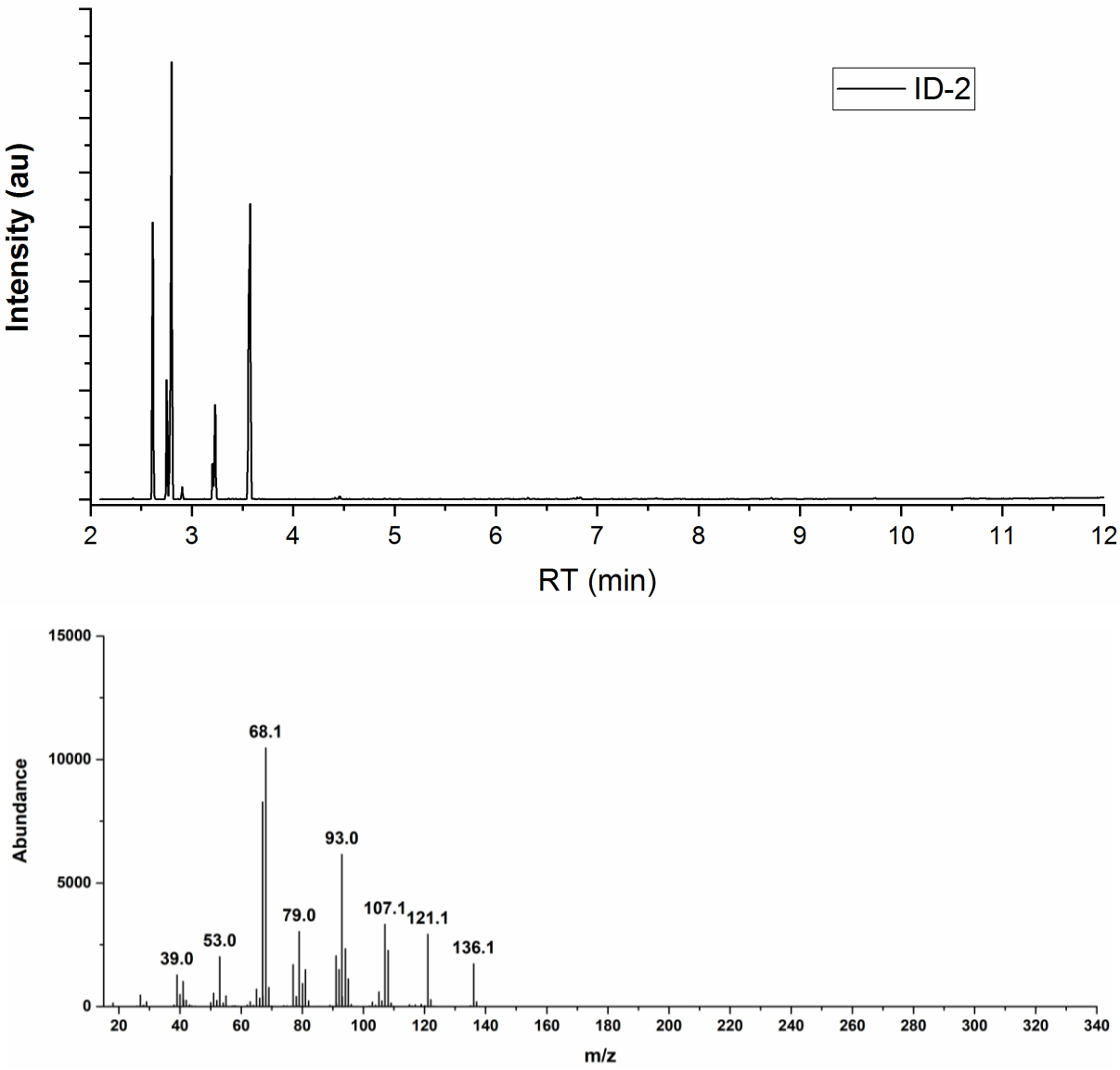


Fig. S32 Gas chromatogram (GC) (top) of isoprene dimers modified at 135 °C (**ID-2**) and the average mass spectrum (bottom) for the region RT = 2.477 to 3.714 min.

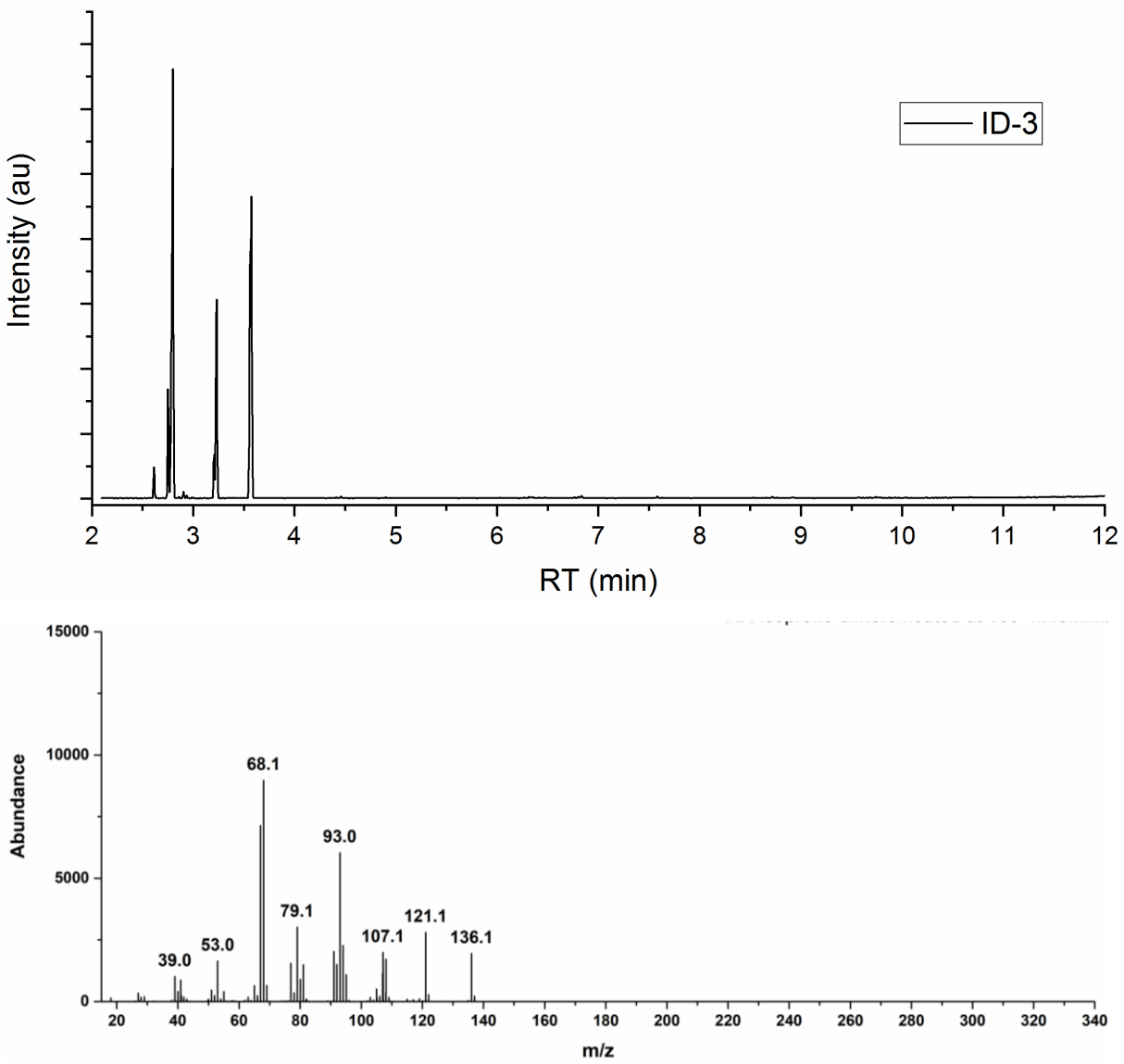
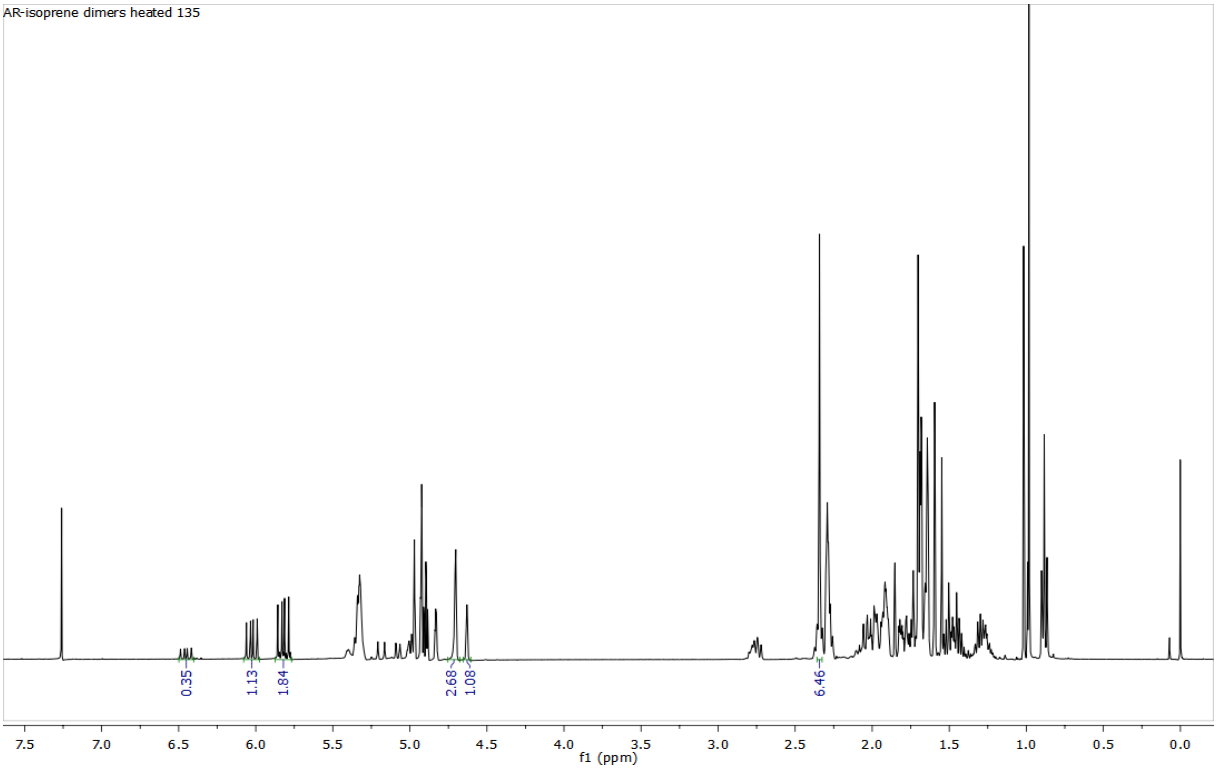
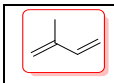
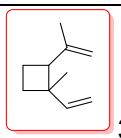
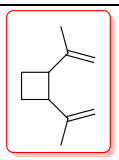
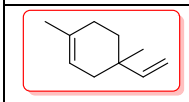
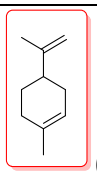
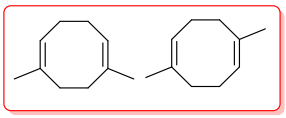


Fig. S33 Gas chromatogram (GC) (top) of isoprene dimers modified at 160 °C (**ID-3**) and the average mass spectrum (bottom) for the region RT = 2.568 to 3.672 min.



 **1** Relative integration= 0.35/1 = 0.35	 **3** Relative integration= 1.13/1 =1.13	 **4** Relative integration= 1.08/2 =0.54
 **5** Relative integration= 1.84/1 =1.84	 **6** Relative integration= 2.68/2 =1.34	Relative integration= 2.68/2 =1.34  **7** and **8** Relative integration= 6.46/4 =1.62
Total integration: 6.82		

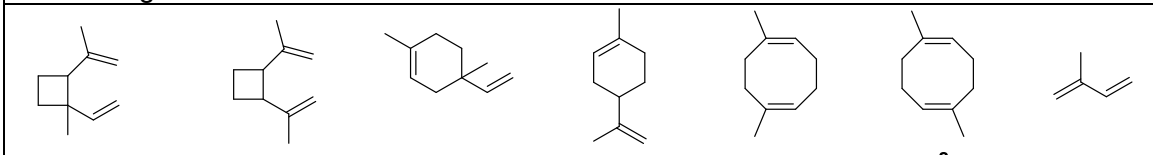
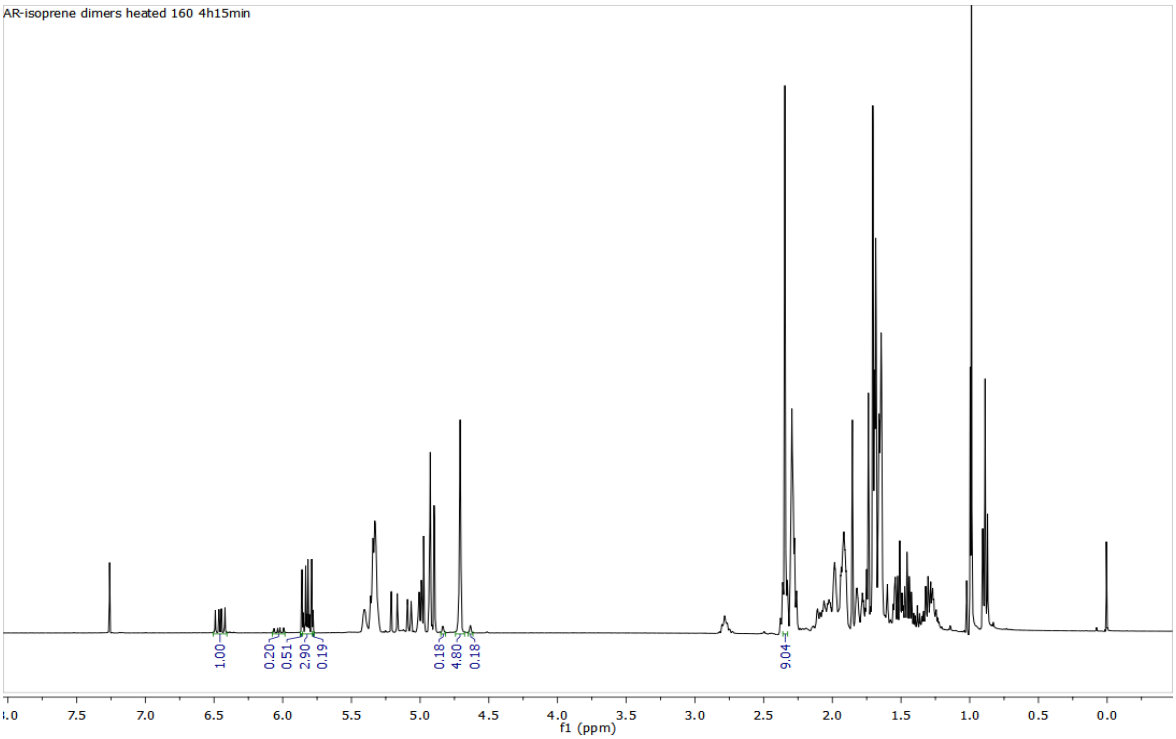
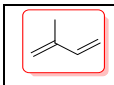
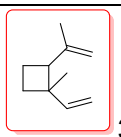
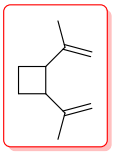
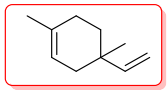
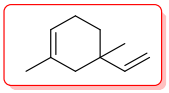
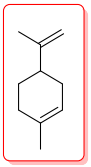
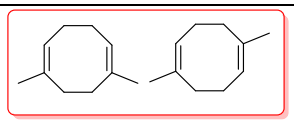


Fig. S34 The % of each isomer (boiling point reported earlier) in the mixture of isoprene dimers modified at 135 °C, obtained by quantitative ^{1}H NMR (the relative concentration method used).



 **1** Relative integration= 1.00/1 = 1	 **3** Relative integration= 0.2/1 =0.2	 **4** Relative integration= 0.18/2 =0.09
 **5** Relative integration= 2.14/1 =2.14	 **27** Relative integration= 0.76/1 =0.76	 **6** Relative integration= 4.80/2 =2.40
 **7** and **8** Relative integration= 9.04/4 =2.26		
Total integration: 8.85		

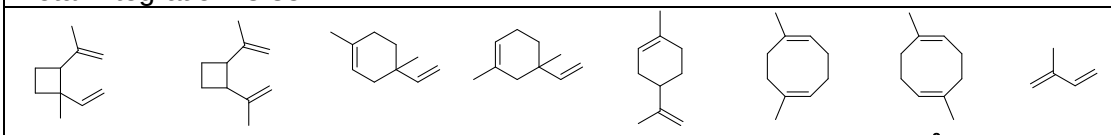


Fig. S35 The mol% of each isomer (boiling point reported earlier) in the mixture of isoprene dimers modified at 160 °C, obtained by quantitative ^{1}H NMR (the relative concentration method used).

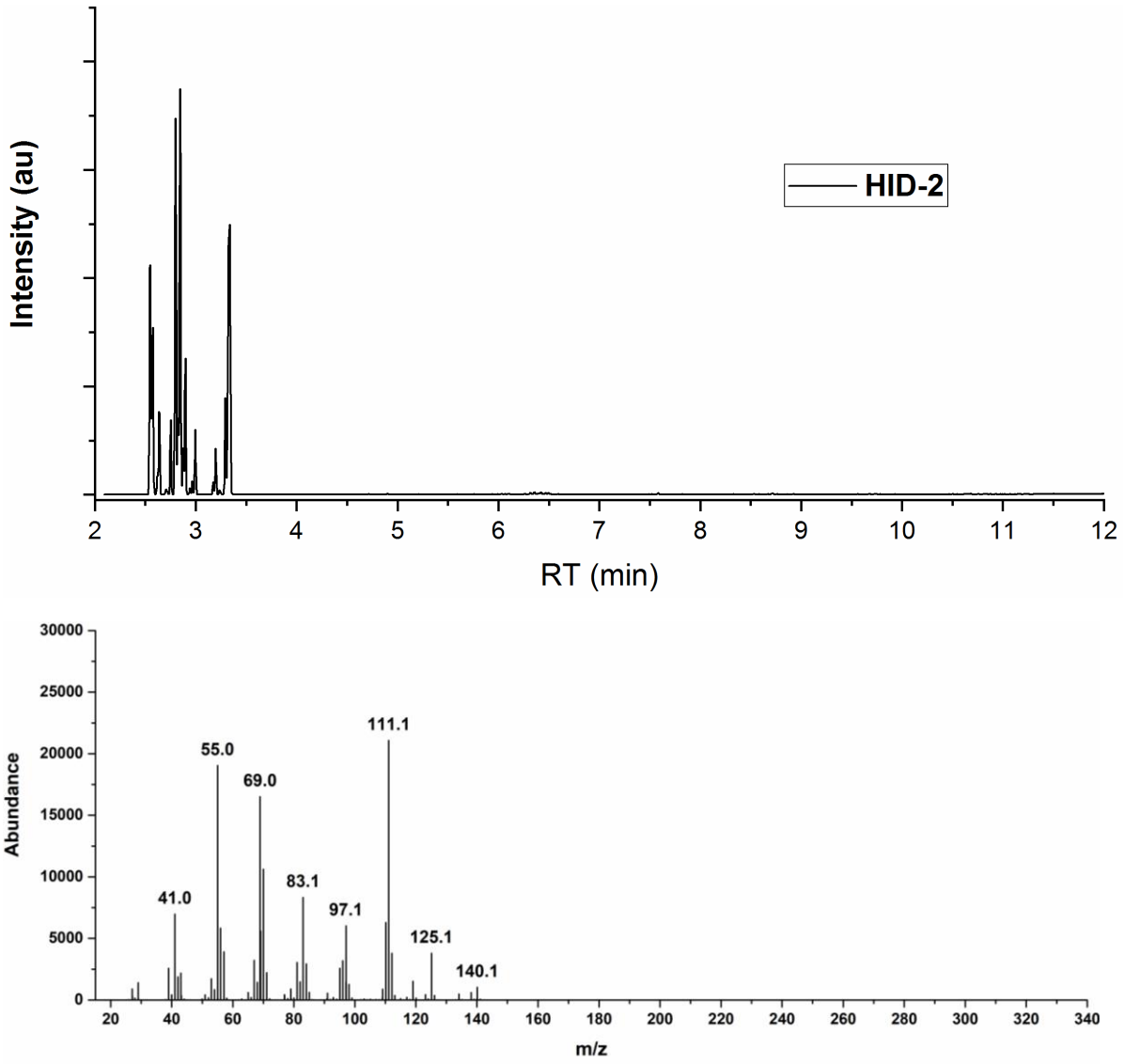


Fig. S36 Gas chromatogram (GC) (top) of hydrogenated isoprene dimers modified at 135 °C (H**ID-2**) and and the average mass spectrum (bottom) for the region RT = 2.440 to 3.422 min.

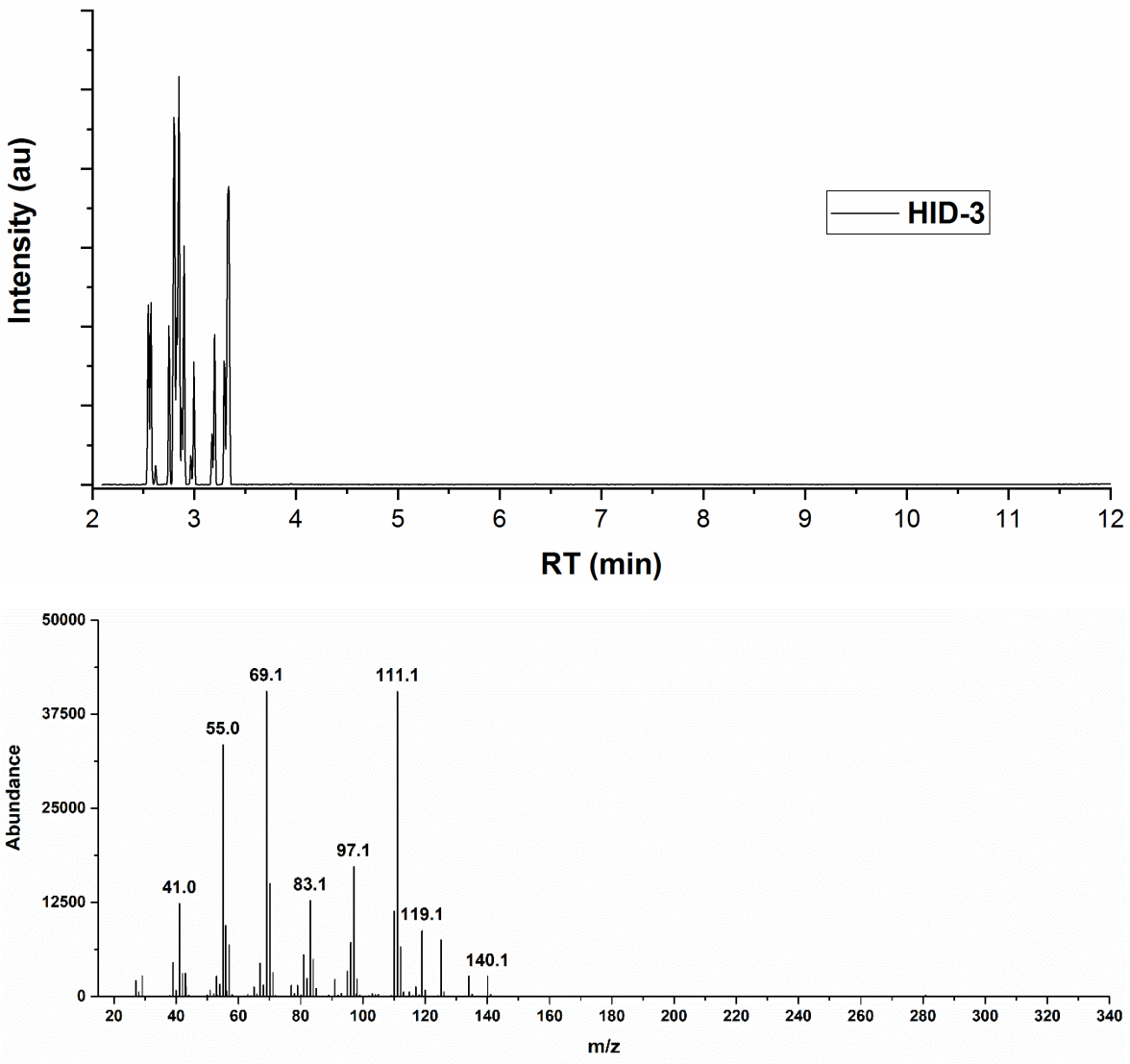


Fig. S37 Gas chromatogram (GC) (top) of hydrogenated isoprene dimers modified at 160 °C (H**ID-3**) and and the average mass spectrum (bottom) for the region RT = 2.477 to 3.416 min.

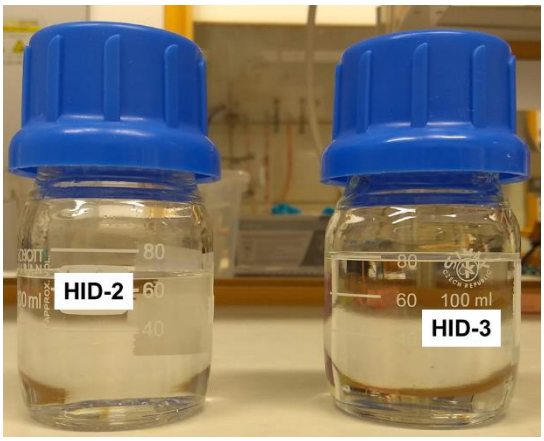


Fig. S38 The modified hydrogenated isoprene dimers (**HID-2** and **3**, ~80 mL) used for testing of fuel properties.

Table S5 Kinematic viscosity (mm^2/s) of **HID's** at different temperature.

Fuel blends	-40 °C	-20 °C	0 °C	20 °C
HID-1	2.60	1.71	1.24	0.96
HID-2	5.40	3.08	2.01	1.45
HID-3	4.93	2.84	1.88	1.36

Table S6 Dynamic viscosity (mPa*s) of **HID's** at different temperature.

Fuel blends	-40 °C	-20 °C	0 °C	20 °C
HID-1	2.12	1.27	0.97	0.73
HID-2	4.60	2.57	1.65	1.17
HID-3	4.20	2.37	1.54	1.09

Table S7 Density (g/ml) of **HID's** at different temperature.

Fuel blends	-40 °C	-20 °C	0 °C	20 °C
HID-1	0.8132	0.7973	0.7815	0.7657
HID-2	0.8507	0.8356	0.8206	0.8054
HID-3	0.8495	0.8343	0.8193	0.8043

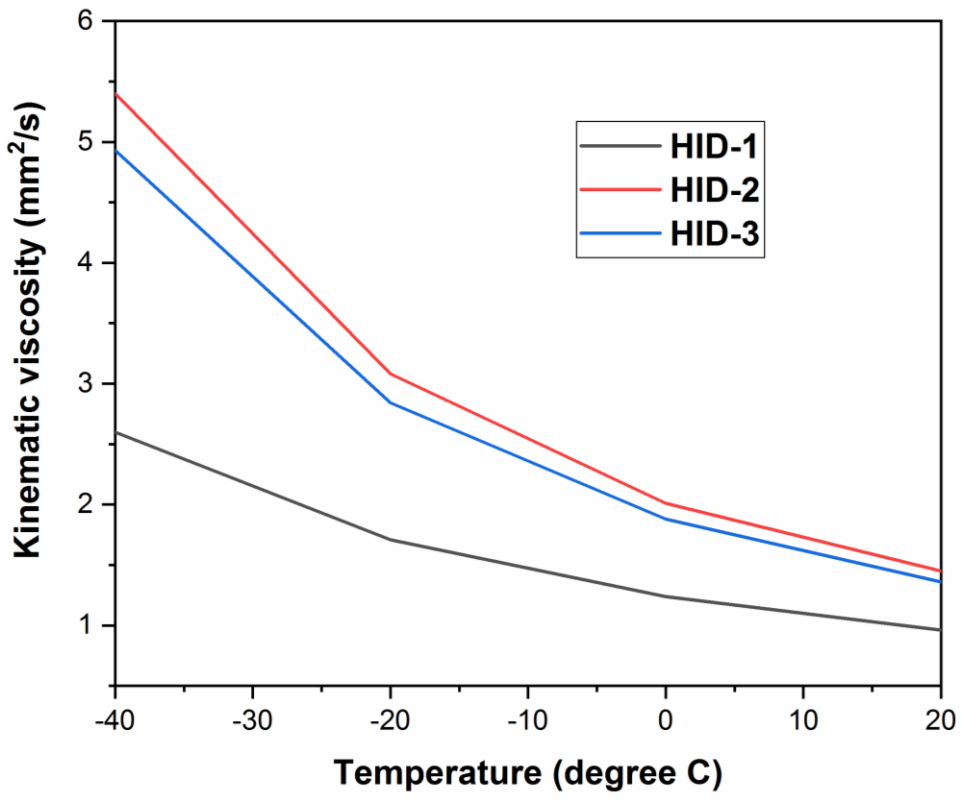


Fig. S39 Kinematic viscosity of **HID's** at different temperature (-40 °C to 20 °C).

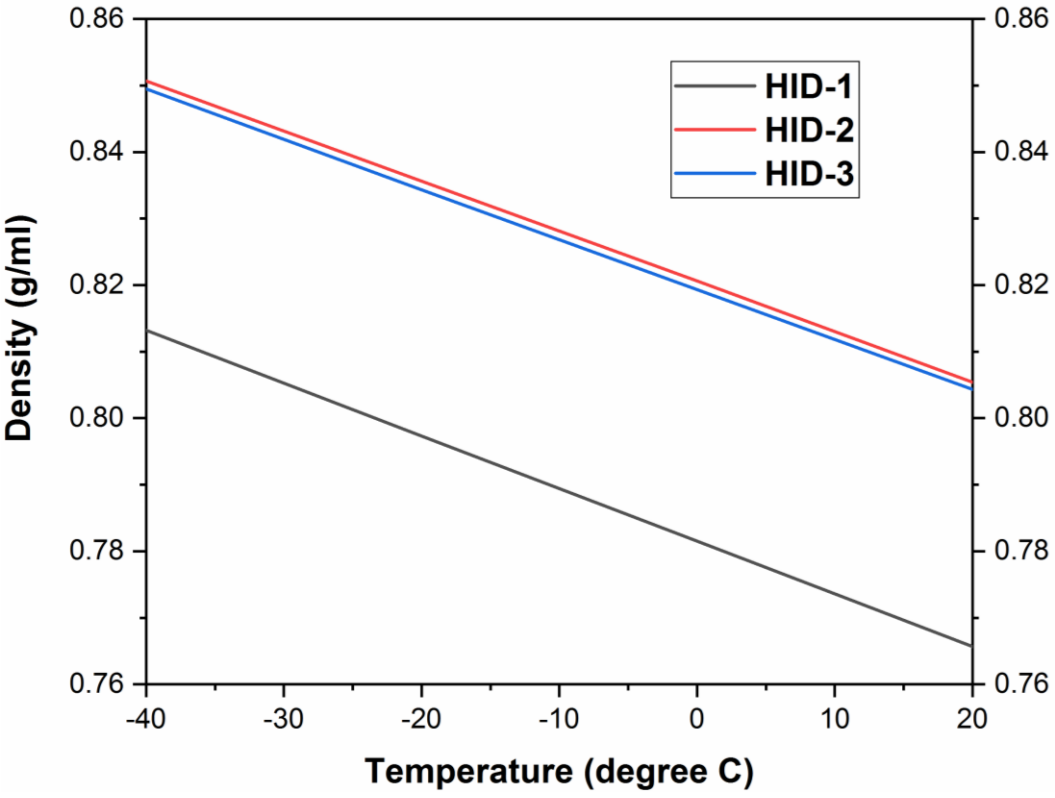


Fig. S40 Density of **HID's** at different temperature (-40 °C to 20 °C).

6. Computational results on the isoprene dimerization mechanism

6.1 Dimers formation

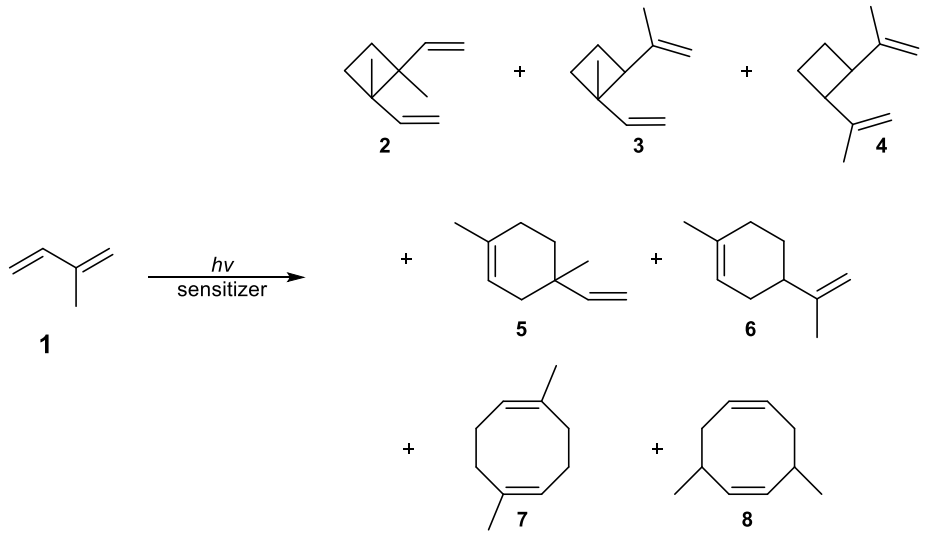


Fig. S41 Dimers formed upon photochemical dimerization of isoprene.

6.1.1 Formation of radical pair intermediates

The first step in the photochemical dimerization of isoprene involves the connection of one isoprene molecule in its T_1 state with another one in the ground state, forming a linear radical-pair intermediate with triplet multiplicity. Fig. S42 shows the various conformers of isoprene in the S_0 and T_1 states, and the barriers for conversion between them.

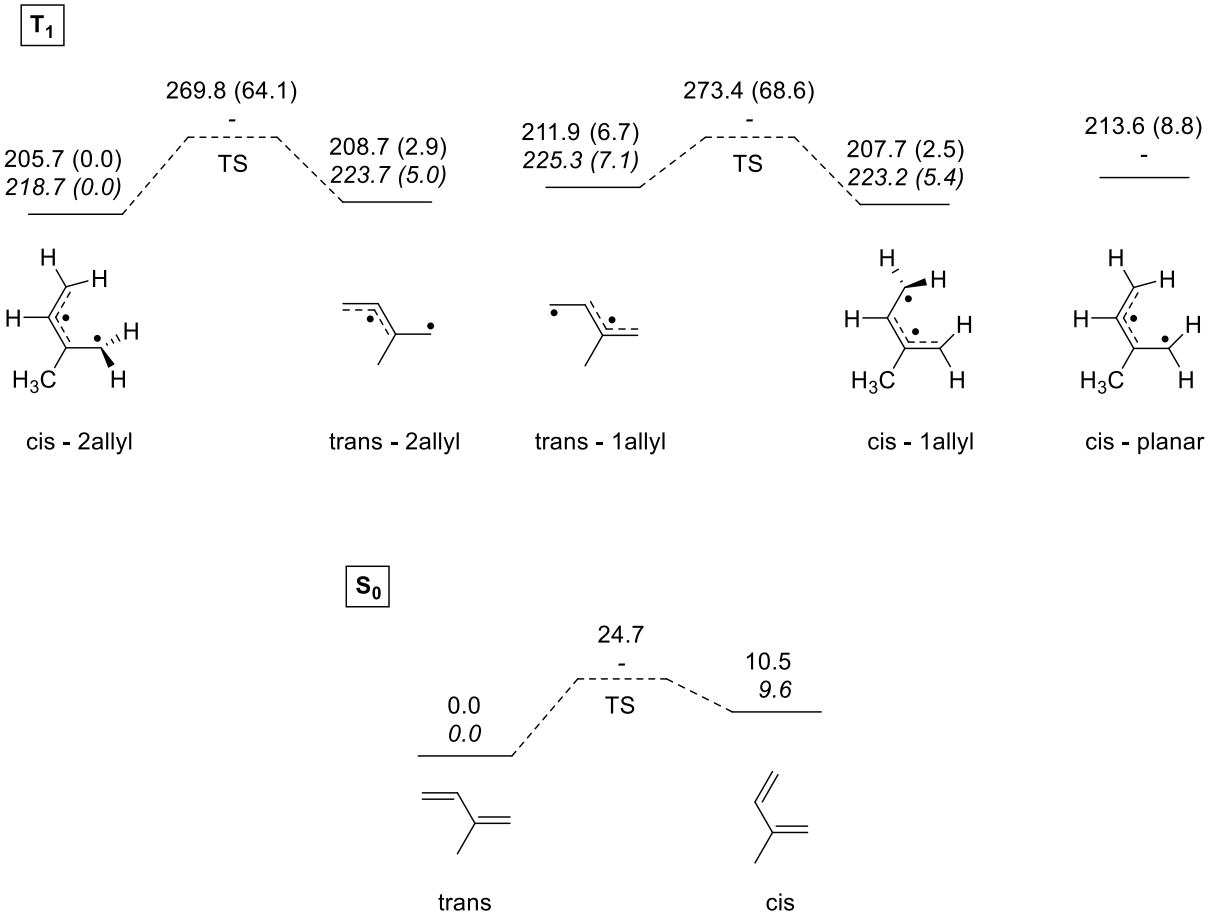


Fig. S42 The isoprene conformers in the S_0 and T_1 states, their energies and the barriers of conversion between them. The values are Gibbs free energies given in kJ/mol, obtained by UB3LYP/6-311G(d,p) (in normal print) and by UM06-2X/6-311G(d,p) (in italics). Values in parenthesis are relative to the T_1 structure that is lowest in energy.

Several possibilities on how the two isoprene reactants connect exist. In Fig. S43 and S44, the activation barriers (energies of the first-order saddle-points) and the energies of the minima of the formed radical-pair intermediates are presented, respectively.

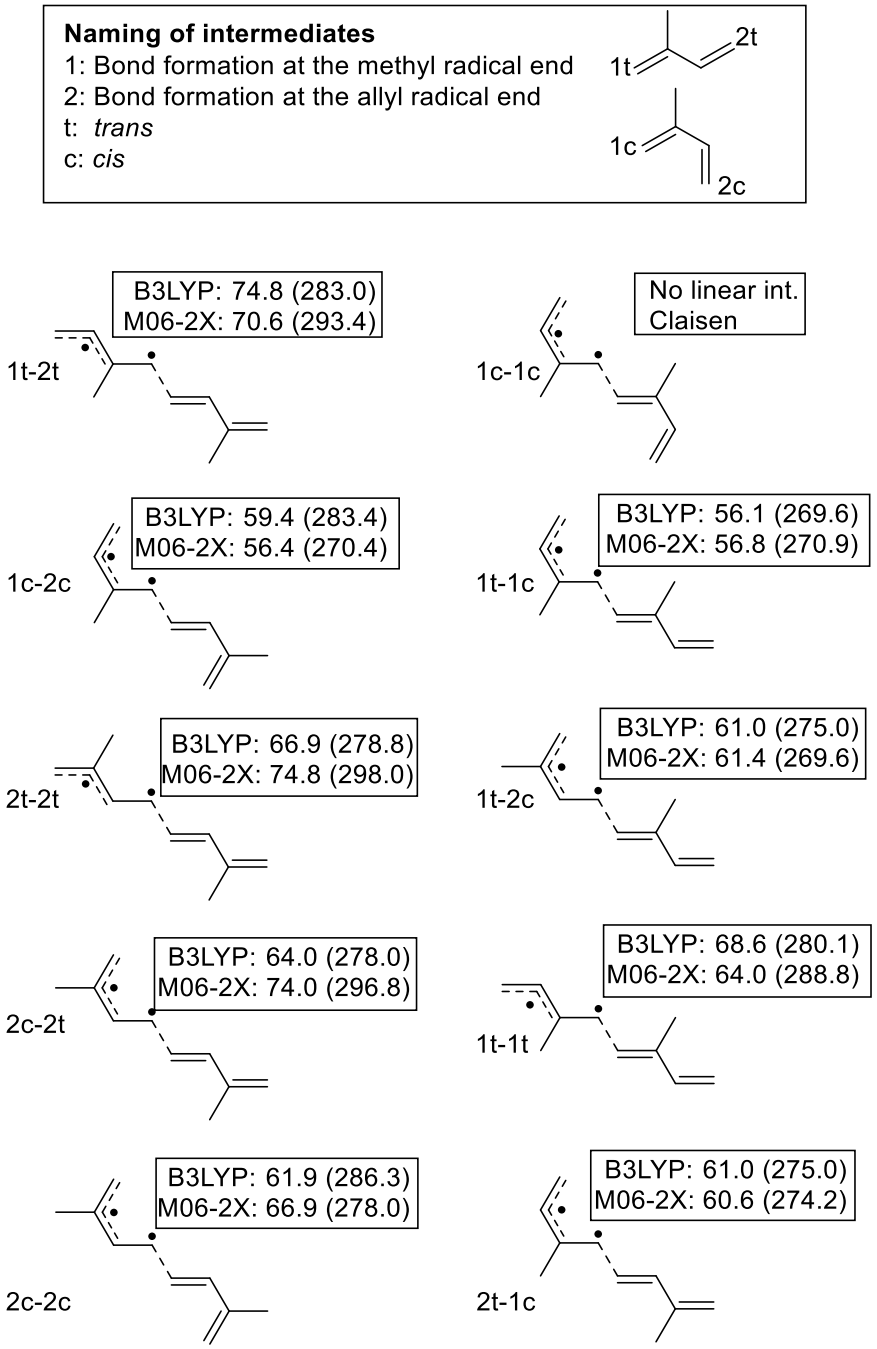


Fig. S43 Activation energies to forming the various triplet radical-pair intermediates relative to the energy of one isoprene in T_1 plus one isoprene in S_0, calculated with both UB3LYP/6-311G(d,p) and UM06-2X/6-311G(d,p). The values are Gibbs free energies given in kJ/mol. Energies relative to the ground state reactants (two S_0 state isoprene molecules in *trans* configuration) are given in parenthesis.

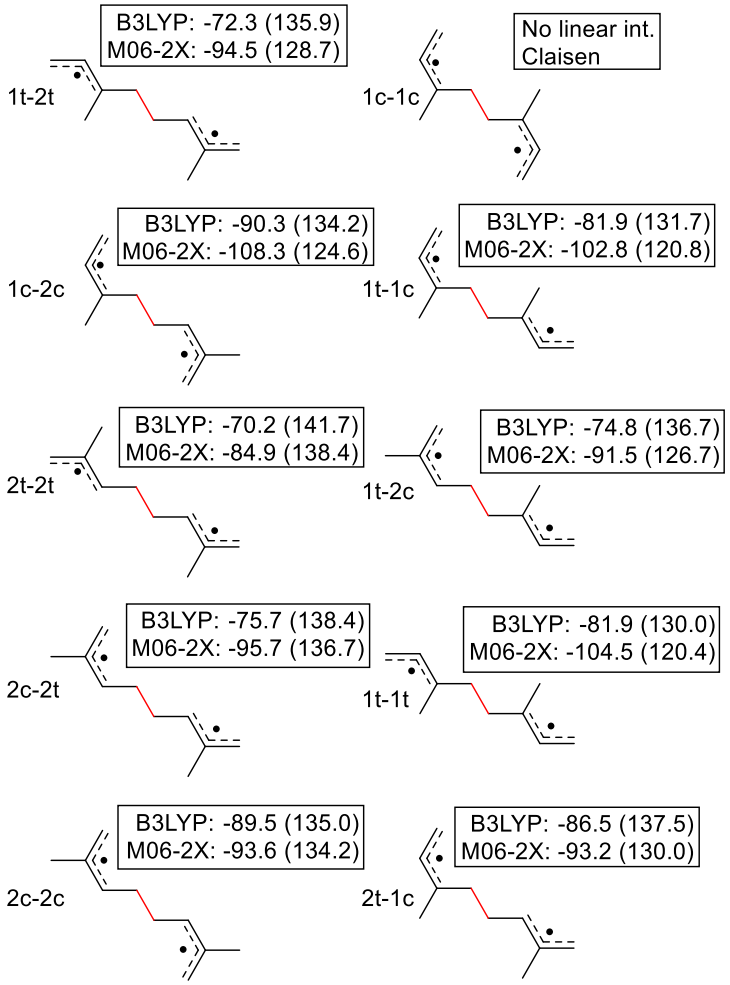


Fig. S44 Energies of the different triplet radical-pair intermediates relative to the energy of one isoprene in T_1 plus one isoprene in S_0, calculated with both UB3LYP/6-311G(d,p) and UM06-2X/6-311G(d,p). The values are Gibbs free energies given in kJ/mol. Energies relative to the ground state reactants (two S_0 state isoprene molecules in *trans* configuration) are given in parenthesis.

Table S8 The final, cyclic dimer products that can be formed from each radical intermediate in Fig. S44.

Intermediates	**Products possible to form (Fig. S41)**
1t-2t	**3** and **7**
1c-1c	-
1c-2c	**3**, **6** and **7**
1t-1c	**2**, **5** and **8**
2t-2t	**4** and **8**
1t-2c	**3**, **6** and **7**
2c-2t	**4** and **8**
1t-1t	**2**, **5** and **8**
2c-2c	**4** and **8**
2t-1c	**3**, **6** and **7**

6.1.2 Relative energies of the radical-pair intermediates

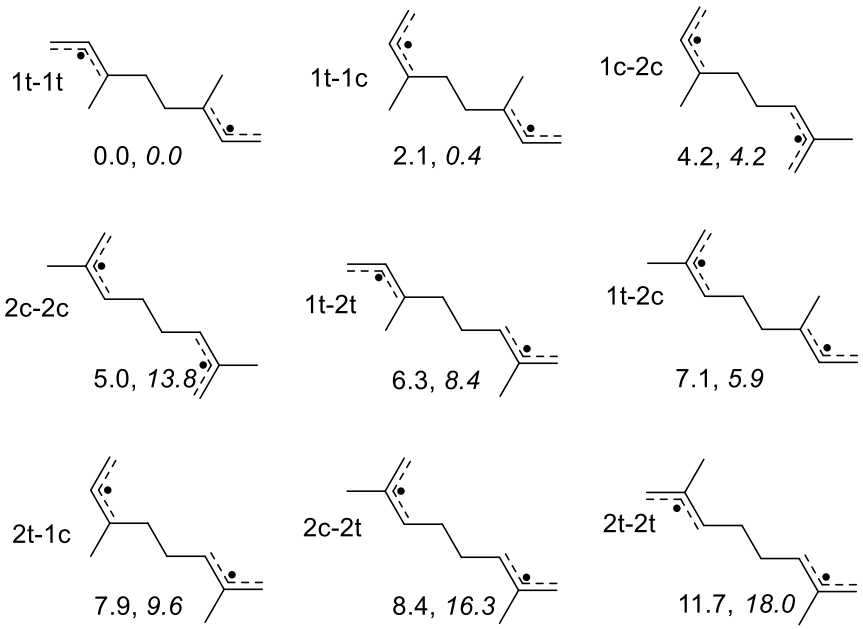


Fig. S45 The relative stabilities of the triplet radical pair intermediates, ordered according to the B3LYP results. Values obtained by UB3LYP/6-311G(d,p) (in normal print) and by UM06-2X/6-311G(d,p) (in italics). With both functionals, the most stable intermediate is 1t-1t, and the least stable one is 2t-2t. Gibbs free energies relative to 1t-1t are given in kJ/mol.

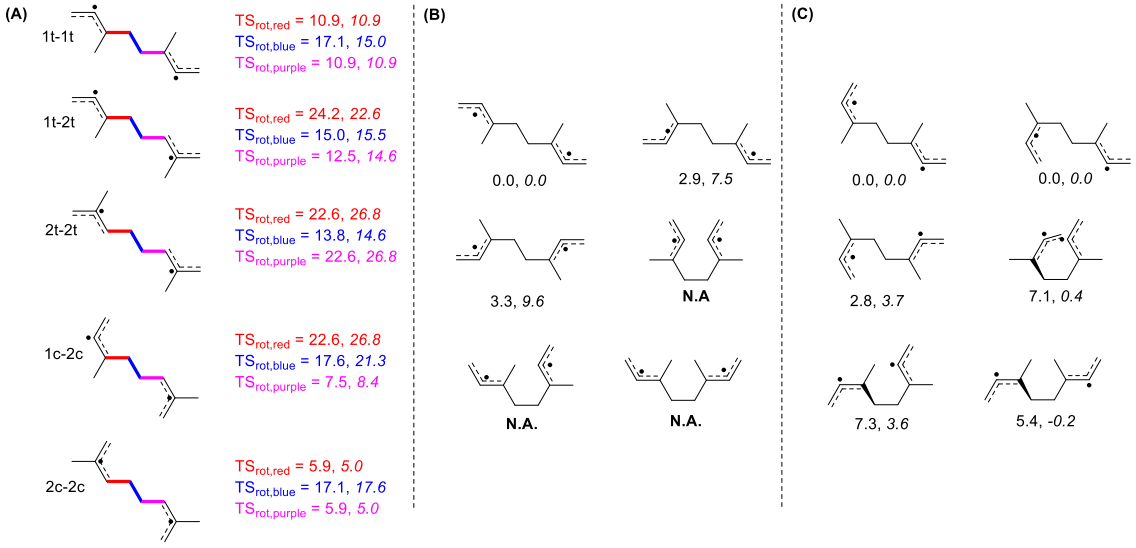


Fig. S46 (A) Single bond rotational barriers for a few of the triplet radical-pair intermediates, and the relative energies of the various rotamers of the (B) 1t-1t and (C) 1t-1c triplet radical-pair intermediates. Gibbs free energies are given in kJ/mol, with UB3LYP/6-311G(d,p) and UM062X/6-311G(d,p) values in normal and italics, respectively.

The barriers range from ~4.2 to ~25.1 kJ/mol, revealing that the single bond rotation process is generally feasible, and that there will be a rapid equilibration between various rotamers of the radical-pair intermediates. As the radical sites of the radical-pairs are spatially separate the triplet and singlet radical-pairs are isoenergetic and there will be a rapid intersystem crossing (ISC) between the singlet and triplet state of these diradical species

6.1.3 Formation of dimers

The activation energies below refer to the ring-closure step that occurs once the dimeric radical-pair intermediate is formed. Upon rapid ISC, the triplet radical-pair intermediate is converted to the singlet radical-pair. The cyclohexene product is more favorable than the cyclobutane and cyclooctadiene products. To compute the barriers, we used the most stable intermediate that directly gives each product.

We first attempted to use 1t-1t, which is the most stable intermediate that potentially can form products **2**, **5** and **8**. However, this was only possible for product **2** (among different attempts to find a transition state that connects 1t-1t and products **5**/**8**, only a photochemical analog of Claisen rearrangement type transition state was found); instead, products **5** and **8** are only formed from 1t-1c, which is 2.1/0.4 kJ/mol (B3LYP/M06-2X) higher than 1t-1t (Fig. S47).

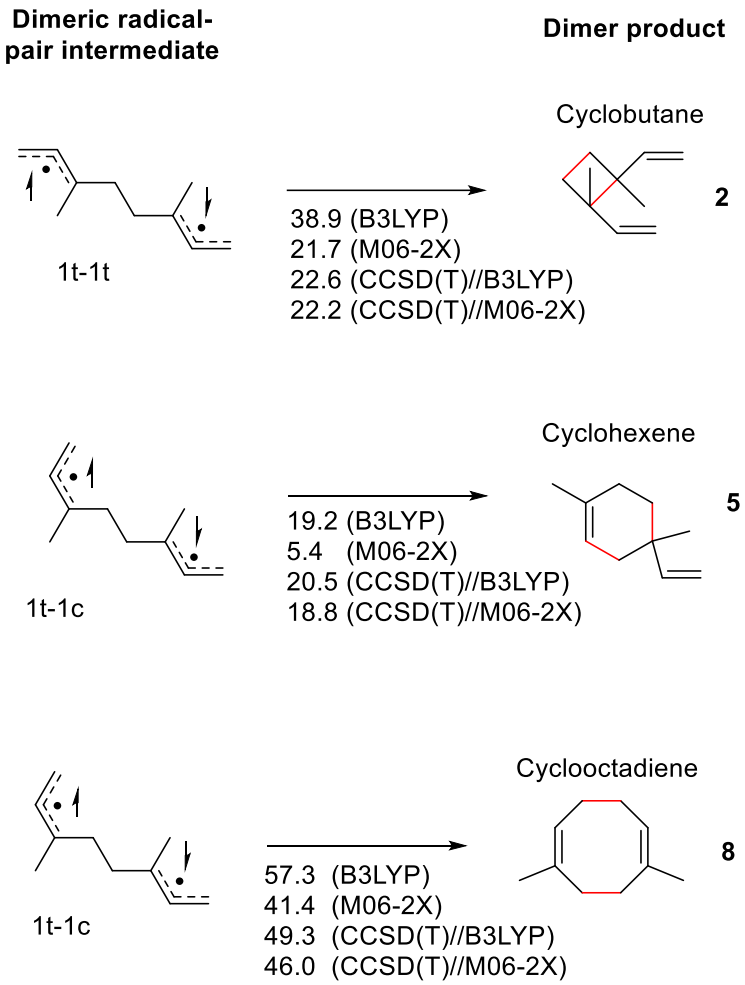


Fig. S47 Activation energies for the ring-closure of the singlet state radical-pair intermediates 1t-1t and 1t-1c, forming the cyclic isoprene dimers **2**, **5** and **8**. Gibbs free energies are given in kJ/mol. Gibbs free energies at CCSD(T) level include thermal corrections from UB3LYP/6-311G(d,p) and UM06-2X/6-311G(d,p) level calculations.

To form products **3**, **6** and **7**, we found that they can be formed using 1c-2c which is the most stable intermediate already (Fig. S48).

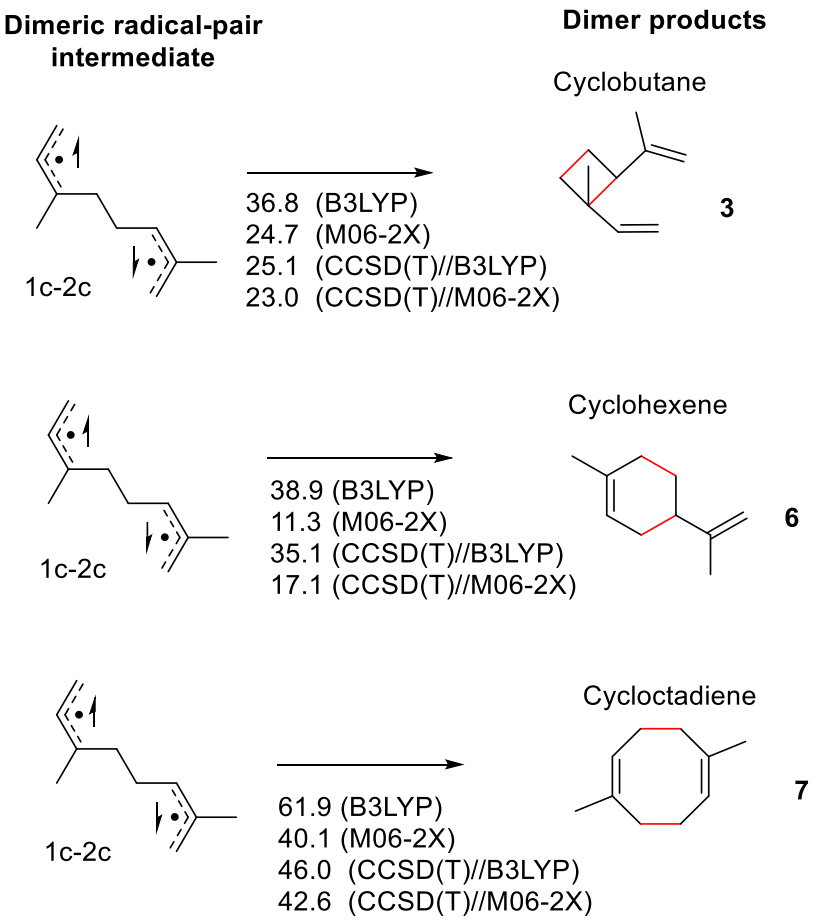


Fig. S48 Activation energies for the ring-closure of the singlet state radical-pair intermediate 1c-2c, forming the cyclic dimers **3**, **6** and **7**. Gibbs free energies are given in kJ/mol. Gibbs free energies at CCSD(T) level include thermal corrections from UB3LYP/6-311G(d,p) and UM06-2X/6-311G(d,p) calculations.

In case of product **4**, this product can be only formed from 2c-2t which is 3.3/2.5 kJ/mol (B3LYP/M06-2X) higher than 2c-2c (Fig. S49).

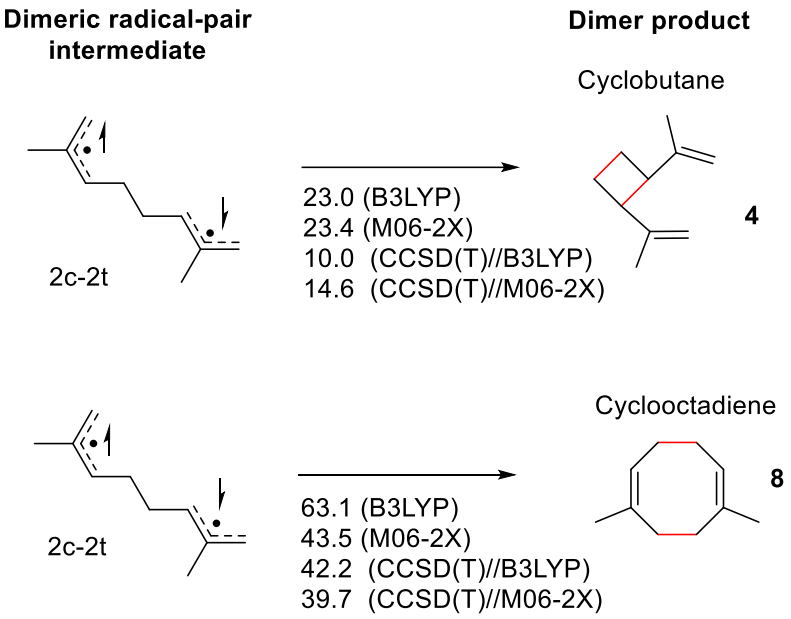


Fig. S49 Activation energies for the closure of the singlet state radical intermediate 2c-2t, forming the cyclic dimers **4** and **8**. Gibbs free energies are given in kJ/mol. Gibbs free energies at CCSD(T) level include thermal corrections from UB3LYP/6-311G(d,p) and UM06-2X/6-311G(d,p) calculations.

6.2 Trimer formation

To investigate why further oligomerization is impeded, the formation of different types of trimers were studied, *i.e.* linear and cyclic. These can either be formed through (*i*) addition of a S_0 state isoprene to a triplet radical-pair intermediate, or (*ii*) by combining one of the cyclic dimers that are formed with isoprene in its T_1 states. One could also argue that a thermal Diels-Alder reaction can take place between a dimer and isoprene in their S_0 states.

6.2.1 Formation of linear trimers

Linear trimers may be formed photochemically by adding an isoprene in its ground state to a radical-pair triplet intermediate, forming a longer *bis*(allyl) radical-pair of triplet multiplicity. Four examples of this are shown below. Considering that the most reactive side of the dimer radical-pair is the one where the unpaired electron is located at the terminal C atom closest to the methyl group position, the activation energies and minimum energies follow expectation. In general, the activation energies for formation of trimer radical-pair intermediates are higher than those for the formation of dimer radical-pair intermediates (up to around 29 kJ/mol from our example calculations), but not always. If some of the dimer intermediates requiring comparatively high activation energy can be formed (*e.g.* 1t-2t or 1t-1t), so can the

corresponding trimer. However, seeing that the barriers for closure into cyclic dimers are lower (by around 25-67 kJ/mol) and do not require an additional isoprene fragment, dimer formation should be favored.

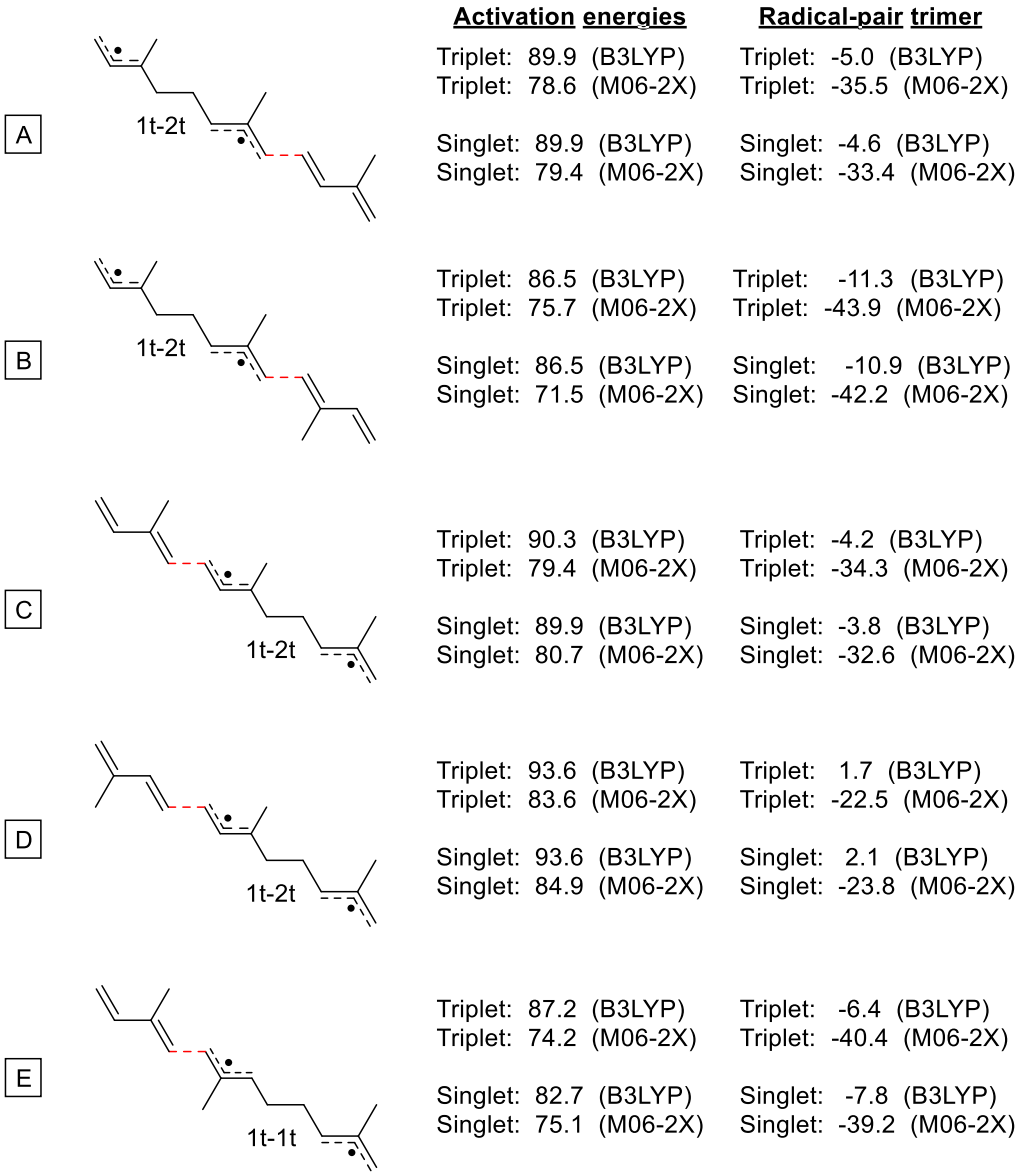


Fig. S50 Activation energies and reaction energies for formation of a few possible linear trimer radical-pair intermediates, calculated with both UB3LYP/6-311G(d,p) and UM06-2X/6-311G(d,p). The values are Gibbs free energies given in kJ/mol.

6.2.2 Formation of cyclic trimers

Cyclic trimers could be formed through a thermal or photochemical process.

An evident thermal pathway that could take place is a Diels-Alder reaction, *i.e.*, concerted addition of an isoprene in its ground state with a cyclic dimer (also in its ground state). This process was investigated but found to have high barriers (146 kJ/mol or higher), and was thus discarded.

In the excited states, however, a T_1 state isoprene could also be thought to add to a C-C double bond of an already formed cyclic dimer. Examples of some of the least sterically hindered trimers formed in this way are shown below. Again, the barriers are in general higher than those for the dimer formation, but not always. Thus, depending on the accessible energy, some amount of cyclic trimers may be formed.

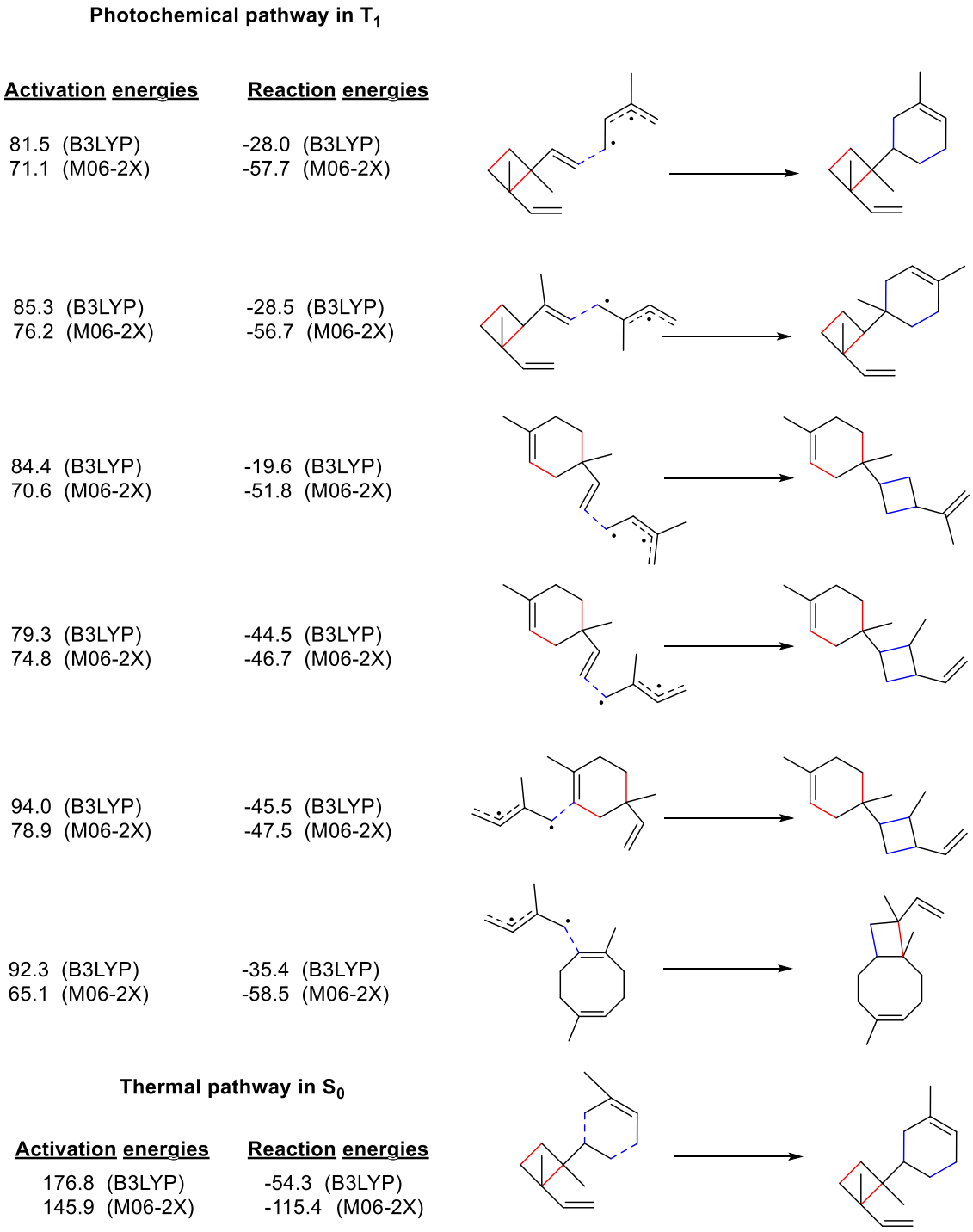


Fig. S51 Activation energies and reaction energies for addition is isoprene to cyclic dimers leading to a few possible cyclic trimers, calculated with both UB3LYP/6-311G(d,p) and UM06-2X/6-311G(d,p). The values are Gibbs free energies given in kJ/mol.

6.3 Investigation of a tentative concerted [4+4] photodimerization mechanism

Attempts to find a concerted [4+4] photochemical mechanism to form **6** and **7** from two isoprene molecules through Baird-aromatic transition states have not been successful.

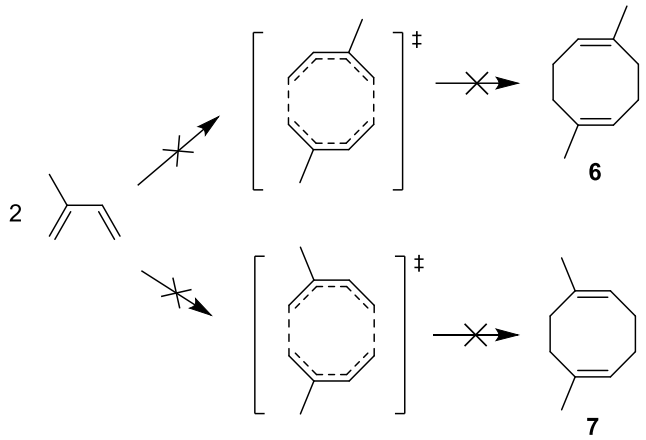


Fig. S52 [4+4] photocycloaddition pathways to generate products **6** and **7** from two isoprene molecules.

If one instead uses two butadiene molecules, a cyclic transition state is found, but it is not the transition state leading to the expected product. Instead it is a TS for the degenerate conversion between two *bis*(allyl) radical pairs through a reaction that may be described as a photochemical analogue of a Claisen rearrangement. The activation energy for this rearrangement (relative to one S_0 state butadiene + one T_1 state butadiene) is 80.7 and 81.9 kJ/mol, at the UB3LYP/6-311G(d,p) and UM06-2X/6-311G(d,p) level of theory respectively.

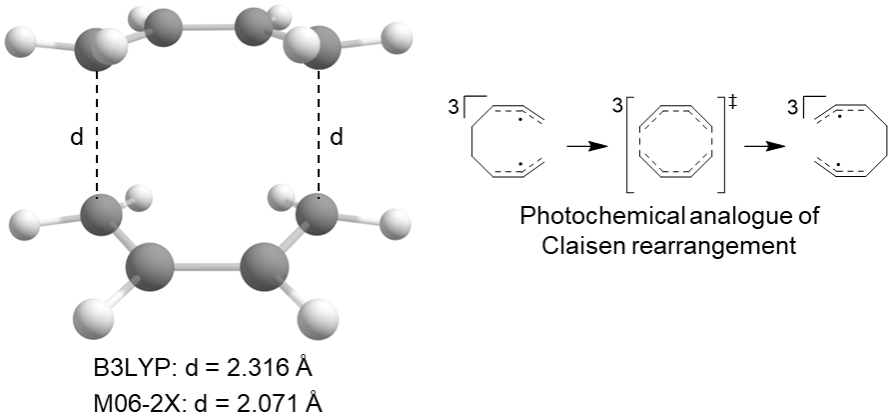


Fig. S53 Transition state of a photochemical analogue of Claisen rearrangement between two isoprene molecules.

7. Life cycle assessment

7.1 Materials and Methods

Process details used for the combined photobiological-photochemical route used for LCA assessment are presented in Fig. S54. and Table S9. The employed LCA followed the method described in International Organization for Standardization (ISO) 14040/44, which has four phases: (1) goal and scope definition, (2) life cycle inventory, (3) life cycle impact assessment, and (4) interpretation (ISO 14040, 2006). LCA modelling was carried out using SimaPro 8.5.2 software (SimaPro, 2018).

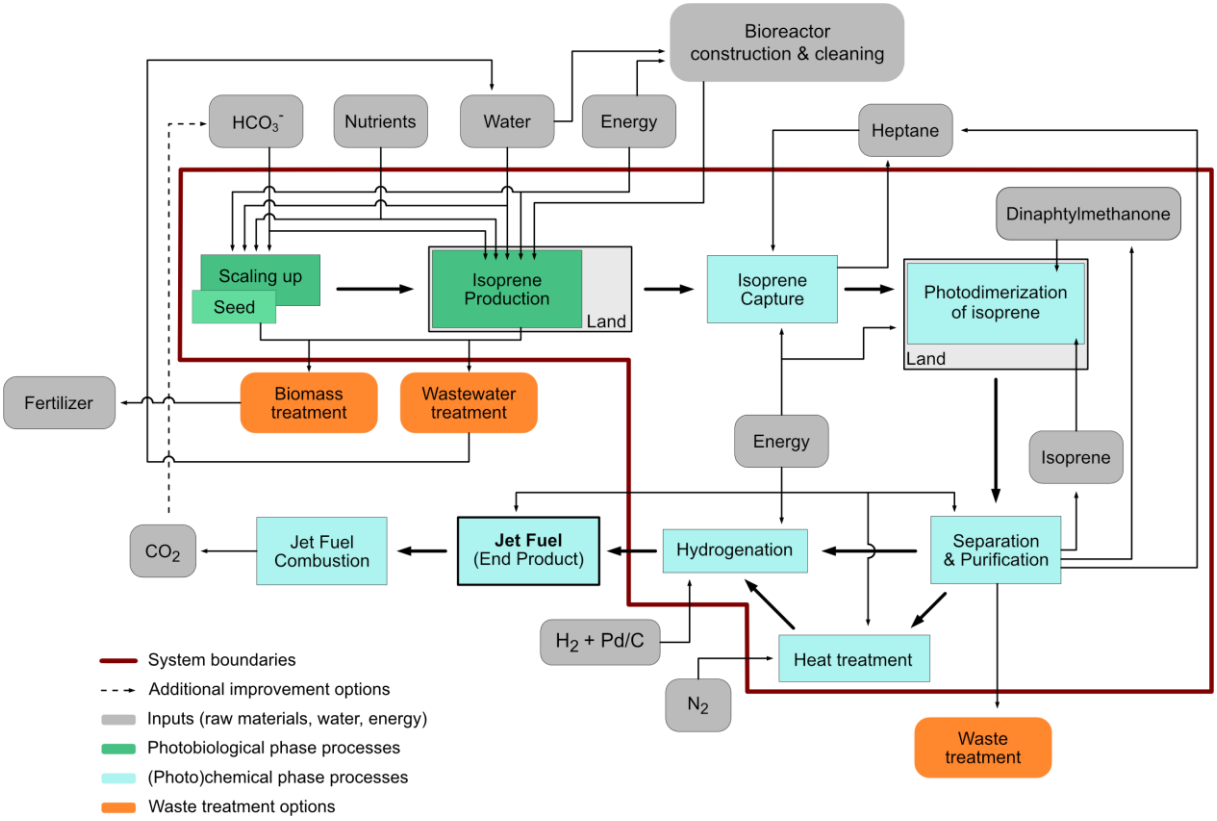


Fig. S54 Process flow chart and system boundary of the combined photobiological-photochemical route.

7.1.1 Goal, Scope and System boundary

The goal of the investigation was to assess the environmental impacts of jet fuel production through the combined photobiological-photochemical route in order to identify the hot spots and improvement options. The employed approach modelled the environmental impacts of a large scale production, using the current production technologies for input materials and energy: estimated process efficiencies from expert knowledge and lab experiments.

The scope of the study was established as a cradle to gate approach, starting from the extraction of raw materials, taking into consideration the production phase. System boundaries are shown in Fig S54. More details about the production phase are presented Table S9.

7.1.2 Life cycle inventory and data collection

Inventory foreground data were based on the experimental results, collected from life-cycle studies and literature. Background data were retrieved from Ecoinvent 3.5 database. Life cycle inventory and related assumptions are presented in Table S9. The functional unit used was 1 tonne biojet fuel produced. The geographical boundaries of the study represent Sweden. The study includes all activities from raw material extraction, and jet fuel production. Transportation of raw materials to the production site was excluded as it is out of scope. Construction and manufacture of capital goods like the bioreactor, photoreactor, mixer, heaters, distillation column and condenser were excluded as well. Energy consumption represents the electricity mix in Sweden provided by the grid, this dataset describes the electricity available on the high voltage level in Sweden for 2014. This dataset includes: electricity inputs produced in Sweden and from imports, transmission network, direct emissions to air (ozone and N_2O), and electricity losses during transmission. Basic data source is IEA World Energy Statistics and Balances (IEA. 2017, Ecoinvent 3.5 database).

7.1.3 Impact assessment

Ten impact categories were evaluated and compared: Climate Change (CC), human toxicity non-cancer effects (HTX), human toxicity cancer effects (CE), particulate matter (PM), photochemical ozone formation (POF), acidification potential (AP), terrestrial eutrophication (TE), freshwater eutrophication (FE), marine eutrophication (ME), and freshwater ecotoxicity (FEC) (Bengtsson et al., 2014).[S18] These categories were chosen, as they are considered environmentally relevant to the study and internationally accepted in accordance with ISO 14040:2006. The selected impact categories were calculated according to ILCD 2011 (Benini et al., 2014),[S19] their related area of protection and units are presented in Table S10.

Table S9 Input/Output data of life cycle assessment of biojet fuel production, functional unit 1 tonne

Route	Process	Item		Unit	Amount	Remarks
		Input	**Output**			
Photobiological	Seed cultivation, 75 m^3	*(Carbon source: HCO_3^-)[a]*		*kg*	*29.5*	
		<u>*Nutrients (medium components):*</u>				
		$MgSO_4 \cdot 7H_2O$		kg	0.39	BG11 medium:[S20]
		$CaCl_2 \cdot 2H_2O$		kg	0.19	
		Citric acid		kg	0.031	
		$Fe_2(SO_4)_3$		kg	0.026	
		K_2HPO_4		kg	0.16	Amounts needed for formation of 100 kg biomass
		$NaNO_3$		kg	7.8	
		EDTA disodium salt		g	5.2	
		H_3BO_3		g	14.9	
		$ZnSO_4 \cdot 7H_2O$		g	1.2	
		$CuSO_4 \cdot 5H_2O$		g	0.4	
		Energy (mixing)		kWh	54.3	Sierra 2008 53 W/m^3[21]
			Seed culture	kg	11.4	
	Isoprene production 750 m^3	*(Carbon source: HCO_3^-)[a]*		*kg*	*5066*	
		Seed culture		kg	11.4	
		<u>*Nutrients (Medium components):*</u>				BG11 medium
		$MgSO_4 \cdot 7H_2O$		kg	7.36	Amounts needed for formation of 1099,7 kg of isoprene, if 90% of fixed carbon is used for production.
		$CaCl_2 \cdot 2H_2O$		kg	3.53	
		Citric acid		kg	0.59	
		$Fe_2(SO_4)_3$		kg	0.48	
		K_2HPO_4		kg	2.95	
		$NaNO_3$		kg	147.5	
		EDTA disodium salt		g	98.4	
		H_3BO_3		g	281.4	
		$ZnSO_4 \cdot 7H_2O$		g	21.8	

		$CuSO_4 \cdot 5H_2O$		g	7.8	
		Water		m^3	11.95	
		Energy (mixing)		MWh	2.3	Mixing power as above
			Isoprene	Kg	1099.7	
Photochemical	Photodimerization of isoprene*	Isoprene		kg	1099.7	
		Photosensitizer		kg	0.45	
			Isoprene dimers	kg	1099.7	yield: 51%
	Separation, purification and heating of isoprene dimers*	Isoprene dimers		kg	1099.7	
		Energy for separation, purification and heating		kWh	1.05	Baral et al.[22-23]
		N_2 production (energy for cryogenic distillation)		kWh	0.16	Liu et. al. [S24]
			Treated isoprene dimers	kg	1011.7	yield: 92%
	Hydrogenation of isoprene dimers	Treated isoprene dimers		kg	1011.7	
		Hydrogen		kg	29.95	
		Energy for hydrogen injection		kWh	9.584	
			Jet Fuel	kg	1000	yield: 96%

[a] Carbon source for cultivation, not included in LCA

Table S10 Environmental assessment of 1 tonne biojetfuel production, Characterization

Impact category	**Unit**	**Total**
Climate change	kg $CO_{2\ eq}$	686.4
Human toxicity, non-cancer effects	CTUh	4.83E-05
Human toxicity, cancer effects	CTUh	3.87E-06
Particulate matter	kg $PM_{2.5\ eq}$	0.2
Photochemical ozone formation	kg NMVOC $_{eq}$	1.1
Acidification	molc $H+_{\ eq}$	1.9
Terrestrial eutrophication	molc $N_{\ eq}$	11.0
Freshwater eutrophication	kg $P_{\ eq}$	0.1
Marine eutrophication	kg $N_{\ eq}$	0.4
Freshwater ecotoxicity	CTUe	273.5

Table S11 Contribution analysis showing percent of impacts originating from the different processes in the different environmental impact categories (cut-off 0.1%).

	Environmental impact									
Process contribution (%)	**CC**	**HTX**	**CE**	**PM**	**POF**	**AP**	**TE**	**FE**	**ME**	**FEC**
Electricity, high voltage	3.7	1.7		1.9	1.3				1.5	
$NaNO_3$ production	96.2	78	83.3	85.1	92.7	94.1	97.1	96	91.6	89.3
Citric acid production		1	1.4	3.3	1.2	1.7		1.1	2.2	1.8
Tap water use		4.1	10.6	2.9	1.6				1.3	3.1
Wood chips	-1.2	5.3								
$MgSO_4 \cdot 7H_2O$ production				4.3	1.1				1.1	
$ZnSO_4 \cdot 7H_2O$ production		7.1								2.4
Others	1.3	2.8	4.7	2.5	2.1	4.2	2.9	2.9	2.3	3.4

Climate change (CC), human toxicity non-cancer effects (HTX), human toxicity cancer effects (CE), particulate matter (PM), photochemical ozone formation (POF), acidification potential (AP), terrestrial eutrophication (TE), freshwater eutrophication (FE), marine eutrophication (ME) and freshwater ecotoxicity (FEC). Note that the use of wood chips as a substitution to fossil fuels for combined heat and power (CHP) production helps in mitigating climate change impacts and appears as a negative value.[25,26]

The use of wood chips as a substitution to fossil fuels for Combined Heat and Power (CHP) production results in a negative value for the climate impact of wood chips. The use of bioenergy from wood chips has some climate impact, but this impact is lower than the impact of fossil fuels. Wood chips are used in a combined heat and power plant, which produces two products, heat and electricity. The heat is used in a process in our production system, causing an emission. There is a surplus of electricity, which is made available in the market and will replace fossil fuels (outside our production system). This reduction of climate impact is included in the calculation of the climate impact of our product as a negative post. The absolute value of substituted fossil fuel electricity is larger than the absolute value of wood chips for heat, making the total impact of the wood chips appear as a negative. This procedure is commonly used in LCA and is known as substitution (European Commission, 2010, page 76-78).[27] Note that this refers to less than 1% of the climate impacts and is thus negligible in the total climate impact, which is mainly caused by the production of $NaNO_3$ (Table S11).

8. NMR spectra

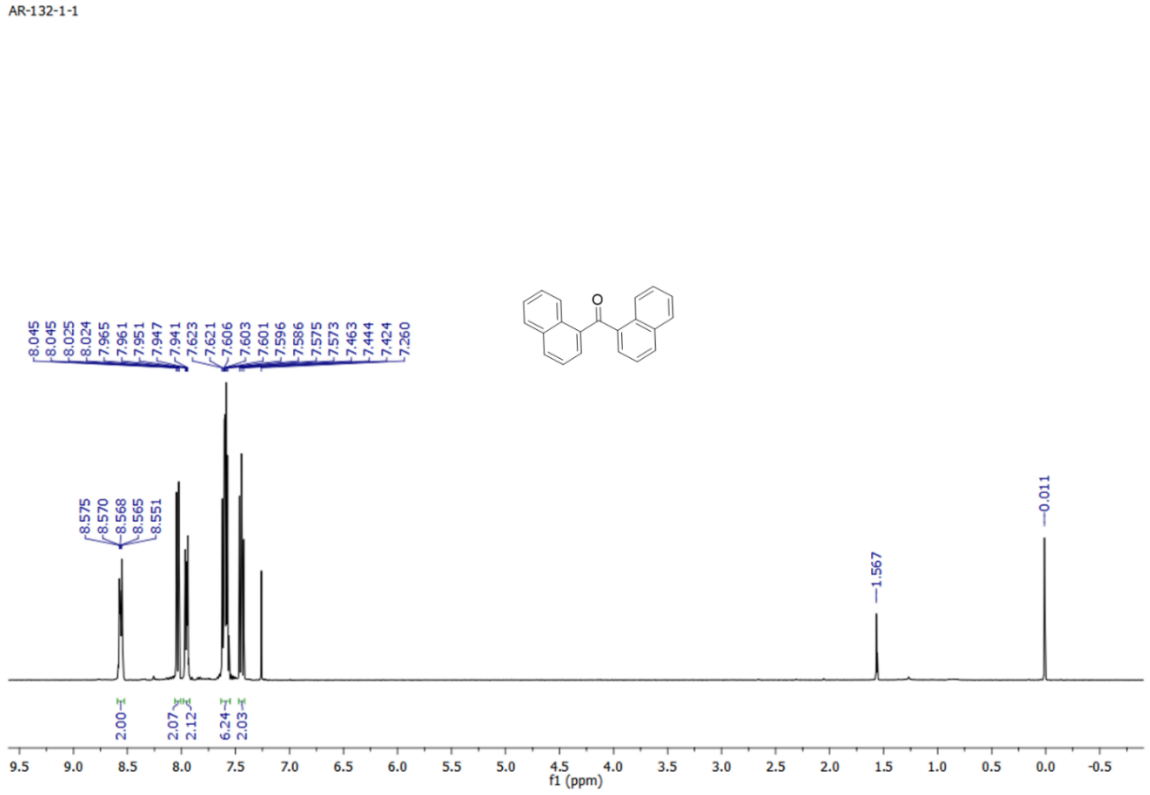


Fig. S55 ^{1}H NMR spectrum of **12** in $CDCl_3$.

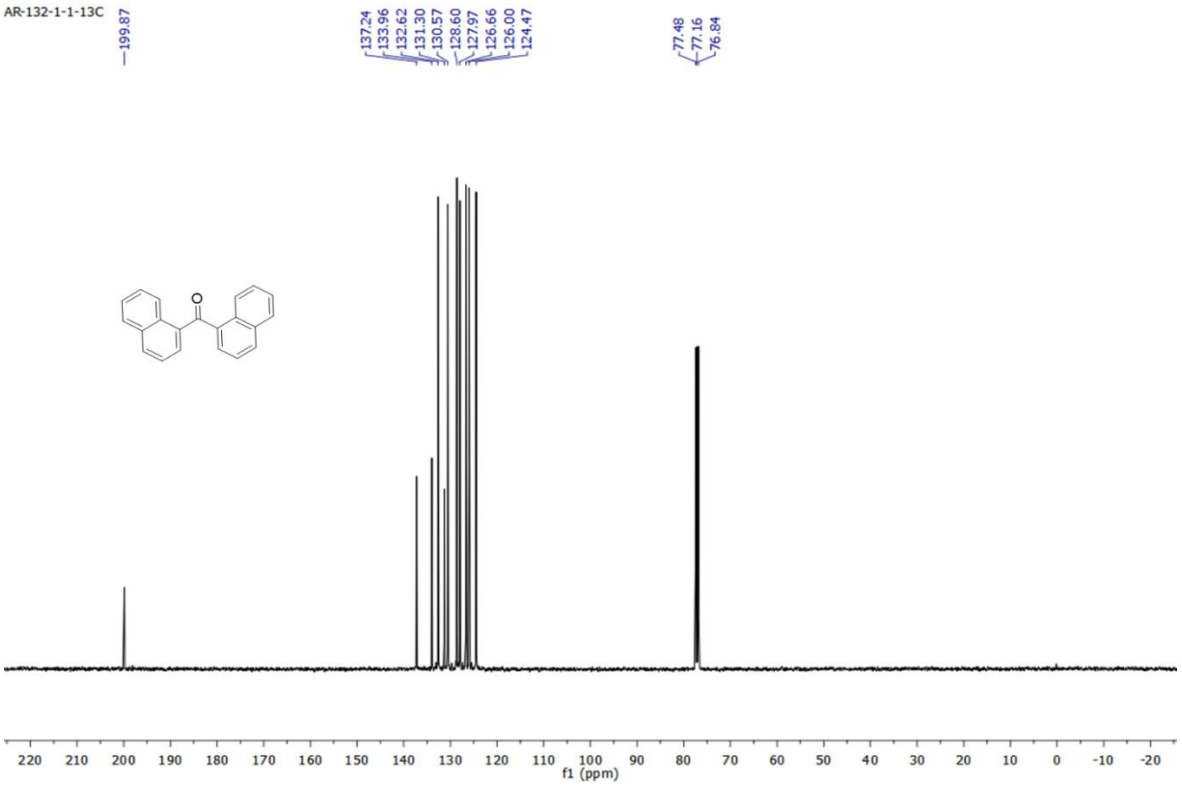


Fig. S56 ^{13}C NMR spectrum of **12** in $CDCl_3$.

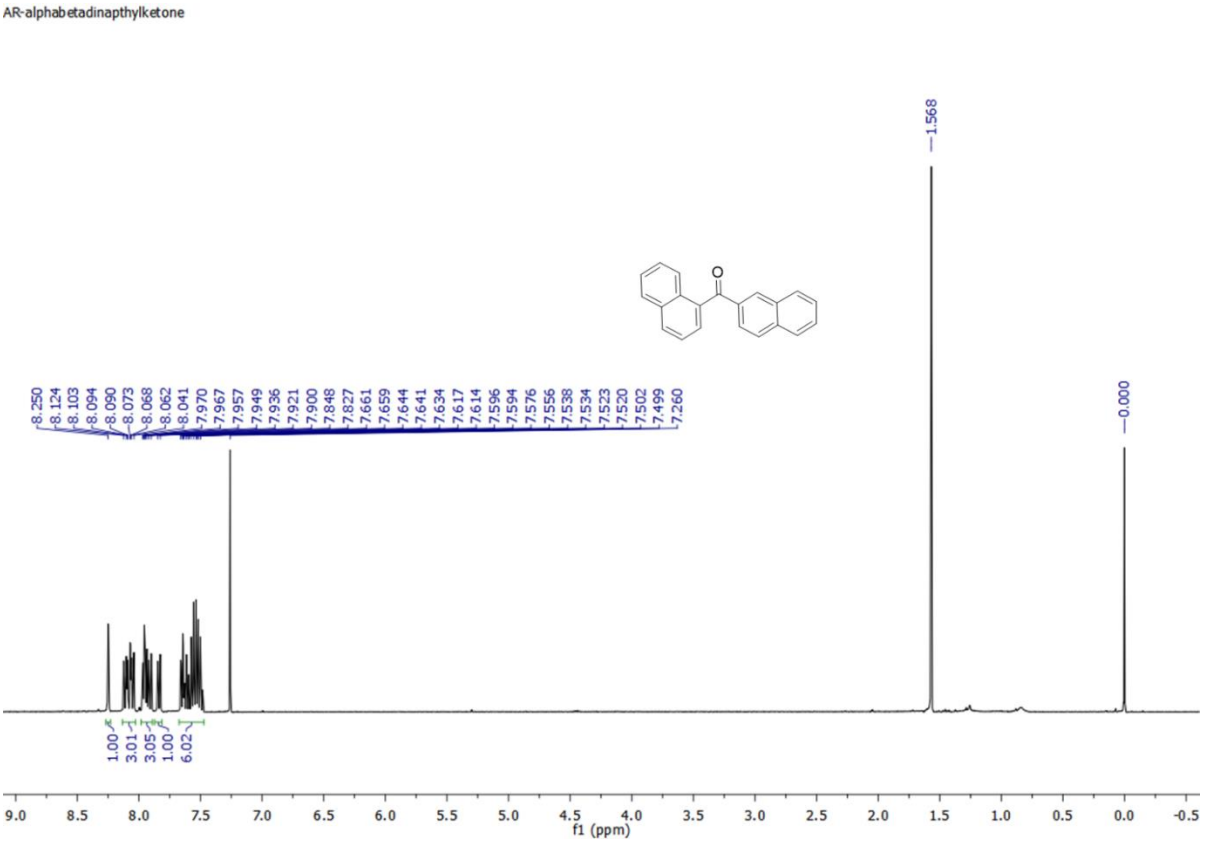


Fig. S57 ^{1}H NMR spectrum of **13** in $CDCl_3$.

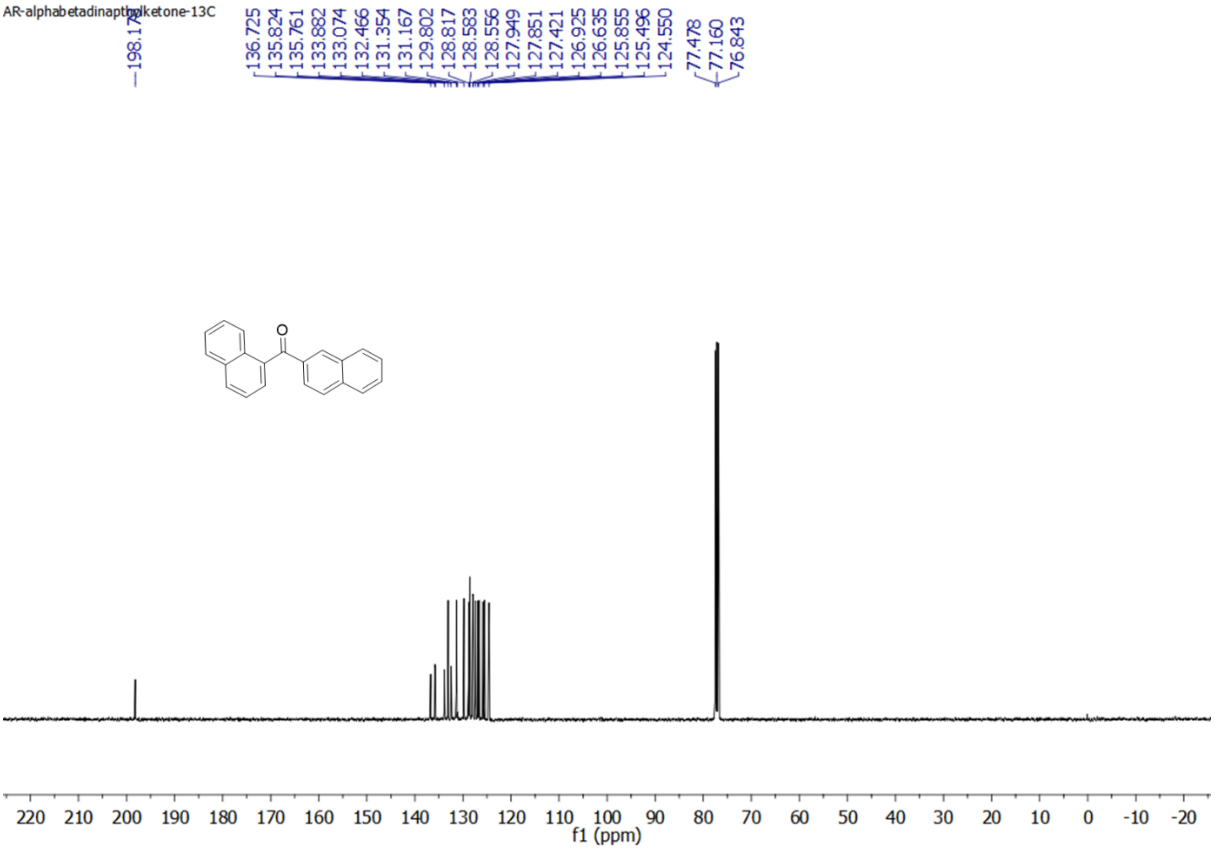


Fig. S58 ^{13}C NMR spectrum of **13** in $CDCl_3$.

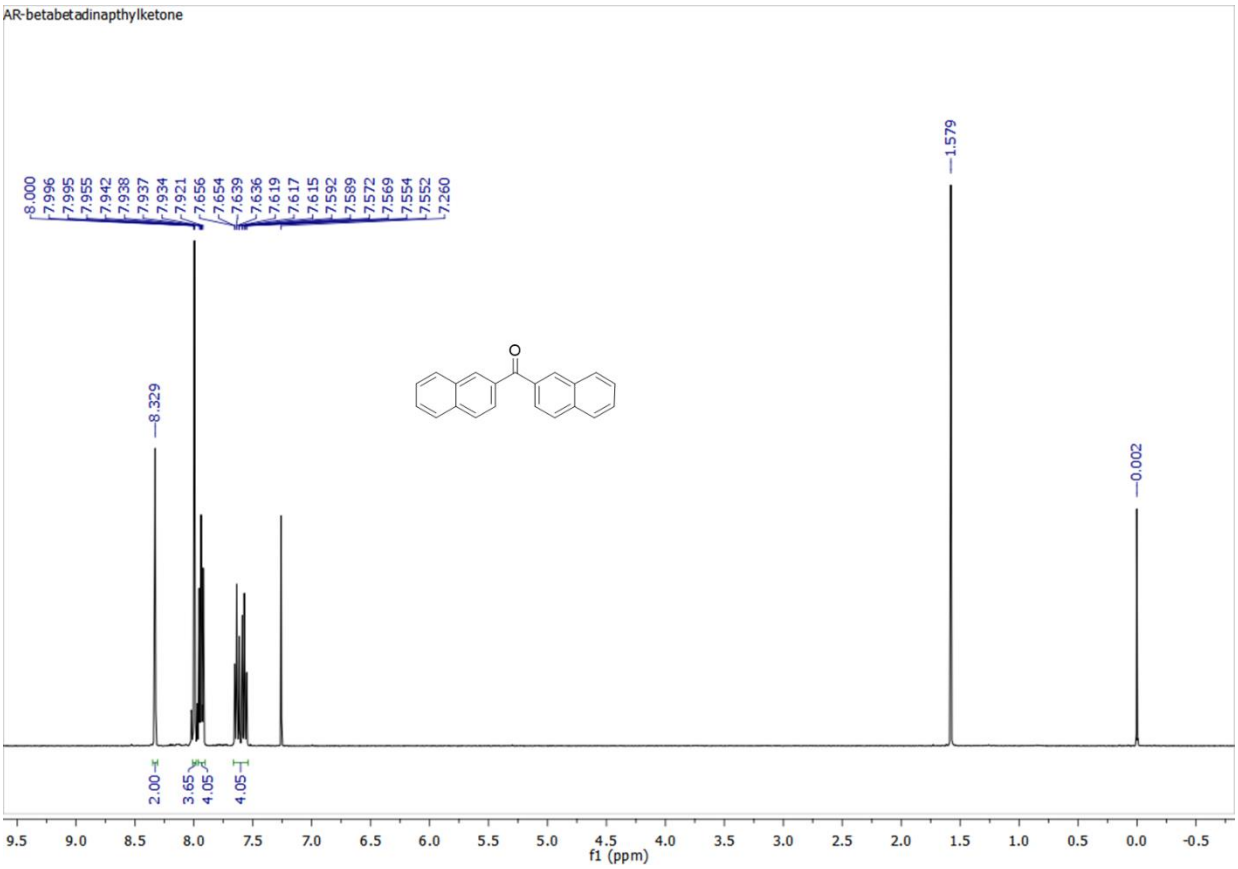


Fig. S59 ^{1}H NMR spectrum of **14** in $CDCl_3$.

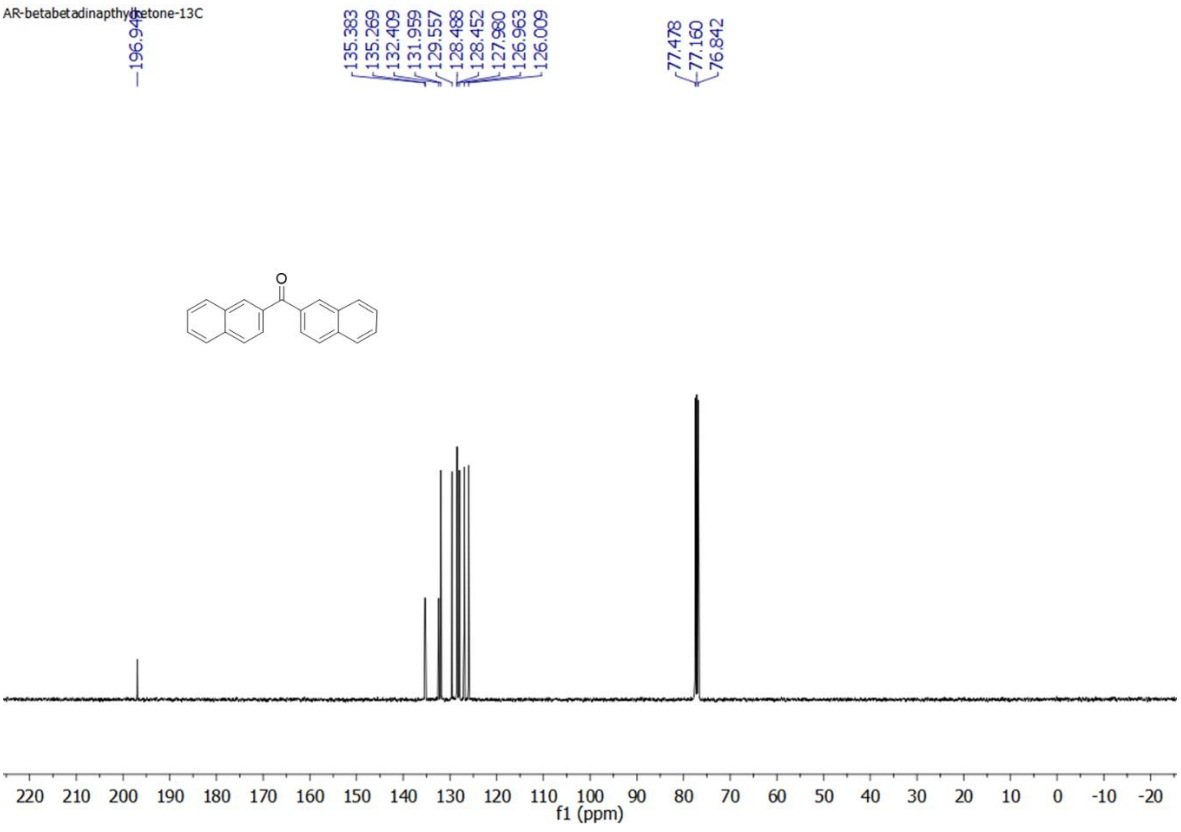


Fig. S60 ^{13}C NMR spectrum of **14** in $CDCl_3$.

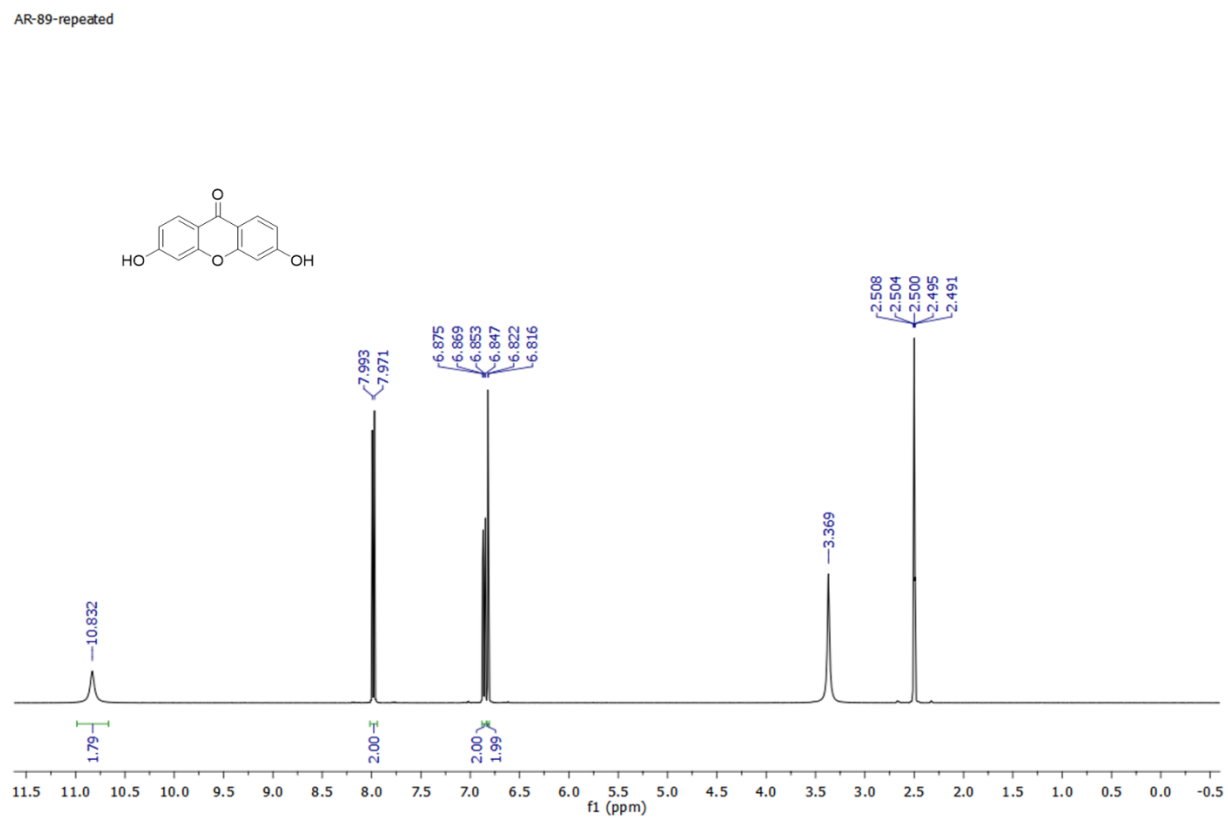


Fig. S61 ^{1}H NMR spectrum of 3,6-dihydroxyxanthone in DMSO-d_6.

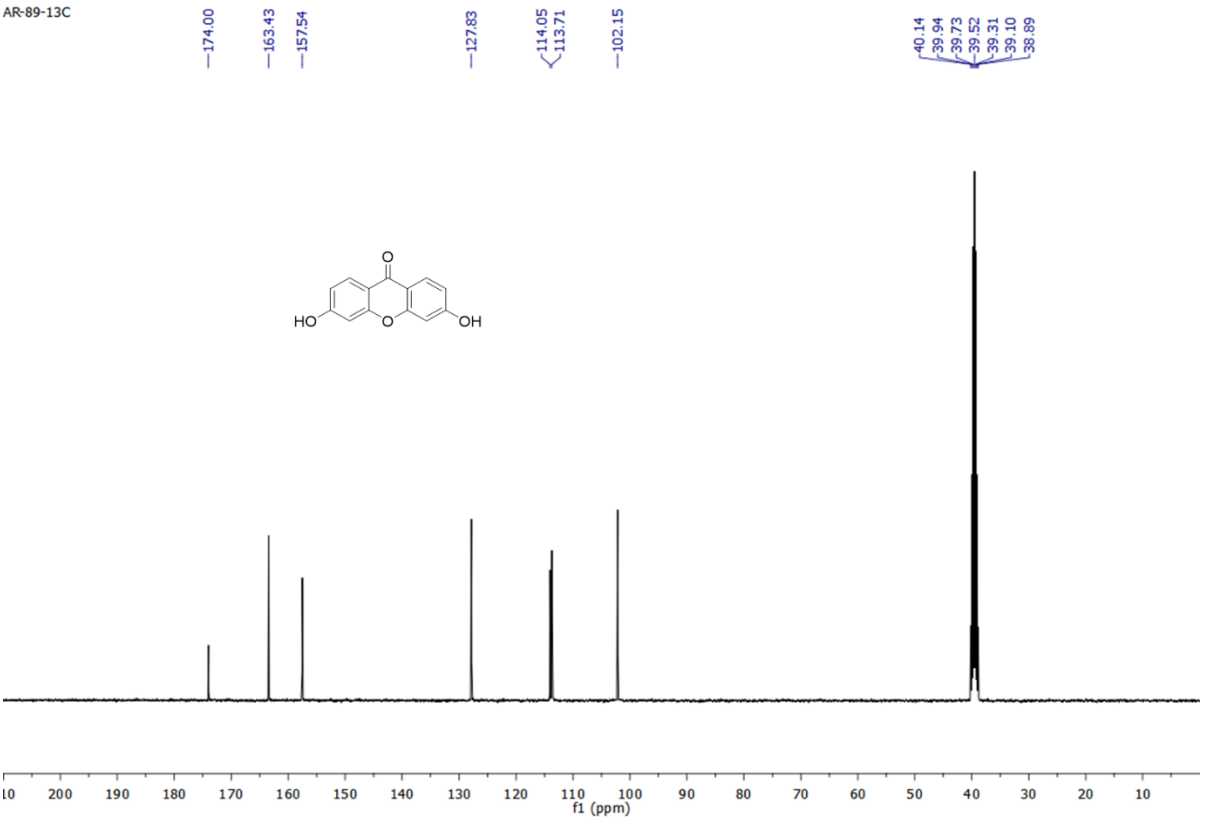


Fig. S62 ^{13}C NMR spectrum of 3,6-dihydroxyxanthone in DMSO-d_6.

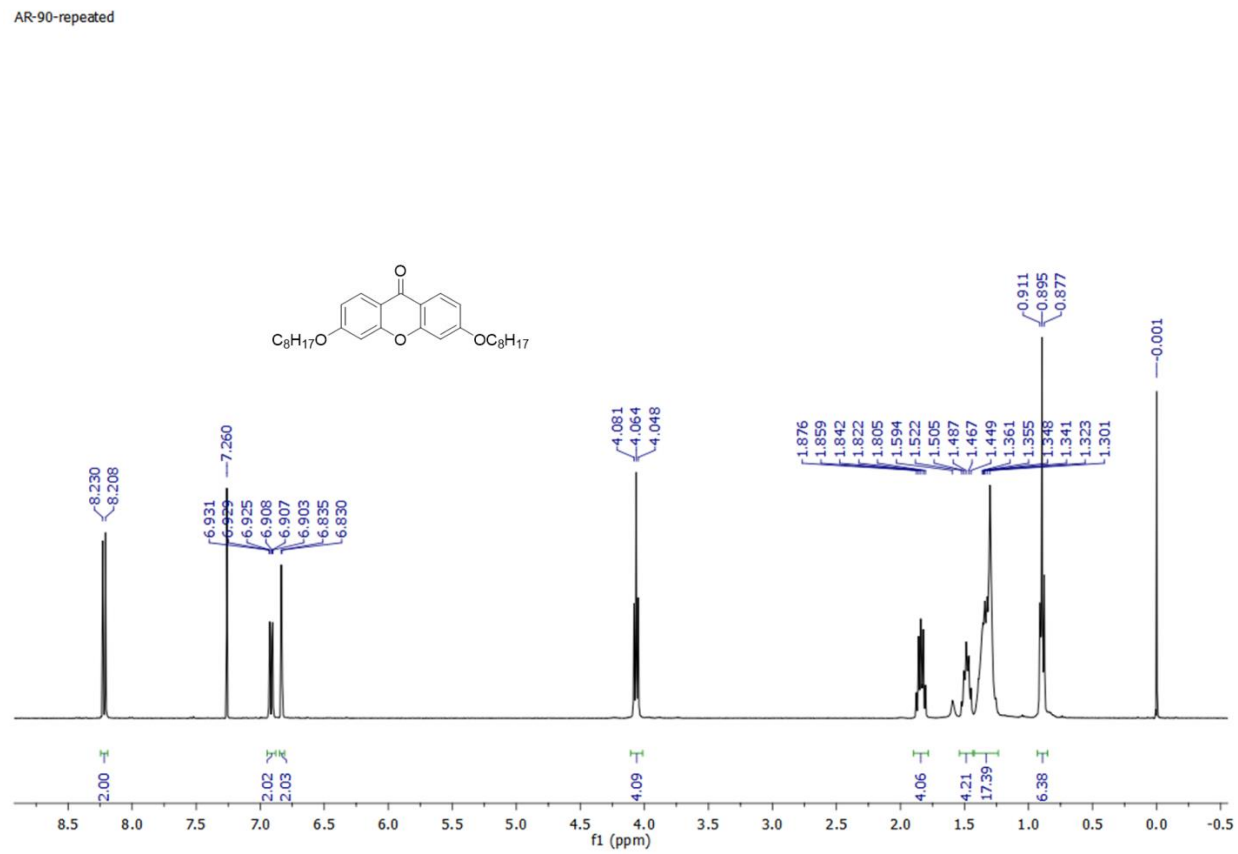


Fig. S63 ^{1}H NMR spectrum of **15** in $CDCl_3$.

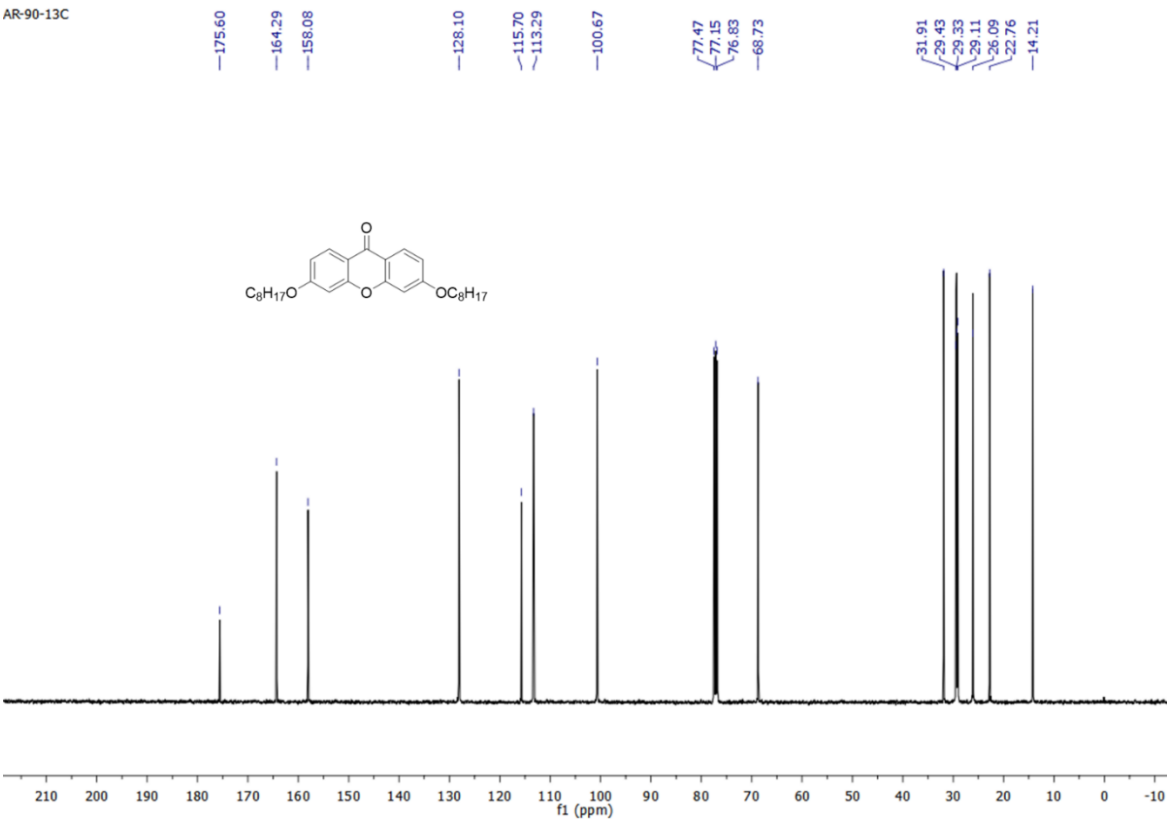


Fig. S64 ^{13}C NMR spectrum of **15** in $CDCl_3$.

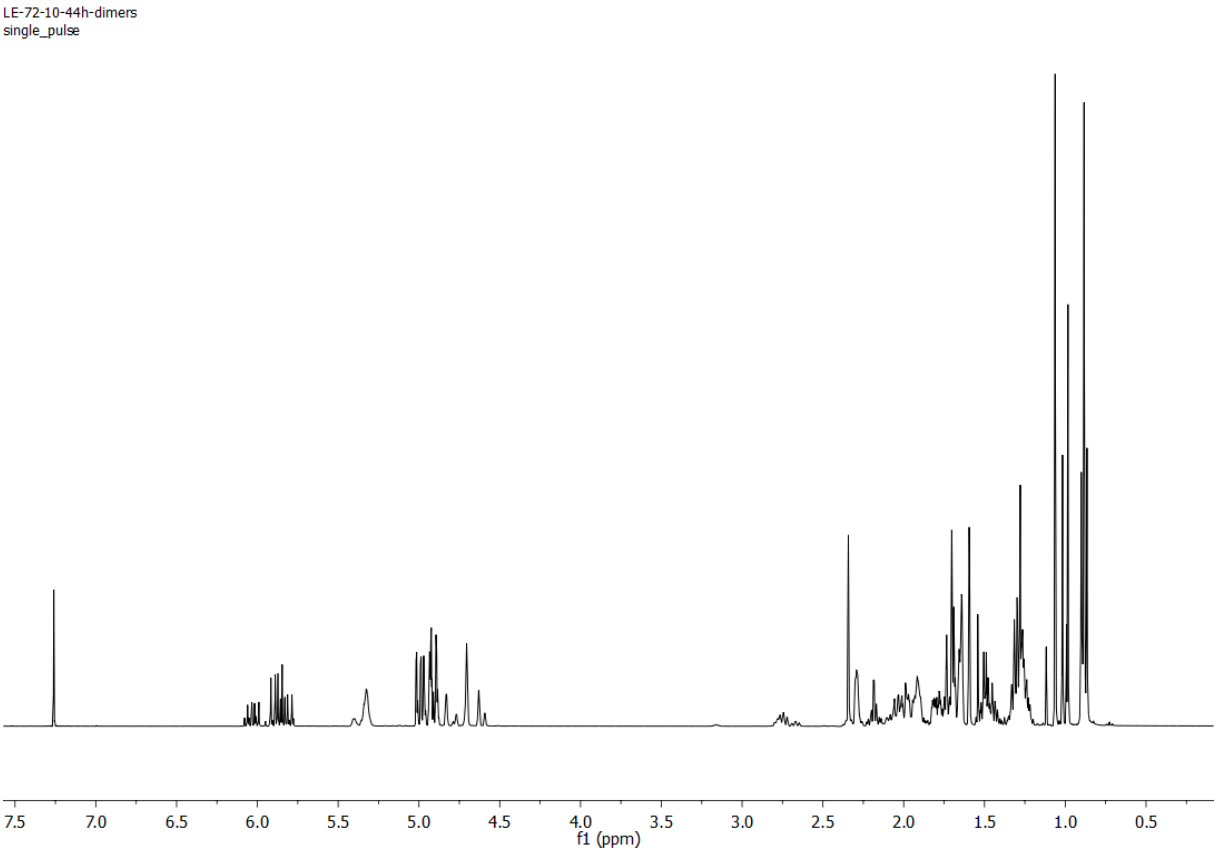


Fig. S65 ^{1}H NMR spectrum of photodimers of isoprene by using **12** as photosensitizers in $CDCl_3$.

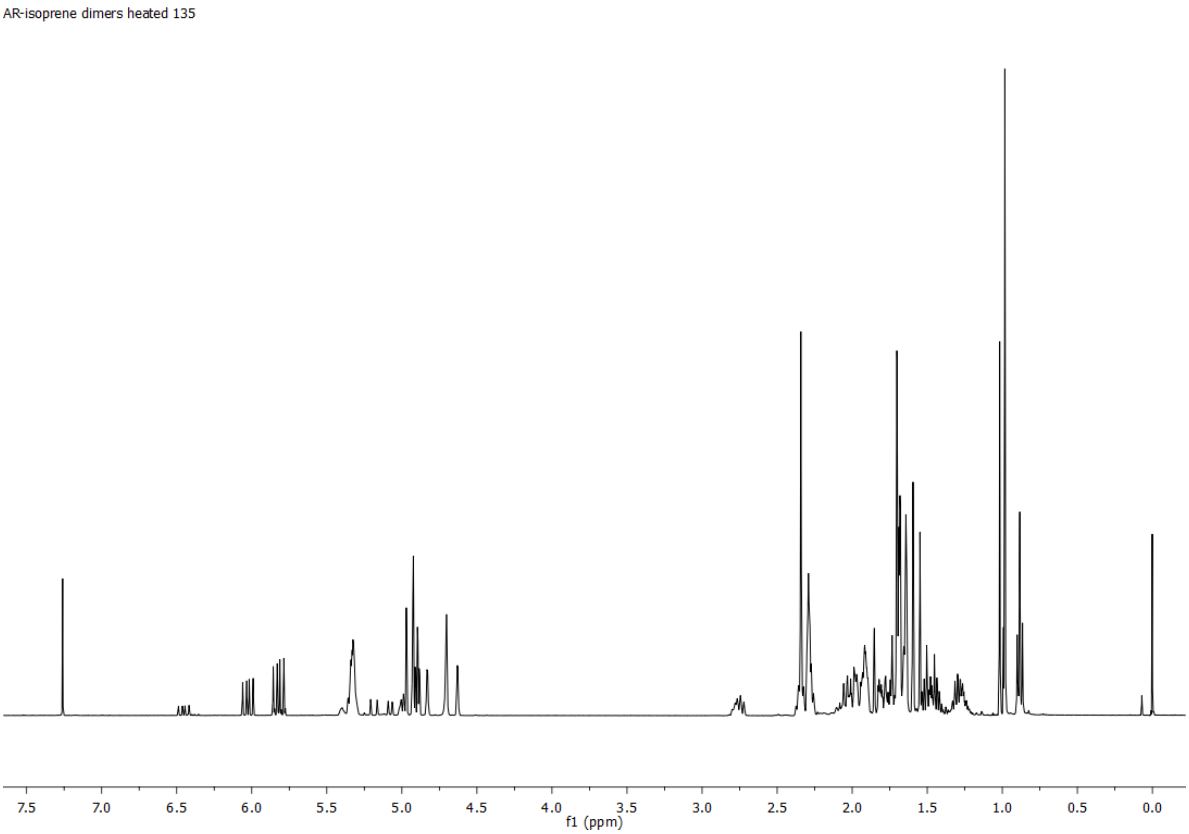


Fig. S66 ^{1}H NMR spectrum of **ID-2** in $CDCl_3$ (with isoprene).

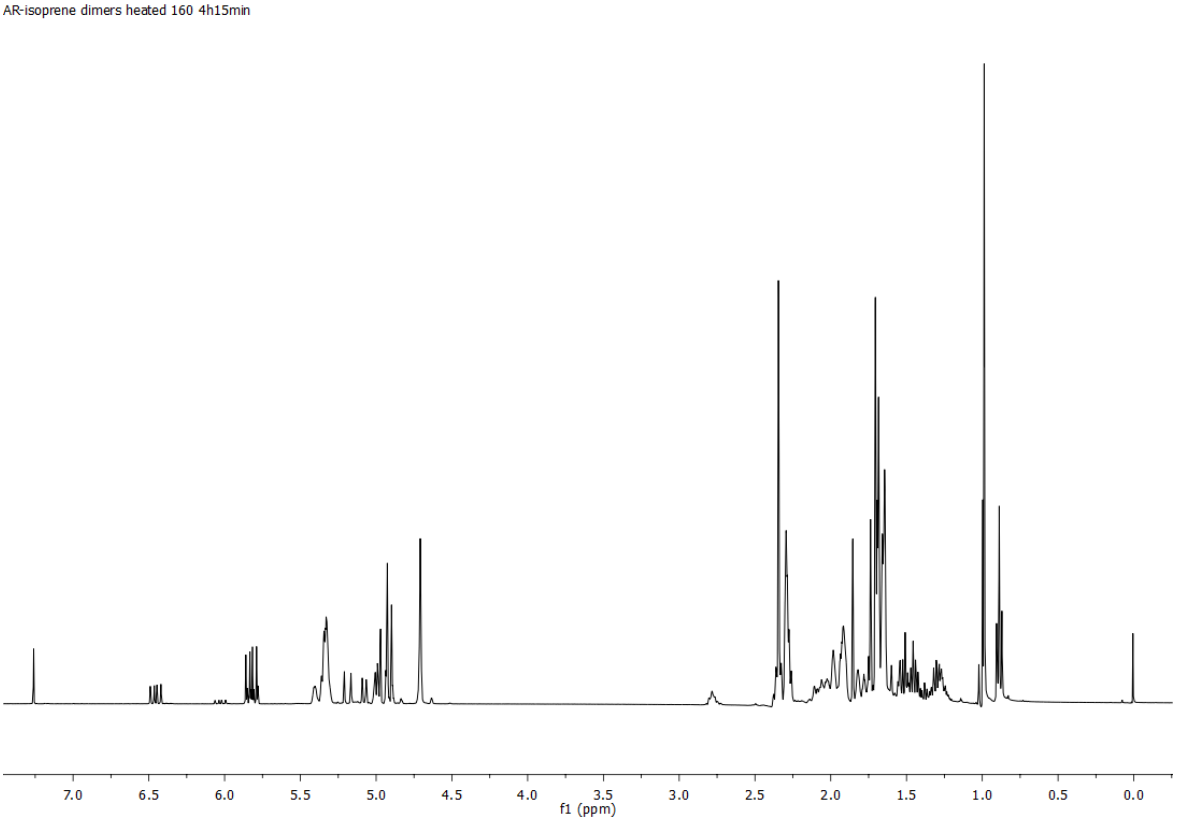


Fig. S67 ^{1}H NMR spectrum of **ID-3** in $CDCl_3$(with isoprene).

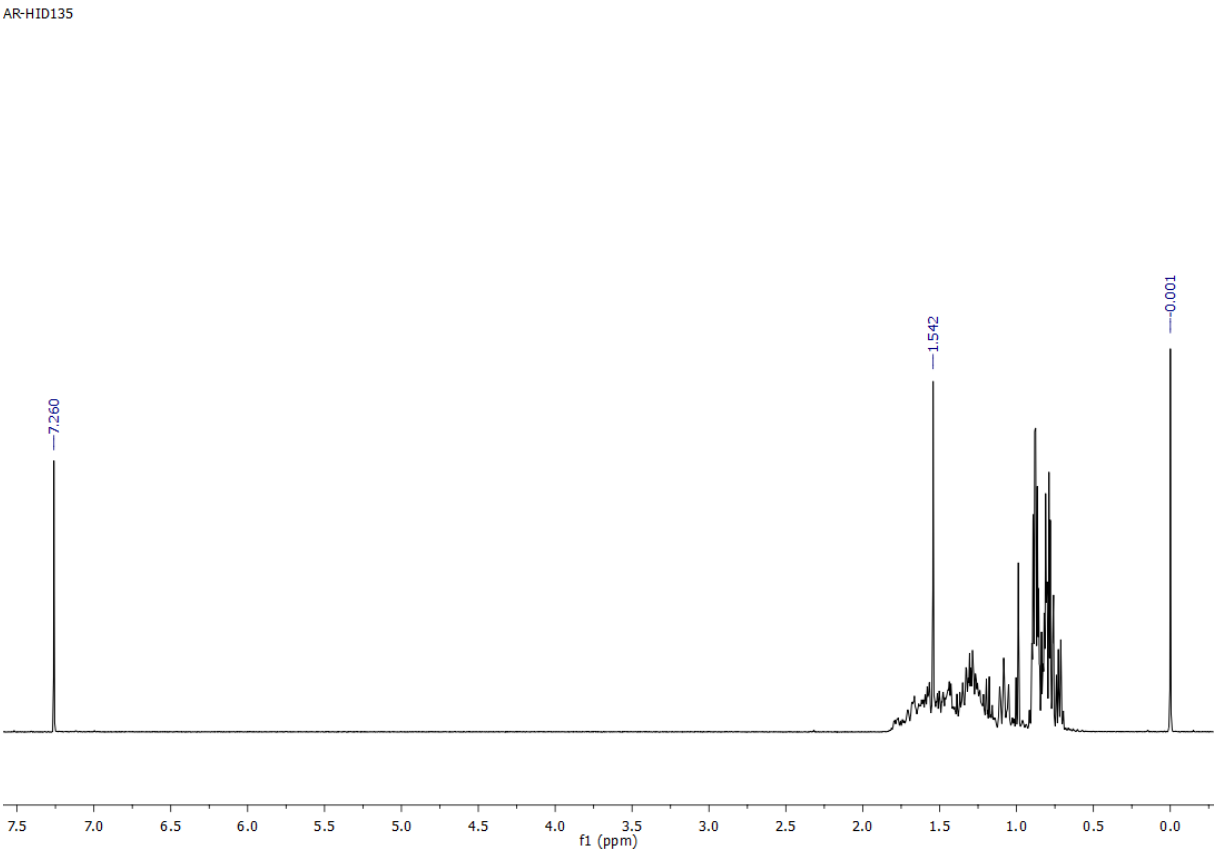


Fig. S68 ^{1}H NMR spectrum of **HID-2** in $CDCl_3$.

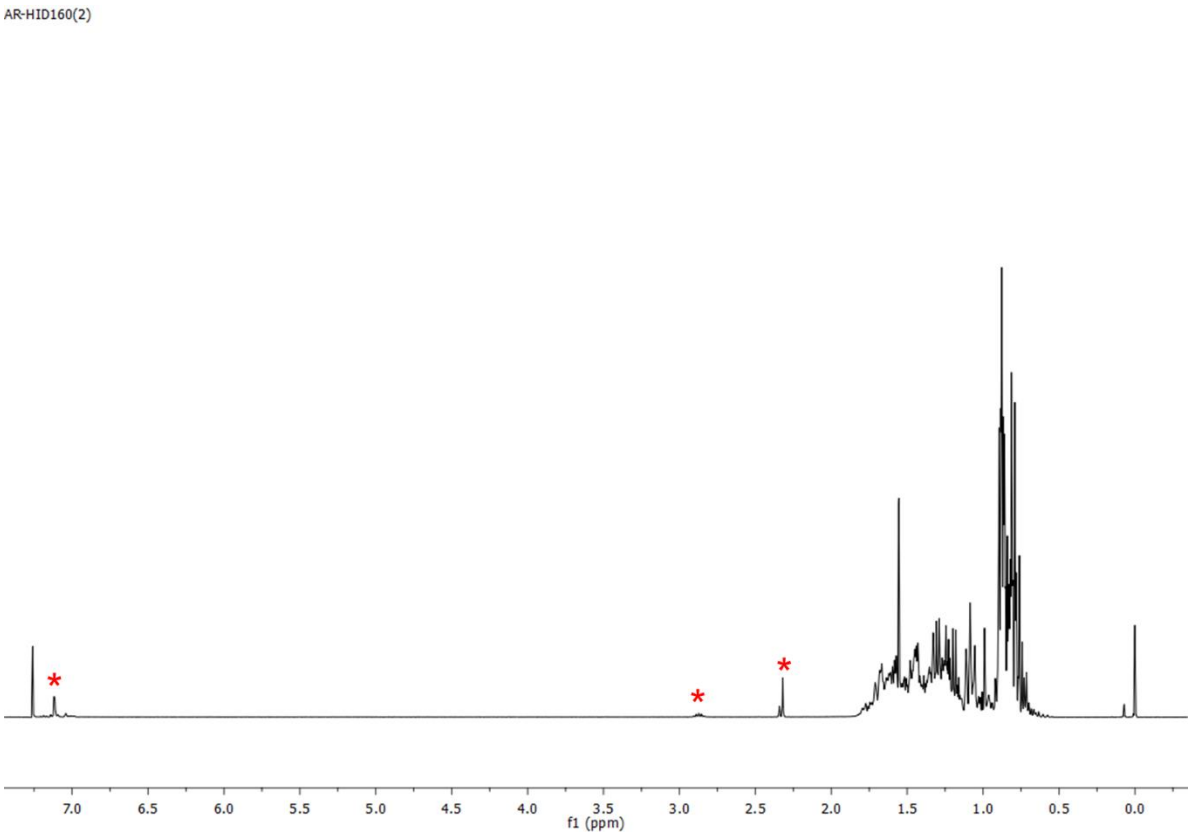


Fig. S69 ^{1}H NMR spectrum of **HID-3** in $CDCl_3$. Small amount of *p*-cymene produced (*, ~0.9%) from the isomerization of limonene during the hydrogenation of **ID-3** at 1 atm H_2 pressure.

9. Cartesian coordinates and absolute energies

B3LYP/6-311G(d,p)

Benzophenone (9)

State: S_0

Absolute Gibbs free energy at 298 K: -576.629152 a.u.

O	-0.00001436	-2.31693392	0.00006620
C	-0.00000283	-1.09647571	0.00002790
C	-1.30012109	-0.34728722	-0.02612368
C	-2.42640095	-0.95804200	0.54265036
C	-1.44343664	0.89287814	-0.66161632
C	-3.66478092	-0.32856679	0.50129316
H	-2.31035172	-1.92823368	1.01026571
C	-2.69061920	1.51141896	-0.72290839
H	-0.58811861	1.36301556	-1.13125667
C	-3.79963911	0.90745931	-0.13374349
H	-4.52735835	-0.80174959	0.95672337
H	-2.79583231	2.46292808	-1.23170659
H	-4.76760676	1.39448177	-0.17368681
C	1.30012926	-0.34730953	0.02613473
C	2.42637462	-0.95802418	-0.54274322
C	1.44347121	0.89280720	0.66171437
C	3.66475284	-0.32853923	-0.50141953
H	2.31030408	-1.92818815	-1.01041126
C	2.69065218	1.51135356	0.72297516
H	0.58816888	1.36289616	1.13143595
C	3.79963869	0.90744411	0.13369311
H	4.52730741	-0.80168329	-0.95693306
H	2.79589066	2.46282940	1.23183072
H	4.76760330	1.39447536	0.17360409

Benzophenone (9)

State: T_1

Absolute Gibbs free energy at 298 K: -576.531183 a.u.

O	-0.00000845	-2.24673647	0.00003368
C	0.00000285	-0.92326018	0.00000117
C	1.30587774	-0.30248088	-0.01671095
C	2.43284310	-1.01946185	0.46330411
C	1.51644608	0.98235817	-0.57409711
C	3.69901968	-0.45348211	0.42105892
H	2.28777528	-2.00388157	0.88995693
C	2.78470628	1.53892731	-0.59333786
H	0.68280556	1.52436717	-1.00221702
C	3.88658891	0.82898922	-0.09768714
H	4.54588874	-1.01172349	0.80451695
H	2.92533573	2.52893119	-1.01314801
H	4.87602490	1.26998501	-0.12460794
C	-1.30587730	-0.30248400	0.01671449
C	-2.43283489	-1.01945263	-0.46333670
C	-1.51645142	0.98234454	0.57412113
C	-3.69901207	-0.45347353	-0.42109658
H	-2.28776172	-2.00386352	-0.89000734
C	-2.78471129	1.53891431	0.59335475
H	-0.68281467	1.52434416	1.00226031
C	-3.88658776	0.82898598	0.09767558
H	-4.54587582	-1.01170543	-0.80457976
H	-2.92534584	2.52891088	1.01318056
H	-4.87602403	1.26998125	0.12459301

Xanthone (10)

State: S_0

Absolute Gibbs free energy at 298 K: -650.694927 a.u.

C	-3.57748524	-0.97058352	0.00032896
C	-2.34643265	-1.60606044	-0.00005942
C	-1.18261471	-0.83197537	-0.00023520
C	-1.24151848	0.56780690	-0.00011356
C	-2.50325866	1.18652276	0.00026604
C	-3.66118834	0.43051046	0.00048652
C	-0.00000033	1.36927101	-0.00048820
C	1.24151817	0.56780673	-0.00013518
C	1.18261421	-0.83197568	-0.00022994
C	2.34643238	-1.60606078	-0.00005347
H	2.26016235	-2.68548942	-0.00017428
C	3.57748499	-0.97058395	0.00032431

C	3.66118752	0.43051016	0.00049071
C	2.50325800	1.18652210	0.00026308
H	-4.48347702	-1.56578696	0.00048832
H	-2.26016191	-2.68548903	-0.00018709
H	-2.52989407	2.26951478	0.00034429
H	-4.63026545	0.91480649	0.00078413
H	4.48347554	-1.56578926	0.00050307
H	4.63026522	0.91480495	0.00077959
H	2.52989468	2.26951419	0.00035146
O	-0.00000015	-1.51731213	-0.00052206
O	0.00000258	2.59276862	-0.00047261

Xanthone (10)

State: T_1

Absolute Gibbs free energy at 298 K: -650.589295 a.u.

C	-3.59004855	-0.98115983	-0.00836015
C	-2.34649816	-1.61052428	-0.01349868
C	-1.19452457	-0.83546375	-0.00800684
C	-1.23527501	0.58707916	0.00972033
C	-2.50799772	1.19545378	0.00573616
C	-3.65961674	0.42004913	0.00900333
C	-0.00000003	1.31669159	0.00000127
C	1.23527493	0.58707910	-0.00971915
C	1.19452463	-0.83546378	0.00800865
C	2.34649824	-1.61052429	0.01349838
H	2.25116443	-2.68915581	0.03221096
C	3.59004857	-0.98115979	0.00835685
C	3.65961665	0.42004918	-0.00900724
C	2.50799762	1.19545377	-0.00573775
H	-4.49587499	-1.57423086	-0.01235353
H	-2.25116430	-2.68915581	-0.03221047
H	-2.56259698	2.27627206	0.01576305
H	-4.62791229	0.90694653	0.03435842
H	4.49587505	-1.57423078	0.01234821
H	4.62791212	0.90694660	-0.03436440
H	2.56259679	2.27627205	-0.01576483
O	0.00000001	-1.50254116	0.00000343
O	0.00000010	2.62191317	0.00000179

Thioxanthone (11)

State: S_0

Absolute Gibbs free energy at 298 K: -973.668398 a.u.

C	-3.79819937	-0.62191398	0.00042259
C	-2.64642269	-1.38963863	0.00021105
C	-1.38469405	-0.77113907	-0.00003307
C	-1.28532320	0.63065755	0.00008423
C	-2.47379092	1.38570518	0.00020965
C	-3.71460399	0.77660560	0.00041606
C	0.00000056	1.37899087	0.00021844
C	1.28532409	0.63065743	0.00008582
C	1.38469425	-0.77113889	-0.00003425
C	2.64642223	-1.38963935	0.00021062
H	2.71302060	-2.47199710	0.00018511
C	3.79819929	-0.62191529	0.00042278
C	3.71460482	0.77660432	0.00041570
C	2.47379190	1.38570491	0.00020954
H	-4.76574675	-1.11102977	0.00057436
H	-2.71302163	-2.47199634	0.00019086
H	-2.37493804	2.46387348	0.00025677
H	-4.61694864	1.37645660	0.00059587
H	4.76574674	-1.11103092	0.00057700
H	4.61694935	1.37645545	0.00059951
H	2.37493903	2.46387320	0.00025502
O	0.00000066	2.60448739	-0.00117156
S	-0.00000146	-1.85923423	-0.00068106

Thioxanthone (11)

State: T_1

Absolute Gibbs free energy at 298 K: -973.573196 a.u.

C	-3.80801467	-0.65097945	0.00024930
C	-2.64520326	-1.40820060	0.00013713
C	-1.39708989	-0.77256677	-0.00001817
C	-1.26603643	0.65355875	-0.00005369
C	-2.47536639	1.38724539	0.00005127
C	-3.70565196	0.75253468	0.00019379
C	0.00000019	1.35427928	-0.00015669
C	1.26603666	0.65355835	-0.00005347

C	1.39708971	-0.77256723	-0.00001794
C	2.64520285	-1.40820140	0.00013750
H	2.69580736	-2.49178328	0.00016498
C	3.80801447	-0.65098058	0.00024980
C	3.70565220	0.75253353	0.00019424
C	2.47536680	1.38724462	0.00005159
H	-4.77595040	-1.13556523	0.00037204
H	-2.69580799	-2.49178249	0.00016461
H	-2.39791406	2.46616304	0.00001649
H	-4.60981672	1.35167447	0.00026740
H	4.77595004	-1.13556669	0.00037265
H	4.60981714	1.35167300	0.00026794
H	2.39791475	2.46616228	0.00001677
O	0.00000033	2.64286302	-0.00018338
S	-0.00000027	-1.82428943	-0.00037274

1,1-Dinapthylmethanone (12)

State: S_0

Absolute Gibbs free energy at 298 K: -883.888815 a.u.

C	-0.00424024	-1.36449647	-0.22814754
O	-0.34770466	-2.32926955	-0.89172954
C	1.47008715	-1.10970013	-0.01845029
C	2.10285539	0.14546047	-0.29362225
C	2.22499059	-2.18270468	0.41341697
C	1.41745245	1.27022103	-0.83016082
C	3.51431196	0.26140108	-0.06690202
C	3.60933698	-2.05644878	0.64909119
H	1.73317091	-3.13365551	0.58112488
C	2.08075684	2.44313188	-1.10182311
H	0.35706429	1.20235528	-1.03488265
C	4.16520132	1.49146460	-0.35067202
C	4.23810582	-0.85721743	0.42000141
H	4.17092615	-2.91057108	1.00973807
C	3.46721443	2.56118724	-0.85370130
H	1.53615139	3.28512875	-1.51398247
H	5.23247498	1.56706673	-0.17023852
H	5.30343286	-0.75164965	0.59684408
H	3.97629221	3.49347937	-1.07022401
C	-1.00111386	-0.47828436	0.45578221
C	-2.32589329	-0.26363119	-0.06391910
C	-0.64015847	0.08829162	1.66621389
C	-2.78056065	-0.77338958	-1.31065621
C	-3.23129871	0.54324959	0.70236468
C	-1.54699996	0.85404064	2.42482064
H	0.35950270	-0.07515301	2.04975924
C	-4.05024164	-0.50007427	-1.76545277
H	-2.12192471	-1.39780938	-1.89512695
C	-4.53607264	0.79781697	0.20423832
C	-2.81454445	1.07837006	1.94870987
H	-1.23580882	1.26436991	3.37837881
C	-4.94096793	0.28806598	-1.00437502
H	-4.37234499	-0.90045716	-2.72027075
H	-5.20803774	1.40859769	0.79809254
H	-3.51935101	1.67315495	2.52063047
H	-5.93923763	0.48877376	-1.37654689

1,1-Dinapthylmethanone (12)

State: T_1

Absolute Gibbs free energy at 298 K:-883.807010 a.u.

C	-0.03406812	-0.49890196	0.46178210
O	-0.10101387	-1.67211704	0.86154406
C	1.28355668	0.22781823	0.59026574
C	2.48251061	-0.30973992	0.02115589
C	1.34075099	1.38325649	1.34347677
C	2.50156090	-1.48725840	-0.77524633
C	3.71761653	0.38366475	0.24014403
C	2.56390109	2.04927394	1.57563805
H	0.42991103	1.78249826	1.77703824
C	3.67398402	-1.94929879	-1.32449352
H	1.58052159	-2.03270266	-0.93078054
C	4.90969029	-0.12486957	-0.34025596
C	3.72624950	1.56152082	1.03193572
H	2.57730228	2.94549153	2.18557167
C	4.89129076	-1.26442898	-1.10633437
H	3.66722488	-2.85077446	-1.92694699
H	5.83979840	0.40660084	-0.16705559
H	4.66955628	2.07045576	1.20091938
H	5.80833675	-1.64272253	-1.54398566

C	-1.17478727	0.21193890	-0.11261774
C	-2.55726467	-0.22586996	0.05515736
C	-0.92601825	1.39669301	-0.93794778
C	-2.92358093	-1.34648492	0.80738598
C	-3.61157478	0.55229936	-0.55078888
C	-1.93797635	2.10084267	-1.50341185
H	0.09983067	1.69010343	-1.11079532
C	-4.28311955	-1.72640896	0.97779562
H	-2.14584878	-1.94021265	1.26319076
C	-4.94588722	0.15127183	-0.36997180
C	-3.30183838	1.70713637	-1.31275115
H	-1.71786665	2.96452789	-2.12076809
C	-5.28283181	-0.98655958	0.39469575
H	-4.51392771	-2.60440669	1.56895985
H	-5.73227493	0.73838379	-0.83222565
H	-4.10389902	2.27961980	-1.76272628
H	-6.32353821	-1.26529811	0.51357001

1,2-Dinapthylmethanone (13)

State: S_0

Absolute Gibbs free energy at 298 K: -883.894495 a.u.

C	4.01022023	2.01095278	-1.29131834
C	2.72876445	1.51460556	-1.26959782
C	2.40623469	0.37329239	-0.48871738
C	3.43637947	-0.25843293	0.27702044
C	4.74745857	0.27903614	0.23311549
C	5.02807302	1.38692538	-0.53253739
H	0.31710006	0.32427954	-1.02557033
H	4.24633821	2.88319578	-1.89005353
H	1.94469966	1.99055668	-1.84905443
C	1.09324626	-0.15783004	-0.44230908
C	3.10688174	-1.40550282	1.05129287
H	5.52958739	-0.19891636	0.81353324
H	6.03532643	1.78733244	-0.55793291
C	1.83160698	-1.90384696	1.06705198
C	0.79907024	-1.27285457	0.31766956
H	3.88850395	-1.88609623	1.63051730
H	1.57933872	-2.78520482	1.64334282
C	-0.56516089	-1.88499811	0.33377347
C	-1.73247351	-1.12635327	-0.25152161
C	-2.21005319	0.10484003	0.29816138
C	-2.37362830	-1.69564020	-1.33276090
C	-1.65427983	0.70772148	1.46007167
C	-3.33362297	0.74125320	-0.32461235
C	-3.47118725	-1.05751523	-1.94855101
H	-2.01924783	-2.64542801	-1.71646293
C	-2.16392934	1.88106519	1.96266150
H	-0.82140295	0.23125677	1.96179473
C	-3.82948390	1.95643936	0.21820970
C	-3.93631456	0.13792007	-1.45836933
H	-3.94411209	-1.51911999	-2.80778133
C	-3.25840097	2.51767874	1.33362595
H	-1.72652984	2.32078226	2.85187053
H	-4.67839652	2.43137222	-0.26259653
H	-4.78120465	0.63307485	-1.92552810
H	-3.64905153	3.44357961	1.74023932
O	-0.73466935	-3.01290024	0.76494117

1,2-Dinapthylmethanone (13)

State: T_1

Absolute Gibbs free energy at 298 K: -883.808416 a.u.

C	4.07937230	-1.81758010	1.33467323
C	2.78407717	-1.35854597	1.35579195
C	2.39031298	-0.25597114	0.55114926
C	3.36766015	0.37711839	-0.28082201
C	4.69507909	-0.12198759	-0.27985857
C	5.04391397	-1.19391773	0.50820539
H	0.32864802	-0.24857444	1.18223868
H	4.36789975	-2.66031989	1.95267103
H	2.04282806	-1.83517748	1.98885299
C	1.06114000	0.23437300	0.54480802
C	2.97064737	1.49128004	-1.06862325
H	5.43529362	0.35840099	-0.91126740
H	6.06268637	-1.56476520	0.50084565
C	1.68070377	1.95485790	-1.03869949
C	0.69620211	1.31236164	-0.23823357
H	3.71154949	1.98040044	-1.69272950
H	1.38533403	2.82148028	-1.61705058

C	-0.66954151	1.91896658	-0.17478339
C	-1.87483665	1.13857993	0.10560626
C	-2.12291472	-0.22749831	-0.32667137
C	-2.94886255	1.84484480	0.81406606
C	-1.36007290	-0.87828192	-1.29832662
C	-3.24785629	-0.93002712	0.23586445
C	-4.00760255	1.16388578	1.32247630
H	-2.82529749	2.90853097	0.96251081
C	-1.60301354	-2.22514012	-1.65875495
H	-0.55697022	-0.34750568	-1.79094100
C	-3.45470946	-2.26997006	-0.11717756
C	-4.14990745	-0.24072755	1.09904404
H	-4.76031452	1.68489969	1.90341393
C	-2.62855788	-2.92068320	-1.05648476
H	-0.97621066	-2.69734570	-2.40553166
H	-4.27656582	-2.81080364	0.33987093
H	-4.99642900	-0.77584770	1.51269255
H	-2.81667439	-3.95748639	-1.31023815
O	-0.79164720	3.14606130	-0.32685435

2,2-Dinapthylmethanone (14)

State: S_0

Absolute Gibbs free energy at 298 K: -883.899078 a.u.

C	4.67125769	-2.35019648	-0.65617770
C	3.36271626	-1.92980222	-0.66928491
C	3.02149177	-0.60726338	-0.28103894
C	4.06194235	0.28874833	0.11889158
C	5.40136859	-0.17666226	0.12270012
C	5.69946990	-1.46507841	-0.25537722
H	0.89923037	-0.83278732	-0.58753676
H	4.92091624	-3.36234623	-0.95341179
H	2.57148553	-2.60592979	-0.97610509
C	1.67936271	-0.14904528	-0.27300172
C	3.71369419	1.61662600	0.48990682
H	6.19096153	0.50224681	0.42718792
H	6.72800209	-1.80797202	-0.24937239
C	2.41074313	2.03777124	0.46507259
C	1.36665533	1.14502087	0.09381486
H	4.50254245	2.29934592	0.78819123
H	2.14631594	3.05559665	0.72326249
C	-0.02853749	1.68711933	0.02180038
C	-2.36984382	1.06897581	-0.47741398
C	-3.52971458	0.27187480	-0.33500197
C	-1.20325358	0.77004464	0.19929563
C	-4.73020386	0.55340348	-1.04166912
C	-3.49569990	-0.84889889	0.55496770
C	-1.17674115	-0.34379486	1.08299222
C	-5.84299690	-0.23450224	-0.87614205
H	-4.75292138	1.40443826	-1.71398194
C	-4.66326104	-1.64179722	0.70330378
C	-2.29478007	-1.12062793	1.26106123
H	-0.27530418	-0.56180047	1.64212372
C	-5.80847089	-1.34264528	0.00457091
H	-6.75416763	-0.01056044	-1.41906212
H	-4.63841558	-2.49035935	1.37896080
H	-2.27199138	-1.95592553	1.95320428
H	-6.69413136	-1.95609605	0.12631360
O	-0.20660395	2.87642638	-0.19125910
H	-2.39088290	1.93511830	-1.12932218

2,2-Dinapthylmethanone (14)

State: T_1

Absolute Gibbs free energy at 298 K: -883.814036 a.u.

C	4.97113573	-2.14333212	-0.69882418
C	3.64739907	-1.79509025	-0.82725401
C	3.17263695	-0.54854141	-0.33996604
C	4.09789124	0.34846532	0.28021850
C	5.45616108	-0.04116458	0.39807203
C	5.88408450	-1.25845103	-0.07875569
H	1.12501574	-0.84221513	-0.94703769
H	5.32111330	-3.09852580	-1.07374613
H	2.94598296	-2.47225997	-1.30392193
C	1.81101382	-0.16544465	-0.44979356
C	3.61976418	1.60474015	0.74343097
H	6.15673821	0.63988216	0.87005739
H	6.92572710	-1.54371837	0.01657786
C	2.30233007	1.95411354	0.60594806
C	1.36642524	1.05487442	0.02134803

H	4.32099172	2.29257649	1.20477089
H	1.94479568	2.92176971	0.93559689
C	-0.04340244	1.52721652	-0.14454011
C	-2.49642105	1.08064107	-0.45018691
C	-3.65586496	0.31895170	-0.25616940
C	-1.17966949	0.61573069	0.01159593
C	-4.93095830	0.73643874	-0.70666844
C	-3.56271543	-0.94620978	0.43136888
C	-1.12121754	-0.59382848	0.69009324
C	-6.08022527	-0.06126914	-0.49874899
H	-5.02051056	1.68695034	-1.22040506
C	-4.70519991	-1.70762548	0.62528249
C	-2.27074399	-1.36372239	0.90183822
H	-0.17796163	-0.94285236	1.09031055
C	-5.98227085	-1.26636772	0.15522585
H	-7.04055709	0.28844813	-0.86014061
H	-4.62878675	-2.65728586	1.14462276
H	-2.19397816	-2.30087830	1.44257114
H	-6.85693036	-1.88325885	0.31995889
O	-0.26025400	2.72104889	-0.39452604
H	-2.54052393	2.04222587	-0.94409591

3,6-di(methoxy)xanthenone (15)

State: S_0

Absolute Gibbs free energy at 298 K: -879.753766 a.u.

C	3.58044892	0.62208158	0.00004287
C	2.33704571	1.25265265	-0.00001187
C	1.18342331	0.47909289	0.00000151
C	1.23620088	-0.92478477	0.00006895
C	2.49940673	-1.53038302	0.00012289
C	3.66456428	-0.78344604	0.00011097
C	0.00000012	-1.72604327	0.00008198
C	-1.23620073	-0.92478492	0.00001904
C	-1.18342332	0.47909273	-0.00004637
C	-2.33704583	1.25265234	-0.00010652
H	-2.27378170	2.33274498	-0.00015636
C	-3.58044900	0.62208116	-0.00010199
C	-3.66456417	-0.78344647	-0.00003717
C	-2.49940652	-1.53038330	0.00002198
H	2.27378146	2.33274528	-0.00006419
H	2.53494764	-2.61327006	0.00017473
H	4.62250929	-1.28417622	0.00015386
H	-4.62250905	-1.28417686	-0.00003300
H	-2.53494731	-2.61327034	0.00007248
O	-0.00000005	1.16530015	-0.00005480
O	0.00000020	-2.95254080	0.00014004
O	-4.65666498	1.45013514	-0.00016313
O	4.65666496	1.45013545	0.00002527
C	5.96443477	0.88512067	0.00007811
H	6.13600843	0.27875700	-0.89484406
H	6.64916595	1.73110741	0.00004872
H	6.13597467	0.27884653	0.89506740
C	-5.96443514	0.88512110	-0.00016241
H	-6.13601023	0.27884497	0.89481876
H	-6.64916579	1.73110825	-0.00021640
H	-6.13597446	0.27875972	-0.89509269

3,6-di(methoxy)xanthenone (15)

State: T_1

Absolute Gibbs free energy at 298 K: -879.643753 a.u.

C	-3.59342527	-0.62129103	-0.00000225
C	-2.34139127	-1.25984352	-0.00000097
C	-1.19982029	-0.49259356	0.00000010
C	-1.23198542	0.93724076	-0.00000003
C	-2.50641804	1.54605852	-0.00000135
C	-3.66656727	0.78409512	-0.00000242
C	-0.00000059	1.66119262	0.00000048
C	1.23198432	0.93724178	0.00000099
C	1.19982035	-0.49259302	0.00000158
C	2.34139189	-1.25984170	0.00000203
H	2.28109721	-2.34006263	0.00000230
C	3.59342584	-0.62128833	0.00000191
C	3.66656657	0.78409809	0.00000153
C	2.50641685	1.54606051	0.00000114
H	-2.28109561	-2.34006439	-0.00000060
H	-2.55226735	2.62671410	-0.00000160
H	-4.62530498	1.28486433	-0.00000349
H	4.62530341	1.28486877	0.00000166

H	2.55226533	2.62671609	0.00000075
O	0.00000034	-1.15619921	0.00000141
O	-0.00000056	2.97859393	0.00000017
O	4.67058188	-1.45044838	0.00000288
O	-4.67058218	-1.45045025	-0.00000303
C	5.97753800	-0.88577172	-0.00000578
H	6.66329948	-1.73091651	0.00000613
H	6.14812532	-0.27880433	-0.89496602
H	6.14812712	-0.27877815	0.89493641
C	-5.97753599	-0.88576824	0.00000295
H	-6.66330086	-1.73091023	0.00000453
H	-6.14811781	-0.27878795	0.89495569
H	-6.14812527	-0.27878557	-0.89494677

B3LYP-D3/6-311+G(d,p)

Benzophenone (9)

State: S_0

Absolute Gibbs free energy at 298 K: -576.647753 a.u.

O	0.00000389	2.32602254	0.00002957
C	0.00000370	1.10551528	-0.00005313
C	1.29716060	0.35338174	0.02937029
C	2.42511848	0.95690106	-0.54278989
C	1.43284473	-0.88602439	0.66771604
C	3.65965112	0.31958966	-0.50253898
H	2.31254772	1.92684719	-1.01187641
C	2.67591042	-1.51258708	0.72761565
H	0.57366703	-1.34881943	1.13763414
C	3.78756519	-0.91647502	0.13455690
H	4.52440315	0.78614940	-0.96057292
H	2.77605110	-2.46398038	1.23754636
H	4.75240740	-1.40972406	0.17302044
C	-1.29715601	0.35338482	-0.02942288
C	-1.43287163	-0.88602276	-0.66775925
C	-2.42508886	0.95691000	0.54278175
C	-2.67594269	-1.51258002	-0.72760638
H	-0.57371675	-1.34882273	-1.13771369
C	-3.65962619	0.31960522	0.50258105
H	-2.31249413	1.92685652	1.01186172
C	-3.78757117	-0.91646130	-0.13450534
H	-2.77610760	-2.46397475	-1.23752961
H	-4.52435800	0.78617085	0.96064712
H	-4.75241715	-1.40970617	-0.17292873

Benzophenone (9)

State: T_1

Absolute Gibbs free energy at 298 K: -576.549622 a.u.

O	0.00000015	2.26132505	-0.00000031
C	0.00000006	0.93821901	-0.00000035
C	1.30263108	0.31196860	0.01964703
C	2.43407091	1.01703737	-0.46633993
C	1.50168013	-0.97138048	0.58460464
C	3.69484017	0.43885663	-0.42488443
H	2.29628497	2.00091273	-0.89680076
C	2.76422488	-1.54042482	0.60268203
H	0.66260121	-1.50121120	1.01745989
C	3.87130827	-0.84329154	0.09947368
H	4.54615046	0.98673241	-0.81333326
H	2.89683772	-2.52936807	1.02745565
H	4.85654085	-1.29362097	0.12541483
C	-1.30263115	0.31196871	-0.01964744
C	-2.43407061	1.01703733	0.46634030
C	-1.50168047	-0.97138010	-0.58460537
C	-3.69483990	0.43885662	0.42488536
H	-2.29628446	2.00091262	0.89680125
C	-2.76422525	-1.54042448	-0.60268227
H	-0.66260173	-1.50121069	-1.01746115
C	-3.87130829	-0.84329138	-0.09947307
H	-4.54614998	0.98673229	0.81333481
H	-2.89683831	-2.52936761	-1.02745612
H	-4.85654090	-1.29362078	-0.12541379

Xanthone (10)

State: S0

Absolute Gibbs free energy at 298 K: -650.713055 a.u.

C	-2.34562314	-1.60588522	-0.00006878
C	-1.18179198	-0.83266533	-0.00003142
C	-1.24079714	0.56742254	0.00003816
C	-2.50139910	1.18711982	0.00005582
C	-3.65995090	0.43137809	0.00001375

C	0.00000037	1.36865245	0.00012991
C	1.24079738	0.56742210	0.00004214
C	1.18179164	-0.83266560	-0.00002847
C	2.34562251	-1.60588583	-0.00006617
H	2.25827670	-2.68516523	-0.00011970
C	3.57673267	-0.96994546	-0.00004219
C	3.65995117	0.43137692	0.00001710
C	2.50139951	1.18711915	0.00005960
H	-4.48263028	-1.56530344	-0.00007376
H	-2.25827774	-2.68516452	-0.00012241
H	-2.52609917	2.27017410	0.00010977
H	-4.62870640	0.91626080	0.00003317
H	4.48262990	-1.56530465	-0.00007355
H	4.62870672	0.91625939	0.00003847
H	2.52609988	2.27017344	0.00011211
O	-0.00000028	-1.51903129	-0.00009076
O	0.00000042	2.59241564	0.00004588

Xanthone (10)

State: T_1

Absolute Gibbs free energy at 298 K: -650.607419 a.u.

C	3.58877156	-0.98067496	0.00823228
C	2.34535856	-1.61075165	0.01329989
C	1.19359170	-0.83613371	0.00788950
C	1.23431034	0.58668251	-0.00965292
C	2.50595889	1.19609206	-0.00564852
C	3.65789667	0.42099060	-0.00888270
C	0.00000007	1.31664281	-0.00000101
C	-1.23431030	0.58668253	0.00965200
C	-1.19359195	-0.83613367	-0.00789088
C	-2.34535849	-1.61075161	-0.01329987
H	-2.24887692	-2.68913943	-0.03177436
C	-3.58877167	-0.98067489	-0.00822994
C	-3.65789675	0.42099048	0.00888526
C	-2.50595873	1.19609199	0.00564946
H	4.49472294	-1.57349012	0.01214114
H	2.24887691	-2.68913948	0.03177354
H	2.55814169	2.27703405	-0.01552125
H	4.62596201	0.90826512	-0.03399496
H	-4.49472307	-1.57349004	-0.01213709
H	-4.62596188	0.90826527	0.03399897
H	-2.55814214	2.27703395	0.01552231
O	0.00000016	-1.50437144	-0.00000219
O	-0.00000004	2.62191465	-0.00000075

Thioxanthone (11)

State: S_0

Absolute Gibbs free energy at 298 K: -973.688265 a.u.

C	-3.79860342	-0.62233001	0.00031507
C	-2.64685264	-1.38986322	0.00012503
C	-1.38476292	-0.77114100	-0.00006549
C	-1.28572421	0.63129898	-0.00007036
C	-2.47463696	1.38570740	0.00013026
C	-3.71526674	0.77636120	0.00032109
C	0.00000018	1.38006504	-0.00028040
C	1.28572436	0.63129856	-0.00007007
C	1.38476274	-0.77114142	-0.00006552
C	2.64685223	-1.38986409	0.00012486
H	2.71501549	-2.47226725	0.00014594
C	3.79860324	-0.62233118	0.00031537
C	3.71526693	0.77636006	0.00032190
C	2.47463735	1.38570662	0.00013100
H	-4.76604039	-1.11157802	0.00047596
H	-2.71501625	-2.47226640	0.00014643
H	-2.37804515	2.46412023	0.00012164
H	-4.61756987	1.37615083	0.00047687
H	4.76604009	-1.11157944	0.00047610
H	4.61757018	1.37614948	0.00047802
H	2.37804586	2.46411947	0.00012267
O	0.00000045	2.60566472	-0.00048679
S	-0.00000028	-1.85993302	-0.00037161

Thioxanthone (11)

State: T_1

Absolute Gibbs free energy at 298 K: -973.593109 a.u.

C	-0.65114208	0.00021963	-3.80824082
C	-1.40865253	0.00011890	-2.64573604
C	-0.77288661	-0.00001526	-1.39715623
C	0.65399420	-0.00003559	-1.26606628
C	1.38747057	0.00006009	-2.47561271

C	0.75253426	0.00017877	-3.70571266
C	1.35542113	-0.00011131	0.00000000
C	0.65399420	-0.00003559	1.26606628
C	-0.77288661	-0.00001526	1.39715623
C	-1.40865253	0.00011890	2.64573604
H	-2.49225520	0.00013775	2.69819063
C	-0.65114208	0.00021963	3.80824082
C	0.75253426	0.00017877	3.70571266
C	1.38747057	0.00006009	2.47561271
H	-1.13558871	0.00032389	-4.77620286
H	-2.49225520	0.00013775	-2.69819063
H	2.46647905	0.00003885	-2.39930381
H	1.35161413	0.00024549	-4.60985156
H	-1.13558871	0.00032389	4.77620286
H	1.35161413	0.00024549	4.60985156
H	2.46647905	0.00003885	2.39930381
O	2.64421725	-0.00019048	-0.00000000
S	-1.82516107	-0.00035118	-0.00000000

1,1-Dinapthylmethanone (12)

State: S_0

Absolute Gibbs free energy at 298 K: -883.923318 a.u.

C	0.01203240	-1.44036956	-0.16413919
O	-0.33647425	-2.45069558	-0.75257594
C	1.48088339	-1.13606605	-0.01813390
C	2.05377897	0.14583537	-0.30025737
C	2.28767720	-2.18097657	0.38723688
C	1.31045304	1.24483537	-0.81256180
C	3.46384336	0.31793441	-0.10433891
C	3.67114364	-2.00071055	0.58855270
H	1.83429336	-3.14939830	0.56259293
C	1.91855021	2.44666774	-1.08607260
H	0.24987686	1.13525986	-0.99500629
C	4.05720937	1.57647775	-0.38924667
C	4.24394825	-0.77414100	0.35534184
H	4.27607676	-2.83311125	0.92910721
C	3.30403810	2.62082894	-0.86543321
H	1.33050779	3.26865016	-1.47835690
H	5.12413269	1.69518673	-0.23143322
H	5.30780989	-0.62611418	0.50921484
H	3.76866391	3.57589078	-1.08251319
C	-0.97617423	-0.52821757	0.49679423
C	-2.28745957	-0.29899932	-0.04254648
C	-0.60905094	0.06543336	1.69133746
C	-2.73576521	-0.83014434	-1.28251796
C	-3.18087936	0.55155457	0.68949657
C	-1.50515285	0.87272196	2.41879828
H	0.38711823	-0.10281492	2.08239878
C	-3.99149831	-0.53787116	-1.76251887
H	-2.08459588	-1.48386611	-1.84316222
C	-4.47228464	0.82408817	0.16650907
C	-2.76312691	1.11255374	1.92400878
H	-1.19266952	1.30518562	3.36204866
C	-4.87268804	0.29180339	-1.03395723
H	-4.31065215	-0.95428322	-2.71137918
H	-5.13746180	1.46715510	0.73333132
H	-3.45773646	1.74152794	2.47125671
H	-5.86043679	0.50686462	-1.42560167

1,1-Dinapthylmethanone (12)

State: T_1

Absolute Gibbs free energy at 298 K: -883.840439 a.u.

C	0.03333796	-0.52393723	-0.45789305
O	0.09787380	-1.70139581	-0.84443240
C	-1.27645740	0.20938278	-0.59935916
C	-2.47898750	-0.31450468	-0.02990122
C	-1.31720038	1.36650413	-1.35032185
C	-2.50799126	-1.49002915	0.76875090
C	-3.70589381	0.39322909	-0.24824352
C	-2.53205128	2.04718560	-1.58200651
H	-0.39815133	1.75628202	-1.77503299
C	-3.68478741	-1.93799048	1.32021295
H	-1.59208983	-2.04395229	0.92428370
C	-4.90281895	-0.10138826	0.33391357
C	-3.70038308	1.57173948	-1.03912119
H	-2.53493683	2.94509255	-2.18946147
C	-4.89514658	-1.24015733	1.10168934
H	-3.68745417	-2.83795392	1.92488298

H	-5.82761293	0.43957421	0.16164733
H	-4.63739620	2.09239089	-1.20741843
H	-5.81557573	-1.60795742	1.54112266
C	1.16774839	0.19200437	0.12000664
C	2.55279377	-0.23289258	-0.04716993
C	0.90494318	1.37401865	0.94559273
C	2.92935170	-1.35484065	-0.79238648
C	3.59965275	0.56228870	0.54975270
C	1.90998101	2.09450327	1.50241853
H	-0.12439028	1.65203636	1.12387929
C	4.29257437	-1.71932026	-0.96519517
H	2.15866698	-1.96225290	-1.24182154
C	4.93781968	0.17657386	0.36665717
C	3.27800296	1.71872480	1.30523804
H	1.68164897	2.95672310	2.11875477
C	5.28546461	-0.96292536	-0.39123968
H	4.53189791	-2.59861432	-1.55094677
H	5.71946291	0.77623144	0.82081763
H	4.07423060	2.30437962	1.74864696
H	6.32899329	-1.22982548	-0.51226377

1,2-Dinapthylmethanone (13)

State: S_0

Absolute Gibbs free energy at 298 K: -883.927653 a.u.

C	3.94151212	-1.99728224	1.30085524
C	2.66462042	-1.48922523	1.28141903
C	2.35465323	-0.33806378	0.51028121
C	3.39168965	0.29127016	-0.24854124
C	4.69788145	-0.25797488	-0.20676206
C	4.96674934	-1.37518123	0.54962841
H	0.26368060	-0.28146901	1.03610094
H	4.16873522	-2.87729049	1.89156939
H	1.87439445	-1.96314037	1.85414853
C	1.04650290	0.20176348	0.46317226
C	3.07377609	1.44644742	-1.01501675
H	5.48530722	0.21808714	-0.78153071
H	5.97023731	-1.78495646	0.57350276
C	1.80169339	1.95358286	-1.03152334
C	0.76322973	1.32269799	-0.29178042
H	3.86074123	1.92517024	-1.58843172
H	1.55617885	2.84020328	-1.60271472
C	-0.60084139	1.93326623	-0.31791194
C	-1.77287622	1.14620467	0.20985571
C	-2.15853983	-0.12767394	-0.31436044
C	-2.49953893	1.72407361	1.23077930
C	-1.51484458	-0.74436032	-1.42238481
C	-3.27764816	-0.79871765	0.27905706
C	-3.59497563	1.05460791	1.81521161
H	-2.20936182	2.70431514	1.59052472
C	-1.93417098	-1.96429217	-1.89623750
H	-0.68445083	-0.24386056	-1.90316760
C	-3.67935990	-2.06137806	-0.23236532
C	-3.96970655	-0.18369174	1.35397998
H	-4.13607872	1.52354448	2.62894388
C	-3.02212463	-2.63592881	-1.29218811
H	-1.42958011	-2.41460528	-2.74351266
H	-4.52494416	-2.56274245	0.22696964
H	-4.81019101	-0.70543525	1.79969561
H	-3.34006968	-3.59894206	-1.67516266
O	-0.76383596	3.07753199	-0.70724284

1,2-Dinapthylmethanone (13)

State: T_1

Absolute Gibbs free energy at 298 K: -883.842119 a.u.

C	4.00653163	1.83861053	-1.29898642
C	2.71564953	1.36775701	-1.32844126
C	2.33770916	0.23633056	-0.55736843
C	3.32497800	-0.41289751	0.25058438
C	4.64763046	0.09833990	0.25820443
C	4.98171898	1.19793347	-0.49765680
H	0.26974633	0.23472166	-1.16824094
H	4.28378265	2.70370666	-1.89064316
H	1.96551627	1.85684170	-1.94120721
C	1.01351437	-0.26365261	-0.55663688
C	2.94229450	-1.55236442	1.00843385
H	5.39563104	-0.39428500	0.87071035
H	5.99685323	1.57837077	-0.48384726
C	1.65461281	-2.02268457	0.97593492

C	0.66200174	-1.36333872	0.20144396
H	3.69126707	-2.05319575	1.61324394
H	1.36579548	-2.90497303	1.53361776
C	-0.70947672	-1.95628363	0.15285462
C	-1.90064553	-1.14379593	-0.08842976
C	-2.08606684	0.22959231	0.35003827
C	-3.01268715	-1.80514770	-0.77976728
C	-1.28961423	0.84183746	1.31913569
C	-3.17423736	0.98534929	-0.21372861
C	-4.04121988	-1.07598685	-1.28379739
H	-2.94074561	-2.87439238	-0.92368426
C	-1.45765596	2.20225924	1.66946647
H	-0.51485637	0.27100738	1.81219984
C	-3.30807546	2.33703224	0.12996351
C	-4.11219694	0.33622280	-1.06980311
H	-4.82384462	-1.56271161	-1.85478527
C	-2.44472273	2.94838175	1.06223437
H	-0.80406392	2.64537771	2.41097137
H	-4.09961657	2.91908109	-0.32997476
H	-4.93339782	0.90931506	-1.48368578
H	-2.57432890	3.99616822	1.30724215
O	-0.84724905	-3.18325003	0.28825148

2,2-Dinapthylmethanone (14)

State: S_0

Absolute Gibbs free energy at 298 K: -883.930353 a.u.

C	4.63869074	-2.36378423	-0.65484329
C	3.33388130	-1.93190545	-0.67320005
C	3.00351867	-0.60641519	-0.28647659
C	4.05019486	0.28073913	0.11780042
C	5.38538040	-0.19616039	0.12656387
C	5.67334141	-1.48737044	-0.25029015
H	0.87988474	-0.81318681	-0.59881154
H	4.88072561	-3.37816040	-0.95067689
H	2.53741149	-2.60072276	-0.98246871
C	1.66608143	-0.13716606	-0.28266976
C	3.71279613	1.61139340	0.48846276
H	6.17963417	0.47589254	0.43407317
H	6.69870271	-1.83944686	-0.24041822
C	2.41337385	2.04332695	0.46052590
C	1.36420461	1.15873935	0.08587690
H	4.50678260	2.28684904	0.78948186
H	2.15505243	3.06272148	0.71891629
C	-0.02769481	1.70665383	0.01743792
C	-2.36637890	1.07774023	-0.47695995
C	-3.51950846	0.27188376	-0.33280042
C	-1.19905696	0.78844749	0.20153292
C	-4.72132889	0.54194478	-1.04119971
C	-3.47670120	-0.84670405	0.55997828
C	-1.16328246	-0.32200907	1.08891915
C	-5.82763986	-0.25507498	-0.87484305
H	-4.75020657	1.39130221	-1.71537946
C	-4.63737746	-1.64914563	0.70906412
C	-2.27461290	-1.10765292	1.26807261
H	-0.25825452	-0.53063223	1.64579697
C	-5.78449117	-1.36115641	0.00850673
H	-6.74023439	-0.04017274	-1.41896150
H	-4.60570517	-2.49588668	1.38669872
H	-2.24573969	-1.94155009	1.96159217
H	-6.66508445	-1.98171099	0.13072276
O	-0.20516399	2.89561622	-0.19822626
H	-2.39199873	1.94182977	-1.13150708

2,2-Dinapthylmethanone (14)

State: T_1

Absolute Gibbs free energy at 298 K: -883.845188 a.u.

C	4.94232491	-2.15729321	-0.70190775
C	3.62188091	-1.79757319	-0.83340094
C	3.15740569	-0.54738480	-0.34625897
C	4.08867580	0.34141182	0.27735263
C	5.44317762	-0.05973984	0.39795410
C	5.86155573	-1.28043909	-0.07898426
H	1.10640806	-0.82219035	-0.95501946
H	5.28510139	-3.11523338	-1.07638924
H	2.91521145	-2.46798801	-1.31183470
C	1.79998384	-0.15311252	-0.45784770
C	3.62089579	1.60106509	0.74189332
H	6.14834509	0.61490845	0.87225923

H	6.90042148	-1.57485267	0.01849698
C	2.30628150	1.96087581	0.60403695
C	1.36565211	1.06899309	0.01719595
H	4.32751861	2.28201276	1.20511892
H	1.95367652	2.93009309	0.93453521
C	-0.04204525	1.54550863	-0.14311657
C	-2.49283755	1.08548437	-0.45173140
C	-3.64689669	0.31684843	-0.25705412
C	-1.17493588	0.63100506	0.01601728
C	-4.92303924	0.72346471	-0.71438488
C	-3.54731332	-0.94395384	0.43799264
C	-1.10996030	-0.57334167	0.70341665
C	-6.06759825	-0.08122957	-0.50637828
H	-5.01675343	1.67068234	-1.23342409
C	-4.68494667	-1.71222707	0.63193477
C	-2.25449772	-1.34983950	0.91626018
H	-0.16548986	-0.91228071	1.10941329
C	-5.96359910	-1.28225169	0.15446172
H	-7.02902451	0.25974310	-0.87310909
H	-4.60406643	-2.65834061	1.15699207
H	-2.17331208	-2.28282862	1.46345175
H	-6.83449599	-1.90437834	0.31928092
O	-0.25897747	2.73983719	-0.39049079
H	-2.54270412	2.04432935	-0.95055339

3,6-di(methoxy)xanthenone (15)

State: S_0

Absolute Gibbs free energy at 298 K: -879.780442 a.u.

C	-3.57906685	0.62137751	-0.00004296
C	-2.33601092	1.25226450	0.00001199
C	-1.18255290	0.47937105	-0.00000129
C	-1.23546500	-0.92466631	-0.00006894
C	-2.49790647	-1.53109805	-0.00012309
C	-3.66329913	-0.78464296	-0.00011122
C	-0.00000006	-1.72606890	-0.00008214
C	1.23546501	-0.92466636	-0.00001908
C	1.18255291	0.47937113	0.00004658
C	2.33601094	1.25226442	0.00010672
H	2.27276522	2.33207680	0.00015668
C	3.57906692	0.62137728	0.00010200
C	3.66329916	-0.78464306	0.00003694
C	2.49790634	-1.53109814	-0.00002224
H	-2.27276492	2.33207692	0.00006441
H	-2.53144779	-2.61404636	-0.00017502
H	-4.62063558	-1.28609997	-0.00015432
H	4.62063542	-1.28610035	0.00003259
H	2.53144781	-2.61404644	-0.00007298
O	-0.00000000	1.16655915	0.00005533
O	-0.00000009	-2.95267902	-0.00014014
O	4.65397255	1.45068819	0.00016319
O	-4.65397257	1.45068813	-0.00002543
C	-5.96270907	0.88635061	-0.00007785
H	-6.13500733	0.27943392	0.89502516
H	-6.64737119	1.73256119	-0.00005131
H	-6.13497214	0.27951851	-0.89524503
C	5.96270923	0.88635064	0.00016230
H	6.13500755	0.27951899	-0.89499833
H	6.64737119	1.73256127	0.00021628
H	6.13497199	0.27943361	0.89527188

3,6-Di(methoxy)xanthenone (15)

State: T_1

Absolute Gibbs free energy at 298 K: -879.671904 a.u.

C	-3.61667689	0.58097560	-0.00000184
C	-2.31505318	1.26083485	-0.00000191
C	-1.17133240	0.52162478	-0.00000088
C	-1.21584909	-0.91227876	0.00000018
C	-2.54102001	-1.56766035	0.00000011
C	-3.69662569	-0.81939323	-0.00000086
C	-0.01297770	-1.68333461	0.00000118
C	1.23772399	-0.91447879	0.00000109
C	1.20755397	0.49012886	0.00000004
C	2.36126764	1.25156140	-0.00000009
H	2.30884755	2.33205324	-0.00000090
C	3.60372418	0.60669956	0.00000085
C	3.67020907	-0.79336877	0.00000189
C	2.49167668	-1.53240061	0.00000200
H	-2.28631493	2.34178910	-0.00000273

H	-2.54668703	-2.64750548	0.00000088
H	-4.65686900	-1.31791684	-0.00000089
H	4.62074227	-1.30797106	0.00000260
H	2.51722371	-2.61530622	0.00000279
O	0.01775354	1.19077308	-0.00000091
O	-0.05030220	-2.94133819	0.00000204
O	4.68625356	1.43316012	0.00000065
O	-4.65244372	1.44053436	-0.00000281
C	5.98667382	0.85501287	0.00000186
H	6.68266456	1.69225354	0.00000182
H	6.15245394	0.24473118	0.89461327
H	6.15245510	0.24473011	-0.89460860
C	-5.98607019	0.92422036	-0.00000243
H	-6.63911074	1.79403429	-0.00000280
H	-6.16742013	0.32260667	-0.89548214
H	-6.16741997	0.32260755	0.89547791

Isoprene (1)

Conformation: trans

State: S_0

Absolute Gibbs free energy at 298 K: -195.290812 a.u.

C	-1.59034652	-0.90587074	-0.00030044
H	-1.48727338	-1.98589912	-0.00031052
H	-2.59969741	-0.51022658	-0.00046571
C	-0.51643010	-0.10034429	-0.00009284
C	0.83135874	-0.68061538	0.00012732
H	0.87158300	-1.76783442	0.00010585
C	1.98176641	0.00335537	0.00034651
H	2.01374106	1.08701766	0.00038073
H	2.93655893	-0.50902684	0.00050010
C	-0.65428812	1.40141446	-0.00007872
H	-0.17228882	1.83809057	0.88053682
H	-0.17199193	1.83813403	-0.88051013
H	-1.70299388	1.70210819	-0.00024807

Isoprene (1)

Conformation: trans

State: T_1

Absolute Gibbs free energy at 298 K: -195.211765

C	1.65698036	-0.90878054	0.00007520
H	2.15489944	-1.17868784	0.92761581
H	2.15497158	-1.17869937	-0.92742338
C	0.44623355	-0.07644750	0.00002297
C	-0.82022189	-0.67174809	-0.00002456
H	-0.82795822	-1.75984416	-0.00001169
C	-2.04917632	-0.04234331	-0.00008717
H	-2.15506909	1.03529386	-0.00010785
H	-2.96264767	-0.62330653	-0.00011899
C	0.66657859	1.41427192	0.00001504
H	1.24908193	1.71682402	-0.87852038
H	-0.26475240	1.98187631	0.00002746
H	1.24910868	1.71682886	0.87853024

Isoprene (1)

Conformation: cis

State: S_0

Absolute Gibbs free energy at 298 K: -195.286693 a.u.

C	0.59774886	1.44273670	-0.09083440
H	-0.24145911	2.09817807	-0.29323643
H	1.56219834	1.91094310	0.07257389
C	0.45515311	0.11183012	-0.06216859
C	-0.85346224	-0.54503539	-0.25897618
C	1.62473193	-0.81963930	0.14856622
H	1.47322052	-1.44001677	1.03839720
H	1.73025726	-1.50383506	-0.70101106
H	2.56184067	-0.27219472	0.26430997
C	-2.02622484	-0.10150292	0.20036937
H	-2.09767434	0.80405707	0.79371749
H	-2.94767832	-0.63786943	0.00483461
H	-0.82838598	-1.48959751	-0.80132420

Isoprene (1)

Conformation: cis

State: T_1

Absolute Gibbs free energy at 298 K: -195.209739 a.u.

C	0.45009074	1.47894089	0.00007952
H	-0.44864539	2.07797691	0.00009437

H	1.40044798	1.99757900	0.00012112
C	0.41410297	0.01750579	0.00000489
C	-0.75903173	-0.68344347	-0.00004221
C	1.74466675	-0.68149595	-0.00001684
H	1.63650491	-1.76761588	-0.00006660
H	2.33495854	-0.39384918	-0.87901694
H	2.33494534	-0.39392820	0.87901797
C	-2.07761273	-0.12028581	-0.00002711
H	-2.25157648	0.94650270	0.00002345
H	-2.94599649	-0.76555814	-0.00006676
H	-0.69393446	-1.76843591	-0.00009607

M062X/6-311+G(d,p)

Benzophenone (9)

State: S_0

Absolute Gibbs free energy at 298 K: -576.380317 a.u.

O	-0.00000522	2.32099828	-0.00001520
C	-0.00000504	1.10984018	0.00006194
C	1.29513376	0.35455142	0.03005604
C	2.42025114	0.96011837	-0.53347341
C	1.41983110	-0.88527156	0.65948257
C	3.65078509	0.31994750	-0.49368182
H	2.30889244	1.93376807	-0.99568529
C	2.65871617	-1.51480620	0.71814096
H	0.55565031	-1.34638954	1.12331714
C	3.77091282	-0.91832793	0.13340615
H	4.51858717	0.78643152	-0.94423570
H	2.75528351	-2.46949502	1.22098849
H	4.73341714	-1.41483116	0.17129156
C	-1.29513920	0.35454659	-0.02999912
C	-1.41979501	-0.88528431	-0.65941819
C	-2.42029077	0.96011392	0.53346135
C	-2.65867287	-1.51482726	-0.71813640
H	-0.55558548	-1.34640310	-1.12319878
C	-3.65081890	0.31993516	0.49361012
H	-2.30896287	1.93376943	0.99566838
C	-3.77090511	-0.91834839	-0.13346959
H	-2.75520700	-2.46952291	-1.22097739
H	-4.51864820	0.78641973	0.94411097
H	-4.73340428	-1.41485805	-0.17140140

Benzophenone (9)

State: T_1

Absolute Gibbs free energy at 298 K: -576.273500 a.u.

O	0.00000671	2.25929095	-0.00004209
C	-0.00000222	0.93166852	0.00005548
C	1.30325884	0.31029507	0.01830599
C	2.42991003	1.02747206	-0.43614672
C	1.49336226	-0.98484218	0.54221490
C	3.69002884	0.45207983	-0.39610271
H	2.29826087	2.02423171	-0.83960056
C	2.75692995	-1.54978759	0.56409326
H	0.65059906	-1.52512588	0.95500729
C	3.86273868	-0.84007648	0.09406992
H	4.54358135	1.01296861	-0.75810607
H	2.88650943	-2.54702617	0.96791126
H	4.84840140	-1.28796728	0.11840502
C	-1.30326276	0.31029426	-0.01824477
C	-1.49334245	-0.98483699	-0.54217741
C	-2.42993539	1.02746254	0.43617095
C	-2.75690727	-1.54978638	-0.56411352
H	-0.65056096	-1.52511313	-0.95494301
C	-3.69005048	0.45206577	0.39607037
H	-2.29830749	2.02421729	0.83964318
C	-3.86273703	-0.84008504	-0.09412504
H	-2.88646701	-2.54702098	-0.96794769
H	-4.54361920	1.01294695	0.75804729
H	-4.84839718	-1.28797914	-0.11850415

Xanthone (10)

State: S_0

Absolute Gibbs free energy at 298 K: -650.432303 a.u.

C	-3.56666233	-0.96669140	-0.00001650
C	-2.33958166	-1.60205903	-0.00007001
C	-1.17650127	-0.83027880	-0.00005366
C	-1.23986269	0.56345481	0.00001325

C	-2.49533268	1.18524703	0.00006643
C	-3.65165188	0.43219000	0.00005202
C	0.00000022	1.36683806	0.00003394
C	1.23986287	0.56345443	0.00001428
C	1.17650100	-0.83027916	-0.00005265
C	2.33958118	-1.60205975	-0.00006804
H	2.25092360	-2.68098953	-0.00012129
C	3.56666203	-0.96669249	-0.00001352
C	3.65165201	0.43218889	0.00005509
C	2.49533305	1.18524627	0.00006852
H	-4.47196222	-1.56201018	-0.00002711
H	-2.25092442	-2.68098885	-0.00012323
H	-2.51686993	2.26867593	0.00011806
H	-4.62007831	0.91596064	0.00009410
H	4.47196174	-1.56201154	-0.00002337
H	4.62007859	0.91595923	0.00009799
H	2.51687061	2.26867517	0.00012017
O	-0.00000023	-1.51382021	-0.00011292
O	0.00000039	2.58049220	0.00007415

Xanthone (10)

State: T_1

Absolute Gibbs free energy at 298 K: -650.311336 a.u.

C	-3.57402593	-0.98256517	-0.00005124
C	-2.33994350	-1.61446088	-0.00007359
C	-1.19004762	-0.83802591	-0.00003447
C	-1.22551023	0.58674318	0.00002811
C	-2.49872793	1.19676727	0.00005011
C	-3.64070920	0.42322345	0.00001101
C	-0.00000000	1.30679577	0.00006256
C	1.22551023	0.58674318	0.00002918
C	1.19004762	-0.83802591	-0.00003343
C	2.33994350	-1.61446088	-0.00007152
H	2.24251076	-2.69268569	-0.00011863
C	3.57402593	-0.98256517	-0.00004809
C	3.64070920	0.42322345	0.00001420
C	2.49872793	1.19676727	0.00005229
H	-4.48249190	-1.57031716	-0.00008172
H	-2.24251076	-2.69268569	-0.00012062
H	-2.54216463	2.27777761	0.00009790
H	-4.61048535	0.90666025	0.00002845
H	4.48249190	-1.57031716	-0.00007774
H	4.61048535	0.90666025	0.00003249
H	2.54216463	2.27777761	0.00010010
O	0.00000000	-1.49308043	-0.00005488
O	-0.00000000	2.62510194	0.00012101

Thioxanthone (11)

State: S_0

Absolute Gibbs free energy at 298 K: -973.401167 a.u.

C	-3.78536523	-0.62222406	0.00025354
C	-2.63543592	-1.38697142	0.00009933
C	-1.37687261	-0.76757967	-0.00005353
C	-1.28454592	0.62799623	-0.00006269
C	-2.46752448	1.38336690	0.00010046
C	-3.70539963	0.77418993	0.00025994
C	0.00000019	1.37876977	-0.00024043
C	1.28454609	0.62799584	-0.00006243
C	1.37687240	-0.76758008	-0.00005337
C	2.63543551	-1.38697223	0.00009956
H	2.69751317	-2.46936371	0.00011108
C	3.78536506	-0.62222521	0.00025394
C	3.70539986	0.77418881	0.00026048
C	2.46752489	1.38336614	0.00010093
H	-4.75152158	-1.11272761	0.00038106
H	-2.69751390	-2.46936289	0.00011089
H	-2.36808284	2.46178777	0.00008828
H	-4.60814640	1.37195903	0.00038815
H	4.75152125	-1.11272905	0.00038147
H	4.60814683	1.37195762	0.00038888
H	2.36808360	2.46178704	0.00008885
O	0.00000037	2.59397693	-0.00039121
S	-0.00000027	-1.85206558	-0.00028396

Thioxanthone (11)

State: T_1

Absolute Gibbs free energy at 298 K: -973.294278 a.u.

C	-0.65749022	-0.01808240	3.79278182
C	-1.40862169	-0.01063455	2.63237481
C	-0.76795467	0.00045701	1.38770071
C	0.65316639	0.00420448	1.26096432
C	1.38358410	-0.00300461	2.46862454
C	0.74468604	-0.01349027	3.69260788
C	1.35542583	0.01187077	-0.00000000
C	0.65316639	0.00420448	-1.26096432
C	-0.76795467	0.00045701	-1.38770071
C	-1.40862169	-0.01063455	-2.63237481
H	-2.49241123	-0.01300731	-2.67542991
C	-0.65749022	-0.01808240	-3.79278182
C	0.74468604	-0.01349027	-3.69260788
C	1.38358410	-0.00300461	-2.46862454
H	-1.14313703	-0.02679384	4.75923120
H	-2.49241123	-0.01300731	2.67542991
H	2.46271941	0.00018120	2.39302581
H	1.34039239	-0.01846387	4.59841107
H	-1.14313703	-0.02679384	-4.75923120
H	1.34039239	-0.01846387	-4.59841107
H	2.46271941	0.00018120	-2.39302581
O	2.63643783	0.01705115	-0.00000000
S	-1.80797652	0.02469612	0.00000000

1,1-Dinapthylmethanone (12)

State: S_0

Absolute Gibbs free energy at 298 K: -883.521107 a.u.

C	0.01112331	-1.44144552	-0.15799107
O	-0.34411223	-2.45199161	-0.72285838
C	1.47991161	-1.13992374	-0.01880995
C	2.04688254	0.14105021	-0.30462859
C	2.28094431	-2.17773311	0.39306848
C	1.29728704	1.23097149	-0.82754844
C	3.44535045	0.31777621	-0.10539267
C	3.66530811	-1.99234333	0.59627987
H	1.82739472	-3.14562007	0.57276135
C	1.90080775	2.42891766	-1.10431074
H	0.23837361	1.11231065	-1.02022775
C	4.03728534	1.57557266	-0.39283420
C	4.23010218	-0.76846802	0.36110385
H	4.27218819	-2.82073725	0.94072787
C	3.28464328	2.61028596	-0.87637197
H	1.31312317	3.24543204	-1.50650167
H	5.10281670	1.69593957	-0.22935277
H	5.29223817	-0.61145567	0.51607358
H	3.74537329	3.56574167	-1.09650063
C	-0.96895746	-0.51721695	0.50078390
C	-2.27877537	-0.29570674	-0.03695541
C	-0.59337636	0.08618601	1.67937835
C	-2.72457601	-0.84023957	-1.27235312
C	-3.16492470	0.55429542	0.68471260
C	-1.48843700	0.90321312	2.40136421
H	0.40587633	-0.07860678	2.06650200
C	-3.97825343	-0.55650650	-1.74837160
H	-2.07021581	-1.49398532	-1.83040502
C	-4.45923650	0.81844144	0.16685017
C	-2.74448836	1.13167812	1.91095863
H	-1.17214645	1.34849090	3.33650000
C	-4.86034093	0.27565368	-1.02300802
H	-4.29942316	-0.98007654	-2.69258713
H	-5.12178376	1.46442458	0.73277554
H	-3.44099229	1.76454785	2.45073174
H	-5.84960373	0.48277624	-1.41317583

1,1-Dinapthylmethanone (12)

State: T_1

Absolute Gibbs free energy at 298 K: -883.427774 a.u.

C	0.02777821	-0.52259196	-0.37184784
O	0.07990882	-1.71422826	-0.67723689
C	-1.27186515	0.21973794	-0.54115270
C	-2.49212831	-0.30801940	-0.01740124
C	-1.28271111	1.38160721	-1.27507150
C	-2.54795479	-1.49131460	0.76846418
C	-3.70077810	0.40131381	-0.26667242
C	-2.48792785	2.06874303	-1.53890038
H	-0.34841886	1.77221124	-1.66606638
C	-3.74024252	-1.93760356	1.27348747
H	-1.63780266	-2.04680782	0.95063114

C	-4.91964712	-0.09280041	0.26723047
C	-3.66919023	1.58878498	-1.04248918
H	-2.46920054	2.97318531	-2.13480981
C	-4.94135839	-1.23487930	1.02000585
H	-3.76631947	-2.84153888	1.87035679
H	-5.83376318	0.45598174	0.06742971
H	-4.60132555	2.10966948	-1.23373256
H	-5.87624463	-1.60469702	1.42400256
C	1.17994491	0.21508387	0.13490194
C	2.55482257	-0.23959576	-0.05387795
C	0.95088636	1.43443021	0.92587852
C	2.88992336	-1.36131117	-0.80470790
C	3.62153659	0.53335770	0.52217315
C	1.97251391	2.13181887	1.46077206
H	-0.07066441	1.74116290	1.10379090
C	4.23842369	-1.75480235	-0.98839905
H	2.10446281	-1.95009622	-1.25327668
C	4.94070698	0.12273658	0.33254435
C	3.33470341	1.71200363	1.26693147
H	1.77238967	3.01231629	2.05958966
C	5.25234058	-1.02393285	-0.42332440
H	4.45376886	-2.63802405	-1.57646088
H	5.73803756	0.70783861	0.77765558
H	4.15011526	2.28327136	1.69097043
H	6.28703271	-1.31724573	-0.55345482

1,2-Dinapthylmethanone (13)

State: S_0

Absolute Gibbs free energy at 298 K: -883.525364 a.u.

C	3.92250224	-2.01146835	1.27979816
C	2.64813514	-1.51118518	1.25124224
C	2.34525352	-0.34982191	0.49415705
C	3.38154930	0.29170501	-0.23639928
C	4.69067514	-0.24986864	-0.18760675
C	4.95461557	-1.37279520	0.55200857
H	0.24624514	-0.30826693	1.00245801
H	4.14667441	-2.89870195	1.85953171
H	1.85094499	-1.99521475	1.80496702
C	1.03404086	0.18603617	0.44328410
C	3.07344225	1.45759502	-0.98993294
H	5.48035406	0.24165681	-0.74539196
H	5.95906643	-1.77793624	0.58318237
C	1.80409966	1.95968509	-1.01423366
C	0.76342211	1.31318327	-0.29439363
H	3.86870010	1.94509796	-1.54346178
H	1.55957552	2.85454308	-1.57325631
C	-0.60060960	1.92877007	-0.32430302
C	-1.77006540	1.14668791	0.21175577
C	-2.15712220	-0.12400734	-0.31267276
C	-2.48182874	1.72118550	1.23612327
C	-1.51708248	-0.73215719	-1.42739284
C	-3.26382027	-0.79205696	0.28229858
C	-3.57482013	1.04959358	1.82644908
H	-2.18681865	2.70030938	1.59562535
C	-1.93918096	-1.94557358	-1.90159971
H	-0.69166358	-0.22490396	-1.91195324
C	-3.67124706	-2.05200250	-0.22951782
C	-3.94990237	-0.18238600	1.36430185
H	-4.11047505	1.51556554	2.64447640
C	-3.02356141	-2.61956705	-1.29247973
H	-1.44231789	-2.39230199	-2.75443918
H	-4.51365379	-2.55254064	0.23566603
H	-4.78685905	-0.70870374	1.81058693
H	-3.34377527	-3.58001834	-1.67803649
O	-0.75587105	3.06401317	-0.71440925

1,2-Dinapthylmethanone (13)

State: T_1

Absolute Gibbs free energy at 298 K: -883.429456 a.u.

C	3.96733539	1.83872829	-1.25552026
C	2.67997473	1.37427705	-1.29286416
C	2.30417322	0.22361661	-0.55089149
C	3.28464286	-0.44510941	0.23153637
C	4.60988332	0.05996407	0.24958664
C	4.94350722	1.17352530	-0.47500054
H	0.23285856	0.24566881	-1.15924368
H	4.24548229	2.71810264	-1.82395429
H	1.92694992	1.87925102	-1.88837057

C	0.97705709	-0.27171557	-0.56175939
C	2.90645344	-1.60336104	0.96151887
H	5.35575102	-0.45351200	0.84673217
H	5.95911654	1.55053350	-0.45522680
C	1.62168185	-2.06852808	0.92059308
C	0.63256084	-1.38441651	0.16640359
H	3.65940461	-2.11942091	1.54754716
H	1.33005593	-2.96548686	1.45345477
C	-0.74307022	-1.97558934	0.11405107
C	-1.92939478	-1.14444582	-0.04356536
C	-2.05698996	0.24866499	0.37781310
C	-3.10262486	-1.78868777	-0.65817369
C	-1.24464111	0.83249584	1.33987516
C	-3.09317748	1.03371582	-0.21724498
C	-4.08005908	-1.03062070	-1.19618591
H	-3.09921218	-2.86824448	-0.72232706
C	-1.36260342	2.19801563	1.66352975
H	-0.49688498	0.23530086	1.84613379
C	-3.17963094	2.38919629	0.09634435
C	-4.05211265	0.40111518	-1.07452229
H	-4.90763074	-1.49652176	-1.71780544
C	-2.30783014	2.97424174	1.02741657
H	-0.70277069	2.62926791	2.40568898
H	-3.94310212	2.99205352	-0.38322730
H	-4.83033275	1.00292949	-1.52603096
H	-2.39411715	4.02995153	1.25452579
O	-0.87329750	-3.19879608	0.17305758

2,2-Dinapthylmethanone (14)

State: S_0

Absolute Gibbs free energy at 298 K: -883.528038 a.u.

C	4.60555311	-2.37214938	-0.64064336
C	3.30652239	-1.93880676	-0.64720696
C	2.98731108	-0.60753346	-0.27391271
C	4.03387867	0.27646569	0.10220878
C	5.36866083	-0.20130866	0.10039328
C	5.64767181	-1.49299791	-0.26149733
H	0.85674967	-0.81360072	-0.55978721
H	4.84160180	-3.39018652	-0.92600846
H	2.50241180	-2.60679253	-0.93670911
C	1.64990053	-0.13580172	-0.26153534
C	3.71008848	1.61392320	0.45945490
H	6.16575634	0.47531762	0.38871248
H	6.67143018	-1.84778622	-0.26073499
C	2.41607459	2.04874713	0.44288188
C	1.36377030	1.16051163	0.09230296
H	4.51308549	2.28733683	0.73898310
H	2.16079759	3.07174068	0.69079611
C	-0.02675340	1.71360578	0.03244489
C	-2.35399161	1.08325020	-0.46826265
C	-3.50514557	0.27208950	-0.32985426
C	-1.19641279	0.79226453	0.21188270
C	-4.70357283	0.54401765	-1.04148538
C	-3.46134077	-0.84222889	0.55192580
C	-1.15617215	-0.31995638	1.09502933
C	-5.80391420	-0.25416044	-0.88306219
H	-4.72952003	1.39678931	-1.71097692
C	-4.61860358	-1.65024625	0.69580984
C	-2.26288433	-1.10620410	1.26520995
H	-0.25085210	-0.52580629	1.65366419
C	-5.76009240	-1.36409411	-0.00434820
H	-6.71504640	-0.04009828	-1.42858151
H	-4.58312755	-2.49861351	1.37065369
H	-2.23899606	-1.94367683	1.95401037
H	-6.63887700	-1.98709872	0.11229652
O	-0.20235302	2.89445833	-0.17413359
H	-2.37987871	1.95048500	-1.11966519

2,2-Dinapthylmethanone (14)

State: T_1

Absolute Gibbs free energy at 298 K: -883.431168 a.u.

C	4.94028908	-2.14400091	-0.69816829
C	3.62501161	-1.78809479	-0.83660933
C	3.15661540	-0.54209865	-0.34457987
C	4.07392911	0.33920622	0.28763955
C	5.42915886	-0.05686143	0.41683818
C	5.85262788	-1.26840794	-0.06287401
H	1.10911399	-0.81998804	-0.97292278

H	5.28870601	-3.09779300	-1.07588461
H	2.92153264	-2.45458348	-1.32428317
C	1.79797325	-0.15188454	-0.46613628
C	3.60473626	1.59583154	0.75756537
H	6.12613361	0.61894744	0.90063419
H	6.89082876	-1.56083277	0.03978189
C	2.29498140	1.95346174	0.61160590
C	1.36517196	1.06153255	0.01145244
H	4.30988459	2.27249030	1.22828277
H	1.93524137	2.91995083	0.94320007
C	-0.04170753	1.54346937	-0.16081833
C	-2.49928667	1.10038039	-0.43828920
C	-3.65509540	0.32277693	-0.24456144
C	-1.17225823	0.62775178	0.00644664
C	-4.92498416	0.73471196	-0.67413603
C	-3.54386282	-0.94708678	0.42079558
C	-1.09539457	-0.57915503	0.66627860
C	-6.06343479	-0.07594260	-0.46783479
H	-5.02651349	1.69194746	-1.17240854
C	-4.66807869	-1.72112921	0.61502461
C	-2.24086733	-1.36230966	0.87859953
H	-0.14613902	-0.92405315	1.05714414
C	-5.94837234	-1.28728004	0.16482537
H	-7.02992004	0.27010368	-0.81410802
H	-4.57397136	-2.67600816	1.12135001
H	-2.15586711	-2.30306881	1.40993568
H	-6.81587636	-1.91360934	0.32782023
O	-0.25029732	2.72215108	-0.42656613
H	-2.55368866	2.07006311	-0.91439798

3,6-Di(methoxy)xanthenone (15)

State: S_0

Absolute Gibbs free energy at 298 K: -879.402629 a.u.

C	3.56894066	-0.62315605	0.00000128
C	2.32996506	-1.25470979	0.00000020
C	1.17746916	-0.48376814	0.00000034
C	1.23454233	0.91477087	0.00000130
C	2.49131736	1.52304670	0.00000222
C	3.65578706	0.77970958	0.00000213
C	0.00000001	1.71809026	0.00000149
C	-1.23454230	0.91477089	0.00000072
C	-1.17746915	-0.48376811	-0.00000027
C	-2.32996511	-1.25470972	-0.00000111
H	-2.26880246	-2.33470293	-0.00000189
C	-3.56894067	-0.62315597	-0.00000096
C	-3.65578704	0.77970969	0.00000005
C	-2.49131734	1.52304677	0.00000087
H	2.26880239	-2.33470300	-0.00000073
H	2.52126519	2.60642876	0.00000291
H	4.61328677	1.28055670	0.00000278
H	-4.61328676	1.28055681	0.00000021
H	-2.52126509	2.60642883	0.00000165
O	-0.00000002	-1.16747886	-0.00000055
O	0.00000004	2.93444562	0.00000223
O	-4.64203331	-1.44409692	-0.00000180
O	4.64203328	-1.44409709	0.00000131
C	5.93160541	-0.86073349	-0.00000455
H	6.08768539	-0.25088508	0.89423655
H	6.63356665	-1.69083459	-0.00000806
H	6.08767635	-0.25088466	-0.89424697
C	-5.93160546	-0.86073333	-0.00000199
H	-6.08768047	-0.25088405	-0.89424337
H	-6.63356665	-1.69083443	-0.00000297
H	-6.08768137	-0.25088540	0.89424014

3,6-Di(methoxy)xanthenone (15)

State: T_1

Absolute Gibbs free energy at 298 K: -879.281795 a.u.

C	-3.59404072	-0.60607202	0.00000085
C	-2.35624542	-1.25345827	0.00000153
C	-1.20252151	-0.49661229	0.00000072
C	-1.23642377	0.90282128	-0.00000075
C	-2.48144165	1.52356947	-0.00000140
C	-3.66143739	0.78982859	-0.00000062
C	0.01675455	1.67502246	-0.00000163
C	1.21569783	0.90693732	-0.00000097
C	1.17151668	-0.54115295	0.00000055
C	2.30627878	-1.26978770	0.00000112

H	2.28017155	-2.35125082	0.00000225
C	3.60266202	-0.59091141	0.00000021
C	3.68142537	0.81655679	-0.00000123
C	2.53780594	1.56396119	-0.00000184
H	-2.30790805	-2.33422135	0.00000267
H	-2.50158534	2.60695524	-0.00000256
H	-4.61114667	1.30551077	-0.00000118
H	4.64415370	1.31093940	-0.00000188
H	2.54321174	2.64370431	-0.00000295
O	-0.02009065	-1.19677784	0.00000148
O	0.05123035	2.92198426	-0.00000290
O	4.64120794	-1.43273066	0.00000096
O	-4.67492308	-1.42295614	0.00000169
C	-5.95512157	-0.82414738	0.00000163
H	-6.10334296	-0.21079605	-0.89374044
H	-6.66945069	-1.64397793	0.00000279
H	-6.10334216	-0.21079419	0.89374256
C	5.95300560	-0.89003889	0.00000005
H	6.11708849	-0.28505105	0.89500001
H	6.62817756	-1.74121963	0.00000075
H	6.11708802	-0.28505290	-0.89500126

B3LYP/6-311G(d,p)

Isoprene

Conformation: trans

State: S_0

Absolute Gibbs free energy at 298 K: -195.281920 a.u.

C	1.983152	0.008987	0.000214
H	2.013620	1.092622	0.000629
H	2.938829	-0.501604	0.000475
C	0.835036	-0.675531	-0.000343
H	0.875792	-1.762553	-0.000237
C	-0.515169	-0.101263	-0.000492
C	-0.664938	1.399426	-0.000045
H	-0.188214	1.843387	-0.879813
H	-1.716866	1.688144	-0.000214
H	-0.188921	1.842507	0.880689
C	-1.582727	-0.912677	0.000181
H	-2.594839	-0.524437	0.000732
H	-1.471527	-1.991714	0.000647

Conformation: trans – 1allyl

State: T_1

Absolute Gibbs free energy at 298 K: -195.201185 a.u.

C	2.038751	-0.071517	0.000000
H	2.568741	0.141807	0.924983
H	2.568741	0.141807	-0.924982
C	0.737631	-0.731278	-0.000000
H	0.728271	-1.823365	-0.000000
C	-0.507987	-0.088135	0.000000
C	-0.561028	1.426716	-0.000000
H	-0.056080	1.837466	-0.879059
H	-1.591330	1.786141	0.000006
H	-0.056070	1.837467	0.879053
C	-1.681720	-0.817177	0.000000
H	-2.649728	-0.331898	0.000001
H	-1.666432	-1.901079	-0.000000

Conformation: trans – 2allyl

State: T_1

Absolute Gibbs free energy at 298 K: -195.202551 a.u.

C	2.048263	-0.045800	0.000013
H	2.158415	1.031312	0.000049
H	2.959775	-0.629649	0.000006
C	0.818940	-0.670783	-0.000016
H	0.824202	-1.758799	-0.000031
C	-0.447677	-0.075504	-0.000019
C	-0.663231	1.416134	-0.000006
H	0.271445	1.977899	-0.000232
H	-1.244278	1.723283	-0.877950
H	-1.243887	1.723330	0.878183
C	-1.657888	-0.909161	0.000015

H	-2.158048	-1.178324	0.926703
H	-2.158072	-1.178364	-0.926649

Conformation: cis

State: S_0

Absolute Gibbs free energy at 298 K: -195.277910 a.u.

C	-2.027610	-0.100505	-0.200746
H	-2.101222	0.802980	-0.796669
H	-2.948920	-0.636224	-0.002889
C	-0.855979	-0.542605	0.258674
H	-0.832876	-1.485507	0.803944
C	0.454583	0.111079	0.061893
C	1.624983	-0.819994	-0.148496
H	1.476280	-1.442824	-1.037029
H	2.559671	-0.269303	-0.265979
H	1.735101	-1.502874	0.701568
C	0.600852	1.440268	0.091150
H	1.566752	1.905648	-0.071759
H	-0.235753	2.098641	0.293968

Conformation: cis - planar

State: T_1

Absolute Gibbs free energy at 298 K: -195.200426 a.u.

C	-2.076438	-0.123281	0.000000
H	-2.252113	0.942969	-0.000000
H	-2.943235	-0.770389	0.000001
C	-0.756412	-0.682856	0.000000
H	-0.688642	-1.767635	0.000000
C	0.414477	0.018861	-0.000000
C	1.744318	-0.681386	-0.000000
H	1.631584	-1.766830	-0.000000
H	2.336739	-0.397049	-0.878657
H	2.336739	-0.397049	0.878656
C	0.447153	1.481409	0.000000
H	1.394966	2.004142	0.000007
H	-0.454628	2.075361	-0.000007

Conformation: cis – 1allyl

State: T_1

Absolute Gibbs free energy at 298 K: -195.202760 a.u.

C	2.096128	-0.156835	0.007369
H	2.635017	-0.012524	0.939825
H	2.647541	0.021193	-0.911809
C	0.735902	-0.686368	-0.011109
H	0.624955	-1.772615	-0.026114
C	-0.438958	0.078667	-0.008604
C	-1.769081	-0.652050	0.005666
H	-1.757362	-1.510784	-0.670401
H	-1.996884	-1.027598	1.008352
H	-2.586253	0.005350	-0.296646
C	-0.416517	1.459484	-0.001119
H	-1.332676	2.037149	-0.006117
H	0.520815	2.002438	0.009695

Conformation: cis – 2allyl

State: T_1

Absolute Gibbs free energy at 298 K: -195.203732 a.u.

C	2.058531	-0.107679	-0.000000
H	2.195786	0.967365	-0.000000
H	2.946374	-0.726888	-0.000000
C	0.799631	-0.670210	-0.000000
H	0.735275	-1.757029	-0.000000
C	-0.414145	0.022606	0.000000
C	-1.728641	-0.715248	0.000000
H	-1.581215	-1.798025	0.000003
H	-2.331686	-0.450879	0.877725
H	-2.331683	-0.450884	-0.877728
C	-0.474242	1.489317	-0.000000
H	-0.539822	2.051811	0.927143
H	-0.539830	2.051812	-0.927142

Intermediates

Combination: 1t-2t

TS

State: T_1

Imaginary frequency: -331.4838

Absolute Gibbs free energy at 298 K: -390.455934 a.u.

C	4.585494	-0.382081	0.412123
H	5.373354	-1.074394	0.680180
H	4.884936	0.633371	0.185610
C	3.273781	-0.805996	0.356081
H	3.093853	-1.851205	0.602179
C	2.138041	-0.064199	0.006181
C	2.200609	1.396317	-0.344473
H	1.831029	1.576390	-1.360324
H	1.563809	1.985329	0.326978
H	3.211405	1.798584	-0.280919
C	0.815952	-0.737718	0.026791
H	0.677802	-1.614447	-0.598864
H	0.283965	-0.789723	0.975769
C	-0.937206	0.453329	-1.116101
H	-0.735747	1.332577	-0.518582
H	-0.356742	0.350741	-2.023391
C	-2.085930	-0.263469	-0.955347
H	-2.298602	-1.061769	-1.662435
C	-3.048609	-0.103260	0.119331
C	-2.830221	0.988190	1.140435
H	-2.805660	1.973919	0.664825
H	-3.626164	0.991360	1.886313
H	-1.876371	0.859667	1.661747
C	-4.123618	-0.914354	0.192000
H	-4.863379	-0.811752	0.977272
H	-4.287257	-1.699201	-0.538488

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.511997 a.u.

C	4.361891	-0.402575	-0.426184
H	5.101964	-1.147850	-0.688304
H	4.675679	0.633413	-0.463349
C	3.083506	-0.774425	-0.066953
H	2.863901	-1.840934	-0.070513
C	2.030005	0.066514	0.298777
C	2.186943	1.560950	0.356498
H	2.038639	2.024402	-0.628152
H	1.454388	2.007757	1.034564
H	3.182617	1.853885	0.698819
C	0.672292	-0.503834	0.606804
H	0.738518	-1.592594	0.698560
H	0.321044	-0.126198	1.576742
C	-0.404986	-0.158933	-0.459149
H	-0.490894	0.925917	-0.554845
H	-0.039872	-0.525727	-1.430029
C	-1.733250	-0.776792	-0.154392
H	-1.732459	-1.853255	0.005473
C	-2.964960	-0.123186	-0.065152
C	-3.059950	1.376277	-0.281630
H	-2.733780	1.656929	-1.287389
H	-4.086915	1.722128	-0.155659
H	-2.433900	1.924931	0.428165
C	-4.119117	-0.832971	0.218951
H	-5.082175	-0.343732	0.294992
H	-4.091004	-1.905226	0.375498

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.511135 a.u.

C	2.132232	1.601248	-0.081140

C	1.953817	0.123752	-0.294371
C	0.574129	-0.376316	-0.595516
C	3.010715	-0.778371	-0.130955
C	4.309320	-0.484526	0.220106
C	-2.850864	1.396079	0.071086
C	-2.892735	-0.120859	0.045521
C	-4.080648	-0.754617	-0.267423
C	-1.745495	-0.863380	0.348537
C	-0.390768	-0.317680	0.647615
H	2.075483	1.868939	0.982895
H	3.102267	1.950634	-0.444116
H	1.355516	2.171360	-0.598025
H	0.614158	-1.410597	-0.949179
H	0.119727	0.219908	-1.395501
H	2.773756	-1.826943	-0.304773
H	4.640291	0.526780	0.422573
H	5.051814	-1.268021	0.302515
H	-3.817255	1.816539	-0.210734
H	-2.601143	1.771542	1.067999
H	-2.101001	1.790069	-0.621047
H	-4.146572	-1.836327	-0.293130
H	-4.980915	-0.195695	-0.490750
H	-1.832785	-1.946700	0.304880
H	0.076830	-0.899812	1.448942
H	-0.448392	0.716353	0.996697

<u>Combination: 1c-2c</u>

TS

State: T_1

Imaginary frequency: -229.5433

Absolute Gibbs free energy at 298 K: -390.455720 a.u.

C	-1.089905	2.135431	0.486579
H	-1.054912	3.185920	0.229348
H	-0.355841	1.774809	1.192243
C	-2.086638	1.295712	-0.069752
H	-2.793071	1.762607	-0.752096
C	-2.249300	-0.047869	0.169942
C	-3.359332	-0.820985	-0.485905
H	-2.964704	-1.662210	-1.069655
H	-4.030948	-1.256214	0.265215
H	-3.954443	-0.193372	-1.151662
C	-1.368518	-0.798101	1.065831
H	-0.666316	-0.286308	1.706708
H	-1.655964	-1.798013	1.367058
C	0.514736	-1.674157	-0.469456
H	0.168795	-2.680413	-0.272205
H	-0.026472	-1.115945	-1.222707
C	1.705061	-1.252080	0.021492
H	2.235908	-1.923000	0.693979
C	2.357822	0.033264	-0.220492
C	3.723503	0.200676	0.408325
H	4.418843	-0.563287	0.043916
H	4.149646	1.180536	0.187637
H	3.671178	0.089161	1.497053
C	1.803297	1.026081	-0.942467
H	2.325808	1.962992	-1.096734
H	0.828144	0.934904	-1.402682

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.512691 a.u.

C	3.178787	-1.766054	-0.176305
H	4.059075	-2.317934	-0.479918
H	2.307956	-2.347846	0.099913
C	3.189027	-0.386307	-0.144450
H	4.116732	0.100642	-0.441248
C	2.143851	0.462904	0.222840
C	2.322995	1.952621	0.196462
H	1.567233	2.439137	-0.433861
H	2.203754	2.382520	1.200100

H	3.307395	2.240212	-0.178685
C	0.789132	-0.052184	0.634583
H	0.879287	-1.029347	1.118399
H	0.349387	0.622314	1.377604
C	-0.204533	-0.174883	-0.557044
H	-0.307694	0.797987	-1.042645
H	0.242771	-0.845586	-1.300558
C	-1.536389	-0.716343	-0.138604
H	-1.544607	-1.760254	0.167360
C	-2.745151	-0.021407	-0.072207
C	-3.983132	-0.790093	0.360808
H	-3.728438	-1.605309	1.041663
H	-4.698890	-0.138327	0.866332
H	-4.490058	-1.228834	-0.504719
C	-2.882830	1.318187	-0.397851
H	-3.843495	1.812259	-0.319583
H	-2.050953	1.919720	-0.739548

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.509947 a.u.

C	3.170417	-1.749994	0.020779
H	4.075394	-2.304401	-0.192313
H	2.292454	-2.328668	0.280588
C	3.159203	-0.372960	-0.036236
H	4.095133	0.111467	-0.310249
C	2.078932	0.479115	0.213146
C	2.227656	1.964434	0.056663
H	1.538298	2.360700	-0.701188
H	1.986653	2.488004	0.990988
H	3.241009	2.245413	-0.237665
C	0.716626	-0.034644	0.570893
H	0.786022	-0.973046	1.127040
H	0.204936	0.681874	1.221484
C	-0.193662	-0.271328	-0.688742
H	-0.267528	0.666444	-1.246419
H	0.319163	-0.986970	-1.338289
C	-1.545961	-0.790179	-0.332819
H	-1.633953	-1.866817	-0.207092
C	-2.685562	-0.016970	-0.065467
C	-3.952795	-0.751947	0.337515
H	-3.848682	-1.193071	1.333770
H	-4.813890	-0.081713	0.357292
H	-4.174224	-1.566085	-0.357975
C	-2.702915	1.360137	-0.139235
H	-3.606823	1.918823	0.069789
H	-1.825585	1.934058	-0.408736

<u>Combination: 2t-2t</u>

TS

State: T_1

Imaginary frequency: -326.3283

Absolute Gibbs free energy at 298 K: -390.457534 a.u.

C	-4.219249	0.939038	-0.290515
H	-5.240633	0.631383	-0.477245
H	-4.015156	2.003470	-0.266583
C	-3.211115	0.016104	-0.089905
C	-1.892588	0.431907	0.150540
C	-0.749099	-0.458589	0.376331
H	-0.644773	-0.966878	1.332517
H	-0.315343	-1.000203	-0.461533
C	1.096017	1.045744	0.706373
H	0.864827	1.462528	-0.265969
H	0.528828	1.439237	1.539925
C	2.247579	0.354130	0.928090
H	2.484579	0.061082	1.948079
C	3.188130	-0.087804	-0.087371
C	2.934883	0.283977	-1.529080
H	2.905302	1.370821	-1.656730
H	3.716146	-0.112814	-2.178787
H	1.972816	-0.105550	-1.876634

C	4.270822	-0.810558	0.262233
H	4.993874	-1.146197	-0.471972
H	4.458384	-1.079846	1.296024
C	-3.528479	-1.465181	-0.129362
H	-2.953187	-1.970840	-0.910678
H	-3.272022	-1.948423	0.818137
H	-4.588402	-1.638005	-0.322680
H	-1.716644	1.507635	0.170138

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.509857 a.u.

C	-4.164743	-0.974550	-0.131301
H	-5.165172	-0.609012	-0.326573
H	-4.028543	-2.048511	-0.075367
C	-3.096890	-0.110358	0.040033
C	-1.814438	-0.606700	0.287839
C	-0.565075	0.189211	0.497898
H	-0.763434	1.261482	0.422759
H	-0.184345	0.019296	1.515510
C	0.565127	-0.189208	-0.498148
H	0.763469	-1.261482	-0.423000
H	0.184391	-0.019288	-1.515754
C	1.814500	0.606694	-0.288129
H	1.705156	1.688313	-0.338744
C	3.096891	0.110357	-0.040006
C	3.342516	-1.385400	0.042299
H	3.095858	-1.883825	-0.899756
H	4.389607	-1.594729	0.265769
H	2.735090	-1.849796	0.824590
C	4.164762	0.974540	0.131228
H	5.165162	0.609032	0.326711
H	4.028631	2.048495	0.074992
C	-3.342627	1.385409	-0.041806
H	-3.095591	1.883603	0.900274
H	-2.735559	1.850046	-0.824231
H	-4.389826	1.594726	-0.264780
H	-1.705035	-1.688325	0.338165

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.508264 a.u.

C	-1.769555	-0.694772	-0.369522
C	-0.483379	0.014760	-0.622681
C	-2.998070	-0.102342	-0.054752
C	-4.108562	-0.881294	0.211417
C	3.131092	-1.409078	0.015447
C	2.998070	0.102342	0.054752
C	4.108562	0.881294	-0.211417
C	1.769555	0.694772	0.369522
C	0.483379	-0.014760	0.622682
H	-0.650318	1.058052	-0.901900
H	0.045473	-0.455543	-1.458538
H	-4.049522	-1.963526	0.190756
H	-5.069963	-0.439636	0.442479
H	4.143287	-1.702889	-0.266094
H	2.912925	-1.854216	0.990786
H	2.440985	-1.855618	-0.706299
H	4.049522	1.963526	-0.190756
H	5.069963	0.439636	-0.442479
H	1.732136	1.781966	0.371470
H	-0.045473	0.455543	1.458538
H	0.650318	-1.058052	0.901901
H	-1.732136	-1.781966	-0.371469
C	-3.131092	1.409078	-0.015448
H	-2.440985	1.855618	0.706298
H	-2.912925	1.854216	-0.990787
H	-4.143287	1.702889	0.266093

<u>Combination: 1t-2c</u>

TS

State: T_1

Imaginary frequency: -314.5034

Absolute Gibbs free energy at 298 K: -390.457684 a.u.

C	1.160120	-0.807411	1.396782
C	1.726486	0.314412	0.573077
C	1.215471	1.576212	0.663135
C	2.762889	0.028542	-0.404259
C	3.291976	-1.176728	-0.674398
C	-3.415591	-0.784517	0.566265
C	-2.242447	-0.280605	-0.239509
C	-1.576988	-1.229281	-1.084597
C	-1.854508	1.030264	-0.147413
C	-0.758859	1.660679	-0.859650
H	0.585783	-1.498226	0.763874
H	1.949238	-1.389837	1.882237
H	0.486057	-0.429226	2.166272
H	1.662368	2.393446	0.108999
H	0.521860	1.843453	1.449728
H	3.126517	0.888057	-0.964077
H	2.976248	-2.076588	-0.159443
H	4.064814	-1.292463	-1.424728
H	-3.113027	-1.600222	1.233211
H	-3.856728	0.006294	1.175685
H	-4.197758	-1.185864	-0.088085
H	-0.722510	-0.960413	-1.688912
H	-1.943542	-2.245272	-1.162666
H	-2.419991	1.670634	0.524853
H	-0.718840	2.742565	-0.890990
H	-0.251796	1.144265	-1.662555

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.511659 a.u.

C	2.884700	-1.562957	-0.533068
C	2.034990	-0.407130	-0.083285
C	0.568530	-0.726483	0.072893
C	2.573276	0.847286	0.199067
C	3.900472	1.226013	0.125748
C	-4.181964	-0.453734	0.252892
C	-2.838349	0.171647	-0.085057
C	-2.734172	0.936816	-1.233370
C	-1.767753	-0.082061	0.776591
C	-0.354606	0.387245	0.610818
H	2.349017	-2.180201	-1.261689
H	3.822280	-1.243972	-0.990279
H	3.136209	-2.220084	0.310775
H	0.474867	-1.607813	0.725651
H	0.176813	-1.062523	-0.898222
H	1.876827	1.616982	0.519286
H	4.688275	0.543927	-0.168094
H	4.196878	2.238383	0.368838
H	-4.243185	-1.476462	-0.132967
H	-4.338877	-0.499966	1.333053
H	-5.005754	0.113993	-0.184364
H	-1.800718	1.385270	-1.547434
H	-3.597009	1.111892	-1.864180
H	-1.961542	-0.713074	1.641022
H	0.024693	0.721174	1.584043
H	-0.309517	1.252614	-0.054813

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.510411a.u.

C	2.830946	1.617356	0.415944
C	2.009984	0.410336	0.056316
C	0.535338	0.679778	-0.110429
C	2.578594	-0.847481	-0.137767
C	3.914380	-1.188833	-0.040871
C	-4.176350	0.389987	-0.288234
C	-2.814584	-0.159631	0.102873

C	-2.657813	-0.714697	1.360530
C	-1.775587	-0.054027	-0.825958
C	-0.353074	-0.478043	-0.615597
H	2.287537	2.264700	1.112193
H	3.784718	1.357123	0.876602
H	3.048678	2.225281	-0.472927
H	0.415980	1.537458	-0.789749
H	0.129894	1.032948	0.848950
H	1.900413	-1.654307	-0.400758
H	4.686000	-0.469987	0.204212
H	4.234386	-2.208495	-0.213284
H	-4.238694	1.462420	-0.077004
H	-4.368881	0.253319	-1.354889
H	-4.977851	-0.102751	0.265876
H	-1.707412	-1.099127	1.707483
H	-3.493399	-0.784743	2.046129
H	-2.002245	0.415798	-1.779870
H	0.051169	-0.846853	-1.564689
H	-0.301302	-1.311255	0.090878

Combination: 2c-2t

TS

State: T_1

Imaginary frequency: -342.2711

Absolute Gibbs free energy at 298 K: -390.457885 a.u.

C	3.210069	-1.407514	0.016365
H	4.133948	-1.822360	-0.366653
H	2.456206	-2.102447	0.357427
C	3.021203	0.013608	0.078165
C	1.877488	0.584391	0.568190
C	0.711700	-0.121899	1.073216
H	0.745692	-1.187987	1.249397
H	-0.012124	0.425793	1.662075
C	-0.771399	-0.292837	-0.887074
H	-0.615215	0.769332	-1.025921
H	-0.009378	-0.939229	-1.299943
C	-1.980462	-0.796717	-0.515841
H	-2.106528	-1.876759	-0.502919
C	-3.131306	-0.025210	-0.082666
C	-3.039742	1.482273	-0.075521
H	-2.828961	1.869299	-1.077587
H	-3.971809	1.929779	0.272259
H	-2.231898	1.827504	0.577498
C	-4.263129	-0.652010	0.298964
H	-5.139833	-0.101324	0.619242
H	-4.336004	-1.734151	0.295330
C	4.153146	0.879188	-0.420035
H	4.382484	0.659957	-1.469184
H	3.914623	1.941195	-0.339531
H	5.070438	0.691864	0.149558
H	1.822954	1.669884	0.576373

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.511163 a.u.

C	-3.251423	1.401137	-0.190019
H	-4.226339	1.772058	-0.481398
H	-2.463795	2.134484	-0.077972
C	-3.042116	0.049749	0.024253
C	-1.810445	-0.498976	0.390323
C	-0.525124	0.233732	0.618464
H	-0.682362	1.314582	0.645328
H	-0.119112	-0.041549	1.600702
C	0.550922	-0.094581	-0.453825
H	0.711529	-1.175372	-0.481539
H	0.136276	0.179769	-1.434218
C	1.836712	0.636518	-0.227468
H	1.768648	1.722207	-0.195990
C	3.104810	0.075603	-0.055864
C	3.293069	-1.430388	-0.089024
H	3.001872	-1.848785	-1.056963
H	4.336650	-1.694704	0.087764

H	2.688803	-1.927768	0.675221
C	4.210849	0.884097	0.143606
H	5.200984	0.467770	0.281214
H	4.116152	1.963661	0.168673
C	-4.221123	-0.898745	-0.122686
H	-3.905501	-1.867726	-0.516477
H	-4.699180	-1.076953	0.845969
H	-4.978528	-0.491012	-0.795114
H	-1.762882	-1.579539	0.508241

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.509135 a.u.

C	-1.797540	0.560767	0.576667
C	-0.479660	-0.094551	0.820834
C	-2.933604	-0.055583	0.032213
C	-2.981135	-1.393172	-0.301415
C	3.105747	1.442946	-0.281927
C	3.010410	-0.059037	-0.085237
C	4.160555	-0.773314	0.193408
C	1.776426	-0.710518	-0.196426
C	0.453525	-0.075401	-0.447674
H	-0.606112	-1.135107	1.134455
H	0.044247	0.417124	1.633116
H	-2.134902	-2.052922	-0.158256
H	-3.879311	-1.833647	-0.716414
H	4.130846	1.788514	-0.140783
H	2.789916	1.734999	-1.287816
H	2.470864	1.982498	0.426903
H	4.129711	-1.847099	0.338923
H	5.125784	-0.288347	0.270139
H	1.771435	-1.786260	-0.032266
H	-0.079101	-0.611396	-1.242056
H	0.563697	0.958290	-0.783297
H	-1.854788	1.628416	0.773966
C	-4.157377	0.811525	-0.209637
H	-4.377813	1.434396	0.661385
H	-3.998760	1.482825	-1.059559
H	-5.039784	0.205749	-0.423268

Combination: 1t-1t

TS

State: T_1

Imaginary frequency: -318.0779

Absolute Gibbs free energy at 298 K: -390.457240 a.u.

C	2.273143	1.407030	0.464688
C	2.123684	0.020897	-0.098007
C	0.758166	-0.506465	-0.336430
C	3.222315	-0.775433	-0.445994
C	4.564164	-0.480486	-0.318320
C	-2.704588	-1.092423	1.200828
C	-2.186139	0.099468	0.439507
C	-1.013355	0.703493	0.796747
C	-2.914602	0.570341	-0.724782
C	-4.053405	0.052713	-1.215672
H	1.759592	2.140863	-0.168460
H	1.817737	1.482292	1.458650
H	3.315370	1.713655	0.550611
H	0.478572	-1.442631	0.137930
H	0.315518	-0.360113	-1.320587
H	2.980608	-1.754144	-0.857194
H	4.923624	0.459838	0.080059
H	5.313906	-1.204755	-0.610229
H	-2.747761	-1.983458	0.563923
H	-2.068863	-1.319632	2.058072
H	-3.720779	-0.916633	1.569216
H	-0.527847	0.460919	1.733233
H	-0.702397	1.621723	0.314278
H	-2.479751	1.430178	-1.230646
H	-4.543731	-0.802117	-0.764310

H	-4.530085	0.479212	-2.089937

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.514338 a.u.

C	-2.243395	1.683365	0.043374
C	-1.918063	0.231264	0.260734
C	-0.492893	-0.123545	0.589126
C	-2.882980	-0.769587	0.127669
C	-4.208761	-0.608594	-0.216109
C	2.243420	-1.683376	-0.043544
C	1.918069	-0.231259	-0.260776
C	0.492907	0.123563	-0.589179
C	2.882965	0.769594	-0.127555
C	4.208727	0.608580	0.216279
H	-3.242536	1.935459	0.408081
H	-1.526118	2.329282	0.557088
H	-2.215051	1.952646	-1.020935
H	-0.434406	-1.173257	0.891198
H	-0.148727	0.473571	1.444713
H	-2.544556	-1.787779	0.313397
H	-4.638194	0.362502	-0.429819
H	-4.870236	-1.462642	-0.286149
H	2.215138	-1.952738	1.020747
H	1.526119	-2.329258	-0.557267
H	3.242543	-1.935435	-0.408324
H	0.148739	-0.473546	-1.444767
H	0.434430	1.173278	-0.891245
H	2.544537	1.787799	-0.313200
H	4.638157	-0.362534	0.429914
H	4.870191	1.462627	0.286442

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.514349 a.u.

C	2.267692	-1.693195	0.021580
C	1.906486	-0.258287	0.289319
C	0.479205	0.054165	0.621035
C	2.840887	0.773748	0.149439
C	4.160899	0.654006	-0.223049
C	-2.267692	1.693195	-0.021581
C	-1.906486	0.258286	-0.289319
C	-0.479205	-0.054166	-0.621035
C	-2.840887	-0.773748	-0.149438
C	-4.160899	-0.654006	0.223049
H	3.260639	-1.940136	0.407408
H	1.549089	-2.374823	0.483885
H	2.281211	-1.916251	-1.053988
H	0.401484	1.063725	1.034764
H	0.106497	-0.639102	1.384183
H	2.478860	1.778435	0.362784
H	4.610039	-0.301930	-0.463465
H	4.801003	1.524892	-0.284656
H	-2.281215	1.916250	1.053988
H	-1.549086	2.374822	-0.483883
H	-3.260637	1.940137	-0.407412
H	-0.106497	0.639102	-1.384183
H	-0.401484	-1.063725	-1.034764
H	-2.478860	-1.778435	-0.362784
H	-4.610039	0.301931	0.463464
H	-4.801004	-1.524891	0.284657

<u>Combination: 2c-2c</u>

TS

State: T_1

Imaginary frequency: -323.4607

Absolute Gibbs free energy at 298 K: -390.454745 a.u.

C	-2.919461	1.473624	0.021032
H	-3.756690	2.119880	0.257153

H	-1.958071	1.954044	-0.117061
C	-3.076064	0.141768	-0.089240
C	-1.985912	-0.775644	-0.419331
C	-0.754164	-0.444972	-0.884561
H	-0.045374	-1.213282	-1.161716
H	-0.520200	0.558474	-1.217376
C	0.743521	0.056249	1.050206
H	-0.009800	0.693049	1.493726
H	0.766727	-0.965239	1.402758
C	1.917725	0.664061	0.451929
H	1.873448	1.737456	0.286984
C	3.059592	0.013676	0.070364
C	4.205559	0.777023	-0.546426
H	5.115791	0.672158	0.055006
H	4.441354	0.391427	-1.545091
H	3.979445	1.840836	-0.637613
C	3.232790	-1.403866	0.235611
H	4.153268	-1.883661	-0.072284
H	2.469293	-2.027764	0.677441
C	-4.423955	-0.502958	0.145042
H	-4.757071	-1.048641	-0.744198
H	-4.370844	-1.229882	0.962989
H	-5.185321	0.236834	0.396919
H	-2.193743	-1.829443	-0.245403

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.512436 a.u.

C	-3.193655	1.449575	-0.022103
H	-4.157928	1.888324	-0.247176
H	-2.371161	2.134186	0.137888
C	-3.039610	0.075997	0.053801
C	-1.824195	-0.555891	0.328418
C	-0.502989	0.100376	0.584639
H	-0.620431	1.169987	0.774559
H	-0.054173	-0.326129	1.490410
C	0.503019	-0.100333	-0.584752
H	0.620444	-1.169947	-0.774676
H	0.054210	0.326181	-1.490523
C	1.824234	0.555909	-0.328524
H	1.819526	1.643771	-0.336886
C	3.039612	-0.076011	-0.053785
C	4.262778	0.803416	0.150017
H	3.999977	1.742466	0.642665
H	5.016846	0.301387	0.759506
H	4.725476	1.053643	-0.810128
C	3.193578	-1.449583	0.022241
H	4.157808	-1.888367	0.247429
H	2.371053	-2.134159	-0.137749
C	-4.262765	-0.803453	-0.149972
H	-3.999932	-1.742559	-0.642494
H	-4.725526	-1.053560	0.810174
H	-5.016786	-0.301488	-0.759571
H	-1.819443	-1.643754	0.336697

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.510041 a.u.

C	1.787171	0.636848	-0.384094
C	0.440970	0.053448	-0.649707
C	2.957168	-0.078234	-0.088361
C	3.015543	-1.455662	-0.046499
C	-4.211776	-0.724105	-0.213085
C	-2.957169	0.078235	0.088362
C	-3.015546	1.455662	0.046509
C	-1.787169	-0.636848	0.384086
C	-0.440968	-0.053448	0.649699
H	0.520299	-0.941318	-1.096118
H	-0.101815	0.678818	-1.365127
H	2.149598	-2.075677	-0.239988
H	3.942037	-1.967876	0.181817
H	-4.128264	-1.231472	-1.179344

H	-4.379592	-1.493255	0.545659
H	-5.095836	-0.085033	-0.246838
H	-2.149601	2.075677	0.239999
H	-3.942042	1.967876	-0.181802
H	-1.845117	-1.722400	0.349180
H	0.101817	-0.678819	1.365119
H	-0.520296	0.941317	1.096111
H	1.845120	1.722400	-0.349196
C	4.211776	0.724105	0.213089
H	4.379576	1.493277	-0.545636
H	4.128275	1.231444	1.179363
H	5.095840	0.085037	0.246811

Combination: 2t-1c

TS

State: T_1

Imaginary frequency: -296.8270

Absolute Gibbs free energy at 298 K: -390.459359 a.u.

C	2.845609	1.345797	-0.275966
C	2.889151	-0.140909	-0.015576
C	3.977740	-0.717740	0.531626
C	1.736269	-0.951065	-0.370711
C	0.567425	-0.495789	-0.893460
C	-2.321963	1.991951	0.031623
C	-2.232438	0.508906	0.251205
C	-1.036517	0.020586	0.956502
C	-3.225931	-0.332617	-0.185201
C	-3.263699	-1.738601	-0.030090
H	2.017406	1.817989	0.262003
H	2.697902	1.555663	-1.340140
H	3.772793	1.826188	0.039388
H	4.014549	-1.785157	0.720302
H	4.854895	-0.140687	0.800141
H	1.827982	-2.014566	-0.162971
H	-0.197795	-1.185605	-1.220822
H	0.449149	0.531786	-1.212978
H	-3.220011	2.268189	-0.523743
H	-2.331868	2.529560	0.988760
H	-1.449436	2.364959	-0.519772
H	-1.011703	-0.981163	1.361407
H	-0.389359	0.740905	1.441121
H	-4.068639	0.124657	-0.698240
H	-2.481302	-2.285080	0.478651
H	-4.098443	-2.310762	-0.412827

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.511380 a.u.

C	-2.990717	1.213628	0.618001
C	-2.808298	-0.172195	0.025773
C	-3.920492	-0.852517	-0.440490
C	-1.539567	-0.752690	-0.044340
C	-0.247526	-0.154884	0.416955
C	2.295056	1.949703	-0.316560
C	2.142523	0.458336	-0.246928
C	0.826463	-0.112939	-0.706650
C	3.175913	-0.339984	0.246458
C	3.187281	-1.713658	0.379265
H	-2.400306	1.961200	0.080145
H	-2.678605	1.245193	1.665995
H	-4.036675	1.520334	0.572469
H	-3.829982	-1.845523	-0.865665
H	-4.911310	-0.417747	-0.397268
H	-1.475765	-1.749896	-0.475568
H	0.161224	-0.750307	1.245297
H	-0.400430	0.852569	0.811126
H	3.249432	2.283394	0.096039
H	2.231479	2.305182	-1.353858
H	1.494051	2.463902	0.230505
H	0.962027	-1.125384	-1.098528

H	0.434967	0.488882	-1.534867
H	4.074364	0.186973	0.564206
H	2.345721	-2.333032	0.094263
H	4.055995	-2.222526	0.776806

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.510727 a.u.

C	2.838509	1.268858	-0.515259
C	2.753722	-0.167262	-0.031180
C	3.897865	-0.784875	0.438758
C	1.536725	-0.857133	-0.072023
C	0.219442	-0.315152	-0.508797
C	-2.217207	1.981454	0.243777
C	-2.085681	0.486447	0.257142
C	-0.766142	-0.079067	0.692860
C	-3.134406	-0.324926	-0.185202
C	-3.149790	-1.701234	-0.260562
H	2.158421	1.921557	0.039847
H	2.574518	1.349763	-1.573893
H	3.849359	1.660571	-0.393231
H	3.874916	-1.810066	0.790282
H	4.850370	-0.270420	0.466742
H	1.538126	-1.880373	0.298103
H	-0.269435	-1.019316	-1.191916
H	0.338770	0.623723	-1.054707
H	-3.186539	2.303864	-0.142154
H	-2.097050	2.399498	1.251919
H	-1.438363	2.448179	-0.374216
H	-0.901121	-1.030207	1.215956
H	-0.283655	0.602716	1.400013
H	-4.036341	0.192699	-0.507975
H	-2.304838	-2.309058	0.039209
H	-4.025358	-2.225793	-0.621061

Cycloadduct formation

<u>Prod. 2</u>

TS

State: Open shell S_0

Imaginary frequency: -416.2908

Absolute Gibbs free energy at 298 K: -390.499537 a.u.

C	-1.254778	-0.003923	1.697626
C	-1.187023	0.368106	0.241672
C	-0.759891	1.787608	-0.108413
C	-1.827123	-0.445503	-0.727105
C	-2.379133	-1.675218	-0.525051
C	1.254786	-0.003978	-1.697616
C	1.187024	0.368110	-0.241679
C	0.759873	1.787617	0.108362
C	1.827101	-0.445474	0.727124
C	2.379160	-1.675174	0.525081
H	-2.288395	0.070287	2.063261
H	-0.920508	-1.029999	1.874098
H	-0.642891	0.656291	2.314766
H	-1.282500	2.544895	0.491156
H	-1.000599	1.995508	-1.154691
H	-1.857421	-0.047733	-1.739719
H	-2.398247	-2.149065	0.448848
H	-2.822139	-2.226683	-1.345080
H	0.920580	-1.030088	-1.874028
H	0.642834	0.656162	-2.314770
H	2.288389	0.070292	-2.063277
H	1.282475	2.544890	-0.491232
H	1.000581	1.995548	1.154633
H	1.857369	-0.047694	1.739735
H	2.398342	-2.148998	-0.448828
H	2.822145	-2.226636	1.345122

TS

State: T_1

Imaginary frequency: -603.8267

Absolute Gibbs free energy at 298 K: -390.436520 a.u.

C	1.104757	-0.002325	-1.687087
C	0.981548	0.342759	-0.208755
C	0.790419	1.844867	0.079533
C	1.752894	-0.442236	0.687782
C	2.204163	-1.806558	0.438775
C	-1.081446	-0.006466	1.691951
C	-0.921944	0.339612	0.225178
C	-0.741349	1.842367	-0.050923
C	-1.720972	-0.445469	-0.713389
C	-2.342312	-1.612418	-0.470313
H	2.121245	0.218744	-2.031387
H	0.912115	-1.061517	-1.868490
H	0.416815	0.580421	-2.302612
H	1.331431	2.502741	-0.607744
H	1.113085	2.089017	1.094666
H	1.924513	-0.034732	1.686013
H	1.563746	-2.666761	0.621220
H	3.220751	-2.019592	0.117063
H	-0.839104	-1.051621	1.896821
H	-0.437291	0.609707	2.322095
H	-2.117941	0.166861	2.005761
H	-1.282160	2.494649	0.642193
H	-1.064015	2.098769	-1.063093
H	-1.796471	-0.039084	-1.719835
H	-2.329887	-2.088619	0.503118
H	-2.891383	-2.123784	-1.252296

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.533708 a.u.

C	-1.020740	-0.036169	1.682967
C	-0.786396	0.272228	0.201505
C	-0.771104	1.816458	-0.047727
C	-1.691342	-0.518814	-0.700222
C	-2.482470	-1.536325	-0.363276
C	1.020740	-0.036169	-1.682967
C	0.786396	0.272228	-0.201505
C	0.771104	1.816458	0.047727
C	1.691342	-0.518814	0.700222
C	2.482470	-1.536325	0.363276
H	-2.068433	0.145219	1.938300
H	-0.783091	-1.074634	1.925657
H	-0.411438	0.602451	2.326156
H	-1.321084	2.419861	0.677858
H	-1.127434	2.075975	-1.047080
H	-1.690012	-0.206175	-1.742011
H	-2.553260	-1.914155	0.650089
H	-3.097243	-2.032808	-1.105970
H	0.783091	-1.074634	-1.925657
H	0.411438	0.602451	-2.326156
H	2.068433	0.145219	-1.938300
H	1.321084	2.419861	-0.677858
H	1.127434	2.075975	1.047080
H	1.690012	-0.206175	1.742011
H	2.553260	-1.914155	-0.650089
H	3.097243	-2.032808	1.105970

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.441165 a.u.

C	1.088855	-0.090446	1.682096
C	0.848334	-0.326905	0.183671
C	0.827671	-1.847465	-0.152767
C	1.742465	0.528809	-0.650309
C	2.074952	1.910697	-0.347143
C	-0.977243	0.087627	-1.666996
C	-0.751897	-0.306657	-0.206374
C	-0.713401	-1.859776	-0.045991

C	-1.652725	0.422698	0.742767
C	-2.456900	1.450304	0.468586
H	2.135391	-0.300238	1.922046
H	0.877919	0.943968	1.962848
H	0.470975	-0.745071	2.301600
H	1.382418	-2.492986	0.532134
H	1.176789	-2.046421	-1.168717
H	2.047686	0.126634	-1.617366
H	1.428774	2.735605	-0.643272
H	2.991950	2.182428	0.171115
H	-0.762362	1.144652	-1.842178
H	-0.339109	-0.491793	-2.337245
H	-2.016822	-0.101492	-1.950683
H	-1.265089	-2.424849	-0.800875
H	-1.059809	-2.178813	0.939551
H	-1.638130	0.055033	1.766409
H	-2.543121	1.878971	-0.523236
H	-3.068121	1.901047	1.242626

<u>Prod. 3</u>

TS

State: Open shell S_0

Imaginary frequency: -382.3259

Absolute Gibbs free energy at 298 K: -390.497556 a.u.

C	0.831241	-0.623100	0.650698
C	0.012271	0.177677	1.631454
C	-1.791063	-1.766438	-0.752704
C	-1.449977	-0.417851	-0.183947
C	-1.433525	-0.241227	1.328279
C	-1.514244	0.713804	-1.042876
C	-1.648953	2.018959	-0.679674
H	0.131737	1.245461	1.437516
H	0.310150	0.010609	2.676868
H	-1.501249	-1.843654	-1.803900
H	-1.313313	-2.581427	-0.202647
H	-2.876257	-1.944228	-0.700155
H	-1.659801	-1.197570	1.809270
H	-2.179827	0.478334	1.685780
H	-1.463060	0.496585	-2.108725
H	-1.749374	2.327550	0.354077
H	-1.682438	2.802488	-1.426539
H	0.685405	-1.699136	0.685749
C	1.964071	-0.170381	-0.076599
C	2.732295	-1.051888	-0.785513
H	3.585606	-0.723108	-1.366336
H	2.507743	-2.112723	-0.792388
C	2.303798	1.305727	-0.086706
H	1.465110	1.897791	-0.463506
H	2.533091	1.669585	0.919834
H	3.170995	1.501758	-0.719374

TS

State: T_1

Imaginary frequency: -620.4770

Absolute Gibbs free energy at 298 K: -390.440012 a.u.

C	-0.592978	0.564752	0.701292
C	0.192559	-0.190411	1.776339
C	1.516970	1.774802	-0.825695
C	1.156367	0.446752	-0.196545
C	1.587862	0.195528	1.254015
C	1.166760	-0.685268	-1.123752
C	1.528732	-1.951910	-0.869895
H	0.036231	-1.267127	1.699139
H	-0.043157	0.111549	2.801406
H	0.970793	1.934277	-1.760240
H	1.298698	2.611888	-0.157020
H	2.589322	1.814569	-1.061432
H	1.936861	1.126517	1.708804
H	2.375324	-0.551596	1.386007
H	0.824008	-0.450334	-2.131147
H	1.895037	-2.271430	0.099128

H	1.475897	-2.711784	-1.640666
H	-0.556911	1.644908	0.841120
C	-1.776532	0.127330	0.068697
C	-2.563470	1.079497	-0.726954
H	-2.335005	1.276676	-1.772491
H	-3.473418	1.526652	-0.334198
C	-2.212160	-1.313516	0.007241
H	-2.089057	-1.720817	-1.005798
H	-1.651587	-1.953661	0.689485
H	-3.277692	-1.405623	0.249451

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.541487 a.u.

C	0.468970	-0.078996	-0.818866
C	-0.259861	-1.373637	-1.246663
C	-1.274019	1.897155	-0.478948
C	-0.913180	0.434662	-0.199380
C	-1.606926	-0.625555	-1.104423
C	-1.001412	0.164093	1.281267
C	-1.800033	-0.691367	1.912831
H	-0.167510	-2.159181	-0.495194
H	-0.004770	-1.786748	-2.224129
H	-0.653596	2.584489	0.104605
H	-1.137878	2.136452	-1.537734
H	-2.318696	2.091017	-0.216793
H	-1.921273	-0.173297	-2.048433
H	-2.453468	-1.175418	-0.692043
H	-0.328516	0.771682	1.885153
H	-2.501110	-1.333658	1.392022
H	-1.778409	-0.779136	2.993344
H	0.650301	0.536181	-1.709976
C	1.733406	-0.100947	-0.003419
C	2.304539	-1.228240	0.423349
H	3.225652	-1.210275	0.996294
H	1.881941	-2.203668	0.215799
C	2.348117	1.248851	0.281883
H	3.270771	1.156176	0.857848
H	2.577459	1.777966	-0.650201
H	1.661487	1.891302	0.843655

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.449051

C	3.012249	-0.515646	0.450889
C	1.703051	-0.108492	-0.178230
C	0.824861	-1.252056	-0.647703
C	1.347241	1.178168	-0.268051
C	0.040698	1.705660	-0.795494
C	-2.689790	-1.003973	-0.471789
C	-1.483679	-0.679141	0.368247
C	-0.313214	-1.626636	0.356034
C	-1.395865	0.625196	1.029604
C	-1.014442	1.896591	0.319812
H	3.643336	-1.054442	-0.265969
H	3.572261	0.346886	0.818035
H	2.847397	-1.197089	1.294448
H	1.449427	-2.139465	-0.795838
H	0.376185	-1.026772	-1.620257
H	2.032135	1.925696	0.129293
H	-0.369040	1.032742	-1.555405
H	0.202447	2.669923	-1.288830
H	-2.885390	-2.081896	-0.495808
H	-3.586467	-0.500076	-0.098835
H	-2.565813	-0.684397	-1.520454
H	-0.670459	-2.631384	0.101205
H	0.127881	-1.689050	1.358675
H	-1.800737	0.726667	2.037511
H	-1.910563	2.358870	-0.131149
H	-0.649251	2.625765	1.053468

Prod. 4

TS

State: Open shell S_0

Imaginary frequency: -331.1651

Absolute Gibbs free energy at 298 K: -390.500378 a.u.

C	1.090588	0.455822	0.576096
C	0.743210	1.835773	0.077574
C	-1.044825	0.416794	-0.627016
C	-0.784854	1.783115	-0.042204
H	1.179994	2.009107	-0.909418
H	1.107200	2.637971	0.733217
H	-1.234225	1.868076	0.951308
H	-1.206036	2.596956	-0.649592
H	0.578739	0.149871	1.484592
C	2.156609	-0.368315	0.132491
C	3.028630	-0.008909	-0.856636
H	2.968807	0.946984	-1.361113
H	3.826575	-0.673437	-1.165107
C	2.297297	-1.719581	0.808018
H	2.463879	-1.604566	1.883736
H	1.386269	-2.312070	0.682006
H	3.132588	-2.288335	0.396065
H	-0.505226	0.191302	-1.542643
C	-2.093510	-0.470946	-0.273195
C	-2.325839	-1.602462	-1.007063
H	-3.107187	-2.303455	-0.739275
H	-1.728862	-1.835188	-1.881606
C	-2.954929	-0.172271	0.937528
H	-2.351598	-0.093476	1.847313
H	-3.490546	0.775075	0.823539
H	-3.694640	-0.958928	1.093428

TS

State: T_1

Imaginary frequency: -667.4183

Absolute Gibbs free energy at 298 K: -390.444898

C	-0.808187	0.455663	-0.571265
C	-0.724534	1.941588	-0.213408
C	0.772783	0.447896	0.603027
C	0.755781	1.920766	0.200341
H	-1.370426	2.156564	0.641999
H	-0.997606	2.624213	-1.024052
H	1.400136	2.101778	-0.663327
H	1.051532	2.619542	0.989380
H	-0.313658	0.205666	-1.509712
C	-1.871775	-0.393157	-0.222834
C	-2.811730	-0.069136	0.856801
H	-3.788549	0.360560	0.650769
H	-2.620642	-0.368772	1.885895
C	-1.974357	-1.775702	-0.818960
H	-2.984868	-1.970155	-1.198590
H	-1.266561	-1.910569	-1.640587
H	-1.770628	-2.551960	-0.069146
H	0.304580	0.267941	1.568982
C	1.835637	-0.496783	0.287336
C	2.009023	-1.613691	1.026686
H	2.764532	-2.350368	0.778325
H	1.396789	-1.812594	1.899627
C	2.712403	-0.232790	-0.916216
H	2.116927	-0.093594	-1.824944
H	3.308202	0.676159	-0.784954
H	3.399977	-1.062340	-1.088713

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.547904

C	-0.718964	0.415136	-0.419521
C	-0.913123	1.930037	-0.155239
C	0.567282	0.474179	0.494688
C	0.579854	2.014189	0.247524

H	-1.562843	2.108494	0.704091
H	-1.255371	2.545870	-0.988616
H	1.210894	2.284764	-0.601930
H	0.848332	2.644147	1.097198
H	-0.397284	0.274368	-1.458974
C	-1.785662	-0.597028	-0.103317
C	-2.999685	-0.260173	0.335811
H	-3.293439	0.771790	0.486623
H	-3.748579	-1.014540	0.552636
C	-1.391955	-2.036654	-0.327735
H	-1.135548	-2.209476	-1.379684
H	-0.504687	-2.299402	0.257102
H	-2.199101	-2.720442	-0.058403
H	0.252142	0.289071	1.525867
C	1.789115	-0.355023	0.201172
C	2.357800	-1.092678	1.159431
H	3.247693	-1.684660	0.972664
H	1.952324	-1.124734	2.165309
C	2.359614	-0.316967	-1.195580
H	1.639887	-0.689601	-1.932000
H	2.619575	0.702928	-1.497022
H	3.260345	-0.928683	-1.268266

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.509954

C	1.452476	0.542851	0.605363
C	0.743162	1.677195	-0.064311
C	-1.395076	0.431697	-0.664429
C	-0.799877	1.593076	0.067358
H	1.008050	1.740891	-1.122636
H	1.065143	2.625978	0.388859
H	-1.071183	1.569950	1.126897
H	-1.216536	2.532187	-0.329606
H	1.186399	0.376765	1.647689
C	2.407067	-0.314245	0.046098
C	2.859761	-0.221484	-1.255676
H	2.497101	0.530971	-1.943501
H	3.603659	-0.910961	-1.635031
C	2.959412	-1.415295	0.936928
H	3.277581	-1.018207	1.904746
H	2.197886	-2.177165	1.129901
H	3.817166	-1.908904	0.476924
H	-1.024027	0.262809	-1.673133
C	-2.386801	-0.435451	-0.198593
C	-2.860698	-1.458992	-1.000373
H	-3.628342	-2.140788	-0.655979
H	-2.472287	-1.609790	-2.001042
C	-2.963084	-0.266854	1.195361
H	-2.187156	-0.354728	1.961679
H	-3.432871	0.713284	1.319760
H	-3.718643	-1.027293	1.398124

<u>Prod. 5</u>

TS

State: Open shell S_0

Imaginary frequency: -204.8747

Absolute Gibbs free energy at 298 K: -390.503868 a.u.

C	-1.964760	1.065473	1.071428
C	-1.237057	0.502536	-0.118527
C	-0.036833	1.255270	-0.597076
C	-1.864958	-0.446175	-0.968874
C	-3.119970	-0.960462	-0.845427
C	3.225453	-0.119762	-0.789656
C	1.998326	-0.119306	0.074549
C	1.282309	1.172499	0.278243
C	1.424039	-1.293857	0.526502
C	0.284199	-1.356452	1.317982
H	-2.537231	0.304333	1.605910
H	-1.275019	1.530334	1.782191

H	-2.672590	1.847192	0.761044
H	-0.298233	2.321389	-0.637054
H	0.217822	0.957471	-1.617517
H	-1.273960	-0.771491	-1.823116
H	-3.787464	-0.678929	-0.039724
H	-3.497425	-1.678917	-1.562200
H	3.595570	-1.131959	-0.967257
H	3.030658	0.345734	-1.765524
H	4.037734	0.458982	-0.331428
H	1.920881	2.011315	-0.011026
H	1.008053	1.333855	1.326130
H	1.853311	-2.232805	0.180914
H	-0.059422	-0.512555	1.895681
H	-0.207161	-2.302520	1.508104

TS

State: T_1

Imaginary frequency: -584.8898

Absolute Gibbs free energy at 298 K: -390.452985 a.u.

C	1.355081	-1.004855	1.328815
C	1.077074	-0.314113	0.011904
C	0.104878	-1.044694	-0.910967
C	2.203043	0.322483	-0.652614
C	3.446025	0.503919	-0.166760
C	-3.435200	0.193021	0.324321
C	-2.042714	0.154703	-0.221296
C	-1.356082	-1.171906	-0.431071
C	-1.174009	1.341326	-0.247647
C	-0.074936	1.371902	0.595612
H	1.868949	-0.347446	2.034372
H	0.435078	-1.349831	1.806164
H	1.994741	-1.883727	1.173239
H	0.500840	-2.054907	-1.087281
H	0.104774	-0.545993	-1.885410
H	1.990015	0.707124	-1.649401
H	3.749746	0.144378	0.809429
H	4.200079	1.019781	-0.749116
H	-3.949208	1.118321	0.047725
H	-4.031875	-0.652955	-0.033965
H	-3.446694	0.146421	1.426827
H	-1.910647	-1.772517	-1.166866
H	-1.401433	-1.766302	0.497643
H	-1.191435	1.997573	-1.119560
H	-0.169872	0.942201	1.588273
H	0.637984	2.187165	0.526147

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.576528 a.u.

C	1.050895	-0.211772	1.533829
C	0.958493	0.018459	0.016885
C	0.171701	-1.134284	-0.662465
C	2.323944	0.098613	-0.633362
C	3.516400	-0.002860	-0.052694
C	-3.473517	0.038365	0.121095
C	-1.979710	0.084975	-0.060214
C	-1.275892	-1.248224	-0.167532
C	-1.298204	1.232673	-0.108304
C	0.196758	1.341061	-0.271954
H	1.513240	-1.176707	1.760893
H	1.647783	0.569970	2.010958
H	0.060806	-0.192985	1.992467
H	0.700411	-2.079898	-0.506433
H	0.164149	-0.953704	-1.743734
H	2.289955	0.253371	-1.712184
H	3.637458	-0.158782	1.013105
H	4.427888	0.067508	-0.635947
H	-3.899504	1.038337	0.226578
H	-3.959333	-0.452289	-0.730683
H	-3.744147	-0.542092	1.011428
H	-1.839708	-1.902369	-0.844169
H	-1.310426	-1.750131	0.809515

H	-1.842699	2.171786	-0.033051
H	0.586346	2.129035	0.383289
H	0.422572	1.676899	-1.293741

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.477520 a.u.

C	-1.384906	0.114615	1.517962
C	-0.917673	0.001812	0.059251
C	-0.032226	1.220302	-0.332562
C	-2.080002	-0.061107	-0.908111
C	-3.380668	-0.034140	-0.629364
C	3.211566	-0.154924	-0.755521
C	2.072597	-0.039973	0.214145
C	1.343302	1.268637	0.386570
C	1.256586	-1.207867	0.567474
C	-0.066580	-1.316223	-0.128473
H	-1.958606	1.031720	1.678059
H	-2.017897	-0.733447	1.792892
H	-0.536543	0.125324	2.204535
H	-0.589262	2.142543	-0.133984
H	0.143919	1.188812	-1.414347
H	-1.780634	-0.141489	-1.953327
H	-3.762059	0.044442	0.382151
H	-4.120609	-0.089995	-1.420144
H	2.864821	-0.251645	-1.799109
H	3.856829	0.728664	-0.717478
H	3.823175	-1.037780	-0.549298
H	1.930402	2.103398	-0.010117
H	1.180909	1.477721	1.452375
H	1.392993	-1.709764	1.524447
H	-0.648356	-2.173069	0.223192
H	0.088949	-1.452230	-1.208076

<u>Prod. 6</u>

TS

State: Open shell S_0

Imaginary frequency: -242.9781

Absolute Gibbs free energy at 298 K: -390.496782 a.u.

C	-0.865306	-0.142216	-0.478102
C	-0.153441	-1.286608	0.176852
C	-2.254474	0.097237	-0.357780
C	-2.882992	1.019355	-1.154486
C	3.452316	-0.041292	-0.756559
C	2.145744	0.016739	-0.014699
C	1.402407	-1.291800	0.095349
C	1.681840	1.210912	0.495070
C	0.534102	1.407906	1.265436
H	-0.486044	-2.228070	-0.286683
H	-0.473390	-1.373340	1.221481
H	-2.331420	1.589987	-1.893019
H	-3.946383	1.208825	-1.073215
H	3.941493	0.934253	-0.793080
H	4.148578	-0.745005	-0.280813
H	3.315990	-0.395176	-1.786746
H	1.776201	-1.849983	0.966582
H	1.697205	-1.899654	-0.767930
H	2.240871	2.104098	0.219512
H	0.199347	2.413559	1.489337
H	0.046690	0.612091	1.804904
H	-0.332055	0.408988	-1.243936
C	-3.059347	-0.678924	0.665164
H	-4.108136	-0.379051	0.647661
H	-3.013641	-1.756767	0.479460
H	-2.680407	-0.512612	1.679011

TS

State: T_1

Imaginary frequency: -599.2971

Absolute Gibbs free energy at 298 K: -390.458314 a.u.

C	-0.873066	-0.085554	-0.554372
C	-0.002610	-1.279552	-0.230275
C	-2.252095	-0.002992	-0.119659
C	-3.155939	0.738993	-0.806058
C	3.645102	0.026342	0.302264
C	2.168949	0.048328	0.071090
C	1.487841	-1.111183	-0.606967
C	1.421026	1.311588	0.039300
C	0.159427	1.377872	0.592888
H	-0.387777	-2.158441	-0.767639
H	-0.074171	-1.523811	0.835373
H	-2.882512	1.258838	-1.717833
H	-4.182628	0.835204	-0.472820
H	3.936451	0.718514	1.097930
H	4.000426	-0.974950	0.564473
H	4.202499	0.334373	-0.600178
H	2.021283	-2.041257	-0.381532
H	1.548325	-0.989592	-1.704988
H	1.711320	2.065847	-0.697574
H	-0.449132	2.265647	0.455924
H	-0.050461	0.811545	1.495354
H	-0.694726	0.342321	-1.538345
C	-2.664047	-0.723836	1.144841
H	-3.704043	-0.509751	1.396036
H	-2.558663	-1.808472	1.040204
H	-2.043722	-0.426049	1.997298

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.582366 a.u.

C	0.715692	-0.009548	-0.370417
C	0.014257	1.218286	0.241861
C	2.221668	-0.008007	-0.173757
C	3.045874	-0.105909	-1.218703
C	-3.660413	-0.063428	-0.066283
C	-2.155898	-0.082732	-0.013530
C	-1.465724	1.256758	-0.157779
C	-1.459087	-1.211722	0.143066
C	0.046483	-1.294089	0.164163
H	0.515135	2.137685	-0.077246
H	0.089015	1.175549	1.334296
H	2.669180	-0.182436	-2.233506
H	4.124075	-0.113169	-1.096601
H	-4.081057	-1.068424	0.008061
H	-4.076578	0.542916	0.747068
H	-4.014679	0.384923	-1.002420
H	-1.994903	2.003171	0.447630
H	-1.567078	1.600871	-1.197241
H	-1.996457	-2.150884	0.258065
H	0.378013	-2.149558	-0.435335
H	0.385373	-1.503550	1.187922
H	0.532500	0.019463	-1.451364
C	2.756436	0.111528	1.233476
H	3.845857	0.046875	1.245137
H	2.470906	1.066014	1.687800
H	2.364966	-0.676263	1.885152

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.582366

C	0.715692	-0.009548	-0.370417
C	0.014257	1.218286	0.241861
C	2.221668	-0.008007	-0.173757
C	3.045874	-0.105909	-1.218703
C	-3.660413	-0.063428	-0.066283
C	-2.155898	-0.082732	-0.013530
C	-1.465724	1.256758	-0.157779
C	-1.459087	-1.211722	0.143066
C	0.046483	-1.294089	0.164163
H	0.515135	2.137685	-0.077246

H	0.089015	1.175549	1.334296
H	2.669180	-0.182436	-2.233506
H	4.124075	-0.113169	-1.096601
H	-4.081057	-1.068424	0.008061
H	-4.076578	0.542916	0.747068
H	-4.014679	0.384923	-1.002420
H	-1.994903	2.003171	0.447630
H	-1.567078	1.600871	-1.197241
H	-1.996457	-2.150884	0.258065
H	0.378013	-2.149558	-0.435335
H	0.385373	-1.503550	1.187922
H	0.532500	0.019463	-1.451364
C	2.756436	0.111528	1.233476
H	3.845857	0.046875	1.245137
H	2.470906	1.066014	1.687800
H	2.364966	-0.676263	1.885152

<u>Prod. 7</u>

TS

State: Open shell S_0

Imaginary frequency: -363.7491

Absolute Gibbs free energy at 298 K: -390.487994 a.u.

C	-1.104067	-1.312112	-0.048382
C	0.247745	-1.833465	0.393412
C	-1.742797	-0.148012	0.298964
C	-1.199135	0.862449	1.134677
C	2.676990	0.449995	0.656071
C	1.677954	0.054075	-0.392094
C	1.413320	-1.425486	-0.556299
C	0.800158	0.940088	-0.974364
C	0.393910	2.167681	-0.438375
H	0.199143	-2.927876	0.444911
H	0.480947	-1.489346	1.406801
H	-0.302120	0.689443	1.712068
H	-1.823055	1.689250	1.452597
H	2.814709	1.530397	0.714070
H	2.395343	0.089103	1.654944
H	3.652471	0.000285	0.434603
H	2.303559	-2.019116	-0.318929
H	1.130302	-1.657673	-1.589669
H	0.191174	0.549701	-1.786870
H	0.897781	2.618207	0.406983
H	-0.312928	2.793725	-0.967811
H	-1.629406	-1.961911	-0.745270
C	-3.102330	0.145576	-0.310354
H	-3.063250	1.044850	-0.934551
H	-3.454219	-0.680704	-0.930625
H	-3.850926	0.326933	0.467226

TS

State: T_1

Imaginary frequency: -605.6222

Absolute Gibbs free energy at 298 K: -390.455909 a.u.

C	1.182588	1.302530	-0.112211
C	-0.072090	1.720525	0.603749
C	1.899883	0.172090	0.099239
C	1.493209	-0.830543	1.054856
C	-3.276639	-0.391694	-0.142847
C	-1.810409	-0.069242	-0.145097
C	-1.397516	1.381052	-0.140438
C	-0.862208	-1.096800	-0.607927
C	-0.162284	-1.949615	0.219414
H	-0.049437	2.807968	0.738538
H	-0.118996	1.287222	1.606779
H	0.933169	-0.513598	1.925359
H	2.169535	-1.659115	1.240577
H	-3.458974	-1.423494	0.169571
H	-3.835705	0.277974	0.519008
H	-3.719340	-0.284915	-1.148741
H	-2.204123	1.972119	0.309122

H	-1.304976	1.745717	-1.178894
H	-0.592505	-1.081162	-1.667786
H	-0.536951	-2.147703	1.217728
H	0.418088	-2.750650	-0.226598
H	1.520203	1.977782	-0.896073
C	3.097162	-0.150860	-0.767154
H	2.926935	-1.070511	-1.339356
H	3.307780	0.651755	-1.476745
H	3.995123	-0.314046	-0.161998

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.544336 a.u.

C	-0.905186	1.415535	-0.127113
C	0.531022	1.791376	-0.451375
C	-1.563189	0.249418	-0.260917
C	-0.977216	-1.066022	-0.778138
C	2.464548	-0.786313	-0.655523
C	1.612144	-0.209113	0.444973
C	1.612180	1.292577	0.578293
C	0.605891	-0.863126	1.041209
C	-0.242209	-1.890442	0.335141
H	0.592467	2.882136	-0.522271
H	0.809184	1.409290	-1.439837
H	-0.247546	-0.857955	-1.565533
H	-1.773482	-1.666492	-1.233132
H	2.288413	-1.852720	-0.803882
H	2.312859	-0.277815	-1.615233
H	3.524151	-0.659018	-0.403877
H	2.576821	1.752532	0.338152
H	1.327703	1.609406	1.585838
H	0.092002	-0.339976	1.842710
H	0.325560	-2.698201	-0.133815
H	-0.961341	-2.354299	1.015738
H	-1.483825	2.232831	0.301190
C	-3.007554	0.148641	0.171740
H	-3.138073	-0.633315	0.929815
H	-3.378169	1.087701	0.587284
H	-3.649310	-0.129297	-0.672896

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.582366

C	-0.905186	1.415535	-0.127113
C	0.531022	1.791376	-0.451375
C	-1.563189	0.249418	-0.260917
C	-0.977216	-1.066022	-0.778138
C	2.464548	-0.786313	-0.655523
C	1.612144	-0.209113	0.444973
C	1.612180	1.292577	0.578293
C	0.605891	-0.863126	1.041209
C	-0.242209	-1.890442	0.335141
H	0.592467	2.882136	-0.522271
H	0.809184	1.409290	-1.439837
H	-0.247546	-0.857955	-1.565533
H	-1.773482	-1.666492	-1.233132
H	2.288413	-1.852720	-0.803882
H	2.312859	-0.277815	-1.615233
H	3.524151	-0.659018	-0.403877
H	2.576821	1.752532	0.338152
H	1.327703	1.609406	1.585838
H	0.092002	-0.339976	1.842710
H	0.325560	-2.698201	-0.133815
H	-0.961341	-2.354299	1.015738
H	-1.483825	2.232831	0.301190
C	-3.007554	0.148641	0.171740
H	-3.138073	-0.633315	0.929815
H	-3.378169	1.087701	0.587284
H	-3.649310	-0.129297	-0.672896

<u>Prod. 8</u>

TS I

State: Open shell S_0

Imaginary frequency: -382.6624

Absolute Gibbs free energy at 298 K: -390.489371 a.u.

C	2.899028	-0.369199	0.557785
C	1.642570	-0.010943	-0.190210
C	0.847737	-1.205418	-0.702927
C	1.314442	1.310833	-0.380806
C	0.174959	1.869252	-0.998022
C	-2.482731	-0.967483	-0.603360
C	-1.360381	-0.759366	0.372106
C	-0.210402	-1.740346	0.305911
C	-1.180579	0.402712	1.083843
C	-1.690293	1.664384	0.748113
H	3.603240	-0.904527	-0.093456
H	3.407099	0.512251	0.954018
H	2.689683	-1.043763	1.397556
H	1.551371	-2.012279	-0.944534
H	0.342574	-0.948449	-1.639838
H	2.003002	2.030537	0.059887
H	-0.495857	1.266824	-1.595071
H	0.130549	2.938732	-1.160804
H	-3.271782	-0.222302	-0.495409
H	-2.137302	-0.947088	-1.646153
H	-2.934091	-1.955668	-0.452089
H	-0.550126	-2.731704	-0.015034
H	0.253664	-1.860616	1.291319
H	-0.379093	0.396590	1.819461
H	-2.458114	1.789654	-0.004518
H	-1.480915	2.525255	1.370064

TS I

State: T_1

Imaginary frequency: -612.5362

Absolute Gibbs free energy at 298 K: -390.458657 a.u.

C	1.629737	-0.397184	0.000179
C	0.733675	-0.839672	1.130909
H	1.233856	-1.632984	1.700060
H	0.562051	-0.017164	1.829513
C	1.762402	0.907294	-0.361982
H	2.357519	1.115117	-1.249893
C	1.123576	2.036963	0.249029
H	0.902461	2.014787	1.308610
H	1.397613	3.020051	-0.120470
C	-0.639470	-1.393217	0.671299
H	-1.153320	-1.776695	1.572794
H	-0.489052	-2.276116	0.037255
C	-0.940087	1.999174	-0.364815
H	-1.145502	3.031722	-0.098755
H	-0.657187	1.832062	-1.397307
C	-1.581393	0.994376	0.329003
C	-1.555596	-0.430644	-0.043370
C	2.341792	-1.487615	-0.753221
H	1.637431	-2.213952	-1.177190
H	2.942180	-1.087252	-1.572745
H	3.007607	-2.054342	-0.089848
C	-2.755021	-1.009402	-0.736557
H	-3.140422	-0.331542	-1.503233
H	-2.524243	-1.971178	-1.206512
H	-3.585167	-1.190909	-0.031586
H	-2.063518	1.257946	1.276456

TS II

State: Open shell S_0

Imaginary frequency: -358.4633

Absolute Gibbs free energy at 298 K: -390.485065

C	-0.847247	1.340203	0.331977
C	0.344999	2.052799	-0.272199
C	-1.570715	0.277330	-0.155921
C	-1.290430	-0.422227	-1.356322
C	1.787069	0.071328	-0.458112

C	1.712165	1.440478	0.154922
C	1.240331	-1.075869	0.066305
C	0.691243	-2.027792	-0.817695
H	0.314699	3.107694	0.026581
H	0.286929	2.038027	-1.366562
H	-0.574561	-0.040898	-2.069785
H	-1.996958	-1.155743	-1.726425
H	2.524277	2.084554	-0.201540
H	1.773614	1.412404	1.246562
H	0.919662	-1.996161	-1.875463
H	0.214830	-2.927780	-0.446873
H	1.958589	0.074899	-1.534313
H	-1.166522	1.736416	1.293650
C	-2.739913	-0.241268	0.664864
H	-2.857619	0.313612	1.597442
H	-3.677006	-0.160403	0.104967
H	-2.605485	-1.299106	0.913710
C	1.011106	-1.275798	1.548552
H	-0.046946	-1.176749	1.806750
H	1.327075	-2.282199	1.840240
H	1.573767	-0.563673	2.152825

TS II

State: T_1

Imaginary frequency: -586.6677

Absolute Gibbs free energy at 298 K: -390.456300

C	3.077826	-0.497337	0.499726
C	1.800689	-0.125039	-0.224099
C	1.052876	-1.208266	-0.812729
C	1.368975	1.163408	-0.224669
C	0.064581	1.660196	-0.777702
C	-2.696139	-0.952525	-0.578348
C	-1.560909	-0.708023	0.387632
C	-0.566779	-1.647777	0.570304
C	-1.486736	0.623082	1.021492
C	-1.028784	1.862936	0.304126
H	3.799049	-0.964072	-0.179276
H	3.552278	0.375162	0.953065
H	2.876791	-1.222609	1.296964
H	1.524059	-2.186368	-0.834883
H	0.412333	-1.011055	-1.662431
H	1.984035	1.907508	0.277060
H	-0.317507	0.980461	-1.544484
H	0.220478	2.625876	-1.272444
H	-3.665487	-0.789181	-0.092324
H	-2.660251	-0.259774	-1.430058
H	-2.679497	-1.972368	-0.971213
H	-0.731884	-2.661294	0.215441
H	0.100443	-1.552858	1.418021
H	-1.997250	0.767934	1.972494
H	-1.893761	2.346650	-0.185123
H	-0.677420	2.592058	1.044785

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.543796 a.u.

C	2.980898	-0.173579	0.268082
C	1.572115	0.041960	-0.238612
C	0.851186	-1.253173	-0.611704
C	1.074427	1.290310	-0.301376
C	-0.311354	1.772258	-0.703501
C	-2.369069	-0.999412	-0.605148
C	-1.307873	-0.794886	0.444942
C	-0.172228	-1.788033	0.455533
C	-1.099720	0.359350	1.092567
C	-1.349423	1.710555	0.472430
H	3.607554	-0.645397	-0.498057
H	3.456583	0.762294	0.567741
H	2.986452	-0.849208	1.132427
H	1.602388	-2.028345	-0.796515
H	0.314451	-1.121024	-1.556704
H	1.742638	2.084548	0.029484

H	-0.701384	1.149838	-1.514628
H	-0.240778	2.793413	-1.094199
H	-3.058603	-0.156524	-0.669915
H	-1.946716	-1.173016	-1.602192
H	-2.959572	-1.890650	-0.361318
H	-0.478941	-2.802761	0.179974
H	0.311762	-1.838240	1.435449
H	-0.319925	0.359090	1.848916
H	-2.357748	1.845564	0.072452
H	-1.171933	2.518312	1.187797

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.486095 a.u.

C	1.614750	-0.250955	-0.008828
C	0.812896	-0.815808	1.143374
H	1.413661	-1.556566	1.682996
H	0.568273	-0.027339	1.860419
C	1.499941	1.018102	-0.418368
H	2.079357	1.321148	-1.288558
C	0.616107	2.085371	0.177924
H	0.679039	2.081830	1.271438
H	0.977645	3.065903	-0.148074
C	-0.500735	-1.490604	0.684392
H	-0.989096	-1.925114	1.575889
H	-0.273442	-2.345965	0.035712
C	-0.889393	1.974155	-0.227469
H	-1.386464	2.909456	0.052159
H	-0.936392	1.895668	-1.321157
C	-1.612065	0.820137	0.402648
C	-1.463459	-0.572077	-0.026136
C	2.525014	-1.224062	-0.715083
H	1.970824	-2.095813	-1.082164
H	3.027902	-0.762154	-1.567126
H	3.292509	-1.607368	-0.031935
C	-2.546858	-1.194433	-0.860628
H	-2.945017	-0.489123	-1.595814
H	-2.186577	-2.081599	-1.392312
H	-3.401638	-1.519022	-0.242192
H	-2.227783	1.037101	1.279754

M062X/6-311G(d,p)

Isoprene

Conformation: trans

State: S_0

Absolute Gibbs free energy at 298 K: -195.171811 a.u.

C	1.968208	0.000239	0.000052
H	1.984709	1.084264	0.000227
H	2.926531	-0.503771	0.000028
C	0.828235	-0.688986	-0.000092
H	0.865643	-1.775412	-0.000245
C	-0.518199	-0.099625	-0.000049
C	-0.638201	1.399573	0.000027
H	-0.150474	1.826577	-0.880520
H	-1.683590	1.706317	-0.000167
H	-0.150855	1.826445	0.880860
C	-1.591049	-0.894472	0.000007
H	-2.596757	-0.490697	0.000079
H	-1.489173	-1.974096	0.000069

Conformation: trans – 1allyl

State: T_1

Absolute Gibbs free energy at 298 K: -195.085990 a.u.

C	-2.019156	-0.082206	0.000001
H	-2.548455	0.119328	-0.925111
H	-2.548454	0.119329	0.925112
C	-0.720641	-0.751694	0.000000

H	-0.702910	-1.841167	0.000000
C	0.510075	-0.086014	-0.000000
C	0.520814	1.425908	-0.000000
H	0.001980	1.815748	0.878996
H	1.540152	1.811779	-0.000003
H	0.001974	1.815748	-0.878992
C	1.693673	-0.787493	-0.000000
H	2.649938	-0.281039	-0.000001
H	1.697191	-1.870732	-0.000000

Conformation: trans – 2allyl

State: T_1

Absolute Gibbs free energy at 298 K: -195.086761 a.u.

C	1.997561	-0.108772	-0.000003
H	2.093550	0.969875	-0.000013
H	2.911713	-0.686447	-0.000003
C	0.773136	-0.726326	0.000004
H	0.746412	-1.812885	0.000009
C	-0.462962	-0.069865	0.000005
C	-0.534872	1.434626	0.000002
H	-0.034690	1.851503	-0.880951
H	-1.568649	1.779616	0.000080
H	-0.034549	1.851514	0.880868
C	-1.714847	-0.834803	-0.000004
H	-2.230944	-1.061170	0.926876
H	-2.230936	-1.061162	-0.926890

Conformation: cis

State: S_0

Absolute Gibbs free energy at 298 K: -195.168143 a.u.

C	2.009802	-0.103398	0.213495
H	2.053925	0.786935	0.831583
H	2.939770	-0.623833	0.019710
C	0.853995	-0.544573	-0.274344
H	0.837373	-1.471216	-0.845358
C	-0.454815	0.111449	-0.067473
C	-1.620390	-0.815893	0.155723
H	-1.452425	-1.440435	1.037347
H	-2.549524	-0.262194	0.290380
H	-1.739785	-1.490028	-0.697832
C	-0.588114	1.437322	-0.095112
H	-1.548687	1.909089	0.077996
H	0.256488	2.082236	-0.307556

Conformation: cis - planar

State: T_1

None

Conformation: cis – 1allyl

State: T_1

Absolute Gibbs free energy at 298 K: -195.086634 a.u.

C	2.082952	-0.159016	-0.000000
H	2.624697	-0.003996	0.926270
H	2.624697	-0.003996	-0.926270
C	0.725486	-0.698645	-0.000000
H	0.607463	-1.782189	-0.000000
C	-0.439284	0.081515	-0.000000
C	-1.771075	-0.637075	0.000000
H	-1.866347	-1.275024	0.881605
H	-2.601083	0.069438	-0.000003
H	-1.866345	-1.275029	-0.881601
C	-0.393840	1.454237	-0.000000
H	-1.301262	2.044117	-0.000000
H	0.552749	1.980577	-0.000000

Conformation: cis – 2allyl

State: T_1

Absolute Gibbs free energy at 298 K: -195.088691 a.u.

C	-2.044813	-0.109249	0.000000
H	-2.166188	0.967287	0.000000

H	-2.938060	-0.718338	0.000000
C	-0.793837	-0.682413	-0.000000
H	-0.730507	-1.768131	-0.000000
C	0.411797	0.015996	-0.000000
C	1.733238	-0.698070	-0.000000
H	1.603185	-1.781576	-0.000001
H	2.326358	-0.419454	-0.877901
H	2.326357	-0.419455	0.877902
C	0.449538	1.483545	0.000000
H	0.521659	2.040405	-0.927574
H	0.521659	2.040405	0.927575

Intermediates

Combination: 1t-2t

TS

State: T_1

Imaginary frequency: -501.1344

Absolute Gibbs free energy at 298 K: -390.231725 a.u.

C	1.889859	1.598850	0.026485
C	1.840612	0.171622	-0.439388
C	0.703852	-0.358776	-0.959162
C	3.011386	-0.670553	-0.242745
C	4.156958	-0.284820	0.330723
C	-2.232364	1.388649	0.348554
C	-2.728013	-0.007774	0.070406
C	-4.062721	-0.122300	-0.460841
C	-1.979240	-1.113387	0.307739
C	-0.622819	-1.142238	0.866085
H	2.026689	1.651194	1.112245
H	2.730018	2.131176	-0.428455
H	0.970945	2.125700	-0.232085
H	0.702024	-1.363007	-1.368349
H	-0.144325	0.266854	-1.212863
H	2.919835	-1.694762	-0.597095
H	4.301388	0.723251	0.702373
H	4.986046	-0.971922	0.442116
H	-2.876028	1.881848	1.082515
H	-1.210692	1.401050	0.725616
H	-2.266920	1.991044	-0.564617
H	-4.494747	-1.092833	-0.663337
H	-4.652308	0.758374	-0.675364
H	-2.418340	-2.075496	0.054396
H	-0.122223	-2.096703	0.952319
H	-0.316422	-0.391404	1.583455

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.29453 a.u.

C	1.999678	1.549540	0.015063
C	1.888352	0.076814	-0.251644
C	0.526191	-0.478891	-0.538917
C	3.007667	-0.751753	-0.192042
C	4.285570	-0.347707	0.112176
C	-2.633514	1.415329	-0.012357
C	-2.837558	-0.084291	0.027893
C	-4.070143	-0.609829	-0.292522
C	-1.777149	-0.914409	0.395230
C	-0.393694	-0.440384	0.706883
H	2.266162	1.749960	1.059099
H	2.777558	2.005145	-0.605348
H	1.058316	2.061816	-0.193466
H	0.600124	-1.510346	-0.893978
H	0.045210	0.101264	-1.336971
H	2.847097	-1.806511	-0.403499
H	4.518425	0.684917	0.340252
H	5.102558	-1.055590	0.136674
H	-3.517323	1.915944	-0.407031
H	-2.438772	1.811049	0.987787

H	-1.781714	1.683851	-0.642683
H	-4.242265	-1.678801	-0.261976
H	-4.897740	0.024476	-0.581955
H	-1.953204	-1.986139	0.404005
H	0.058458	-1.067975	1.480744
H	-0.415292	0.580419	1.099765

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.294134 a.u.

C	2.006906	1.559899	0.009922
C	1.878347	0.093894	-0.282389
C	0.514901	-0.440734	-0.573024
C	2.981948	-0.756819	-0.195111
C	4.257821	-0.377759	0.139744
C	-2.618479	1.411305	0.012663
C	-2.824934	-0.088153	0.034368
C	-4.054056	-0.609199	-0.297908
C	-1.766668	-0.923028	0.406528
C	-0.384728	-0.453661	0.704654
H	2.251438	1.739377	1.063467
H	2.806816	2.012435	-0.583897
H	1.078987	2.090402	-0.212878
H	0.573257	-1.457606	-0.969347
H	0.015909	0.175863	-1.329309
H	2.806765	-1.807365	-0.416286
H	4.503600	0.649398	0.379016
H	5.062617	-1.099154	0.174163
H	-3.501545	1.918479	-0.375225
H	-2.422260	1.793342	1.017850
H	-1.766435	1.687160	-0.614122
H	-4.225887	-1.678608	-0.282573
H	-4.882010	0.028651	-0.578681
H	-1.943647	-1.994576	0.402427
H	0.092924	-1.106655	1.439631
H	-0.396873	0.554388	1.129089

Combination: 1c-2c

TS

State: T_1

Imaginary frequency: -521.8090

Absolute Gibbs free energy at 298 K: -390.233243 a.u.

C	0.579815	-1.629977	1.143004
C	1.436050	-0.474726	0.711552
C	1.370899	0.734900	1.321352
C	2.265909	-0.701191	-0.472864
C	2.753804	0.242654	-1.284528
C	-3.138467	-0.697096	0.023846
C	-1.915718	0.082639	-0.382613
C	-1.249895	-0.343926	-1.586025
C	-1.472904	1.121081	0.370946
C	-0.292568	1.927221	0.095205
H	-0.086628	-1.933003	0.325467
H	1.197945	-2.498114	1.394965
H	-0.034341	-1.373314	2.006546
H	2.090461	1.512951	1.095691
H	0.783743	0.859896	2.223573
H	2.456775	-1.743560	-0.720949
H	2.566660	1.297382	-1.113488
H	3.359577	-0.016504	-2.143714
H	-2.879052	-1.742502	0.222186
H	-3.598736	-0.281309	0.920462
H	-3.882636	-0.697147	-0.777964
H	-0.319509	0.093524	-1.917068
H	-1.680316	-1.131199	-2.190948
H	-2.030234	1.368524	1.270406
H	-0.167478	2.860333	0.629285
H	0.202225	1.854575	-0.863707

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.296099 a.u.

C	-0.810861	1.557637	-1.436093
C	-1.389983	0.639616	-0.406642
C	-1.152007	0.973379	1.040201
C	-2.090446	-0.507012	-0.777190
C	-2.652709	-1.428020	0.076806
C	3.242082	0.049847	-0.534980
C	1.913372	-0.418511	0.024134
C	1.351928	-1.578227	-0.457082
C	1.308893	0.387293	0.995784
C	-0.007063	0.132022	1.658969
H	0.274634	1.642105	-1.310511
H	-1.012770	1.207814	-2.449369
H	-1.221222	2.568957	-1.331570
H	-2.064001	0.809943	1.623998
H	-0.898273	2.034000	1.133367
H	-2.189163	-0.691224	-1.844541
H	-2.606985	-1.319126	1.153318
H	-3.180721	-2.289611	-0.308188
H	3.102394	0.922750	-1.178653
H	3.924594	0.337112	0.267346
H	3.719906	-0.731141	-1.126676
H	0.385399	-1.934718	-0.126178
H	1.866660	-2.167306	-1.205474
H	1.823298	1.302747	1.278390
H	0.067935	0.385246	2.721745
H	-0.270923	-0.925694	1.599547

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.296348 a.u.

C	0.658707	1.271223	-1.639683
C	1.327707	0.333598	-0.687334
C	1.066180	-1.125850	-0.870733
C	2.151917	0.802274	0.344532
C	2.803206	0.033930	1.273394
C	-3.251453	0.515483	0.000323
C	-1.885736	0.032632	0.444700
C	-1.176354	0.782710	1.359779
C	-1.379708	-1.130410	-0.135468
C	-0.020395	-1.685388	0.108358
H	-0.414460	1.053027	-1.694205
H	0.788590	2.314142	-1.347248
H	1.056897	1.143346	-2.653853
H	1.982620	-1.700674	-0.709257
H	0.738399	-1.320052	-1.895834
H	2.262797	1.881857	0.419312
H	2.751077	-1.047963	1.266773
H	3.410448	0.491112	2.042681
H	-3.165746	1.145995	-0.889270
H	-3.903316	-0.323446	-0.248458
H	-3.734929	1.103760	0.781091
H	-0.196163	0.494467	1.712755
H	-1.603167	1.689384	1.771011
H	-2.004563	-1.651739	-0.855195
H	-0.042888	-2.770893	-0.018422
H	0.309976	-1.483534	1.130916

<u>Combination: 1t-1c</u>

TS

State: T_1

Imaginary frequency: -524.2442

Absolute Gibbs free energy at 298 K: -390.236705 a.u.

C	2.587901	-1.600824	0.285141
C	1.717119	-0.565246	-0.365642
C	0.498460	-0.881026	-0.877245
C	2.150316	0.824770	-0.359259
C	3.290700	1.278510	0.174015

C	-3.278423	-1.144675	-0.182291
C	-2.227661	-0.147495	0.200844
C	-1.053623	-0.681390	0.917513
C	-2.337007	1.172344	-0.122051
C	-1.377642	2.169197	0.189235
H	3.582874	-1.619981	-0.169045
H	2.724399	-1.380537	1.349193
H	2.148445	-2.594174	0.193726
H	0.198200	-1.915894	-0.995712
H	-0.085910	-0.137048	-1.407024
H	1.469265	1.530255	-0.830456
H	4.004311	0.616359	0.651328
H	3.544049	2.330540	0.140643
H	-4.090828	-0.681332	-0.742414
H	-2.843955	-1.942958	-0.795172
H	-3.697580	-1.626500	0.707944
H	-1.066502	-1.725033	1.207969
H	-0.461809	-0.027637	1.543970
H	-3.225877	1.486007	-0.662025
H	-0.483975	1.947376	0.755233
H	-1.535941	3.195573	-0.109715

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.297583 a.u.

C	2.244868	-1.593236	0.182529
C	1.712011	-0.259305	-0.251424
C	0.269044	-0.172809	-0.646343
C	2.519293	0.877314	-0.236505
C	3.833499	0.919656	0.163299
C	-2.790474	-1.627414	-0.126634
C	-2.120811	-0.317811	0.147842
C	-0.678206	-0.364367	0.562678
C	-2.788687	0.891097	-0.029298
C	-2.260518	2.146887	0.169897
H	3.176048	-1.834820	-0.338912
H	2.467691	-1.606802	1.255693
H	1.527755	-2.390837	-0.019901
H	0.038127	-0.944873	-1.391791
H	0.054925	0.794218	-1.108464
H	2.061180	1.806063	-0.569600
H	4.352238	0.035955	0.513367
H	4.392198	1.845208	0.143148
H	-3.800403	-1.495135	-0.516609
H	-2.217166	-2.216397	-0.852543
H	-2.850745	-2.233368	0.785097
H	-0.462815	-1.327813	1.036469
H	-0.456925	0.409267	1.303923
H	-3.822690	0.831220	-0.361380
H	-1.239497	2.296338	0.498613
H	-2.860029	3.031706	0.006647

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.297493 a.u.

C	2.272587	-1.599624	0.163189
C	1.706791	-0.282128	-0.277460
C	0.265892	-0.230055	-0.665367
C	2.475471	0.882989	-0.232249
C	3.778767	0.965012	0.189617
C	-2.788335	-1.618304	-0.101976
C	-2.112184	-0.312625	0.174966
C	-0.671188	-0.365098	0.573226
C	-2.768852	0.901588	-0.024105
C	-2.225069	2.154182	0.137962
H	3.221182	-1.810857	-0.339437
H	2.474293	-1.608664	1.240921
H	1.584189	-2.418176	-0.054711
H	0.029546	-1.044000	-1.361056
H	0.034100	0.711566	-1.169587
H	1.991465	1.798954	-0.564813
H	4.320287	0.095910	0.542004

H	4.308455	1.907725	0.182527
H	-3.806234	-1.481058	-0.468748
H	-2.231104	-2.195656	-0.850202
H	-2.827710	-2.238493	0.800874
H	-0.455575	-1.313968	1.074880
H	-0.425241	0.433587	1.277737
H	-3.806273	0.845393	-0.346025
H	-1.198021	2.300600	0.449106
H	-2.816637	3.041515	-0.040281

Combination: 2t-2t

TS

State: T_1

Imaginary frequency: -515.8024

Absolute Gibbs free energy at 298 K: -390.230012 a.u.

C	-1.406605	-0.537368	-0.559551
C	-0.575314	0.421088	-1.040907
C	-2.737729	-0.291493	-0.023131
C	-3.466651	-1.302527	0.472424
C	1.967452	-1.436378	0.223153
C	2.726993	-0.136943	0.101789
C	4.102433	-0.213645	-0.261402
C	2.134328	1.067959	0.330973
C	0.732845	1.284656	0.736037
H	-0.933970	1.426697	-1.224904
H	0.361738	0.152342	-1.513677
H	-3.084019	-2.317049	0.479621
H	-4.458877	-1.141833	0.876797
H	2.584879	-2.192379	0.712706
H	1.045268	-1.320318	0.791285
H	1.703039	-1.821852	-0.766999
H	4.697585	0.683789	-0.365497
H	4.580212	-1.167463	-0.438630
H	2.751557	1.956584	0.216858
H	0.340292	2.290513	0.659694
H	0.316424	0.691864	1.544017
H	-1.054390	-1.564558	-0.512624
C	-3.259084	1.121366	-0.035217
H	-2.592761	1.784084	0.524643
H	-3.316478	1.505197	-1.057448
H	-4.252508	1.174099	0.409152

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.290846 a.u.

C	1.740479	-0.738681	0.361143
C	0.444062	-0.045280	0.633916
C	2.943130	-0.098843	0.057377
C	4.078900	-0.826166	-0.224702
C	-3.004733	-1.413654	-0.043406
C	-2.943105	0.098864	-0.057309
C	-4.078823	0.826213	0.224909
C	-1.740485	0.738667	-0.361250
C	-0.444119	0.045214	-0.634066
H	0.611942	0.965773	1.015105
H	-0.116707	-0.582608	1.405603
H	4.061879	-1.909146	-0.211766
H	5.015755	-0.341212	-0.465838
H	-3.979160	-1.757789	0.302411
H	-2.837164	-1.821476	-1.043495
H	-2.241862	-1.836353	0.614976
H	-4.061777	1.909193	0.211995
H	-5.015692	0.341281	0.466033
H	-1.730557	1.825006	-0.351019
H	0.116668	0.582506	-1.405765
H	-0.612033	-0.965849	-1.015210
H	1.730571	-1.825020	0.350833
C	3.004703	1.413669	0.043401
H	2.241775	1.836334	-0.614935
H	2.837197	1.821521	1.043490

H	3.979098	1.757828	-0.302490

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.290261 a.u.

C	-1.730363	-0.745435	-0.383969
C	-0.435474	-0.059135	-0.647910
C	-2.927005	-0.098596	-0.059764
C	-4.060301	-0.819032	0.239043
C	2.980151	-1.414053	0.052207
C	2.927005	0.098599	0.059767
C	4.060294	0.819042	-0.239049
C	1.730363	0.745430	0.383987
C	0.435477	0.059124	0.647927
H	-0.592673	0.946312	-1.046344
H	0.145651	-0.610335	-1.392425
H	-4.047061	-1.902197	0.233896
H	-4.994252	-0.329409	0.482325
H	3.951556	-1.765276	-0.294946
H	2.812692	-1.816100	1.054664
H	2.213107	-1.836037	-0.601893
H	4.047048	1.902206	-0.233900
H	4.994242	0.329424	-0.482353
H	1.724858	1.831682	0.365245
H	-0.145649	0.610319	1.392444
H	0.592681	-0.946324	1.046358
H	-1.724862	-1.831687	-0.365221
C	-2.980147	1.414056	-0.052229
H	-2.213109	1.836047	0.601872
H	-2.812676	1.816088	-1.054690
H	-3.951555	1.765287	0.294908

<u>Combination: 1t-2c</u>

TS

State: T_1

Imaginary frequency: -503.8259

Absolute Gibbs free energy at 298 K: -390.237124 a.u.

C	0.918383	0.435644	-1.638870
C	1.512061	-0.411198	-0.553337
C	1.239246	-1.738475	-0.449043
C	2.310201	0.236194	0.475457
C	2.502002	1.556745	0.585161
C	-2.840474	1.028602	-0.631517
C	-1.853629	0.312080	0.252463
C	-1.123964	1.123751	1.190665
C	-1.667689	-1.028578	0.136009
C	-0.724367	-1.827231	0.901608
H	0.284005	1.218719	-1.206846
H	1.703204	0.933985	-2.216577
H	0.306957	-0.162797	-2.314297
H	1.753317	-2.350010	0.284257
H	0.709004	-2.260255	-1.237147
H	2.756313	-0.423941	1.216313
H	2.073709	2.257300	-0.122468
H	3.098820	1.971295	1.387866
H	-2.328909	1.767769	-1.257437
H	-3.370976	0.334939	-1.284197
H	-3.577192	1.570718	-0.031566
H	-0.355888	0.717872	1.830904
H	-1.357019	2.175591	1.291714
H	-2.256604	-1.556882	-0.608892
H	-0.818358	-2.905397	0.874956
H	-0.251007	-1.414113	1.781834

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.295411 a.u.

C	0.907928	-0.417249	1.621741
C	1.411810	0.369848	0.449706

C	0.872589	1.747032	0.193054
C	2.319493	-0.196497	-0.450809
C	2.803261	-1.478153	-0.393505
C	-3.039103	-0.928143	0.495284
C	-1.881158	-0.355982	-0.296816
C	-1.199047	-1.174729	-1.169392
C	-1.534424	0.976515	-0.058044
C	-0.402140	1.719509	-0.692214
H	0.384441	-1.321056	1.288749
H	1.735689	-0.737525	2.264076
H	0.210527	0.167309	2.223007
H	1.626931	2.356353	-0.314283
H	0.633704	2.241853	1.139998
H	2.658240	0.437710	-1.268306
H	2.499448	-2.166371	0.385462
H	3.508026	-1.842165	-1.128658
H	-2.716681	-1.182538	1.509083
H	-3.854982	-0.207797	0.577223
H	-3.427920	-1.833971	0.029286
H	-0.324817	-0.842463	-1.712805
H	-1.516643	-2.198106	-1.324498
H	-2.119812	1.521985	0.677859
H	-0.708490	2.753494	-0.881505
H	-0.142922	1.280380	-1.658708

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.295498 a.u.

C	0.910321	-0.532883	1.572251
C	1.380983	0.330924	0.441451
C	0.794642	1.698951	0.292757
C	2.366979	-0.104050	-0.454570
C	3.001901	-1.316683	-0.433357
C	-3.075001	-0.999725	0.415893
C	-1.905671	-0.370949	-0.313290
C	-1.132328	-1.152595	-1.141303
C	-1.633712	0.977422	-0.065099
C	-0.478258	1.736976	-0.617359
H	0.804995	-1.576988	1.269105
H	1.621080	-0.497990	2.407599
H	-0.057582	-0.190893	1.943960
H	1.531313	2.373788	-0.152378
H	0.527260	2.105233	1.273196
H	2.654724	0.600471	-1.233411
H	2.781561	-2.065002	0.317464
H	3.757031	-1.561374	-1.167858
H	-2.791824	-1.259923	1.439827
H	-3.920095	-0.311129	0.469976
H	-3.407911	-1.910861	-0.081990
H	-0.268228	-0.766756	-1.664260
H	-1.370431	-2.198612	-1.289236
H	-2.284240	1.504838	0.627291
H	-0.758389	2.787150	-0.737891
H	-0.198403	1.363720	-1.605634

Combination: 2c-2t

TS

State: T_1

Imaginary frequency: -518.8135

Absolute Gibbs free energy at 298 K: -390.226773 a.u.

C	-1.895036	-1.021726	-0.039395
C	-0.589005	-1.253796	-0.314842
C	-2.562199	0.271312	-0.195525
C	-1.882880	1.422973	-0.290778
C	2.714403	-1.175182	-0.593917
C	2.599997	0.233153	-0.056728
C	3.526968	1.190981	-0.534812
C	1.653969	0.580570	0.866594
C	0.644071	-0.310545	1.474746
H	-0.012369	-0.550506	-0.906488

H	-0.178859	-2.250612	-0.207434
H	-0.799388	1.454072	-0.245522
H	-2.400726	2.366319	-0.418612
H	3.763081	-1.474165	-0.646706
H	2.184152	-1.893017	0.030994
H	2.303265	-1.239803	-1.605252
H	3.488935	2.216859	-0.192891
H	4.290389	0.920195	-1.251535
H	1.655406	1.613188	1.212373
H	-0.245210	0.155585	1.878274
H	0.975997	-1.203081	1.997486
H	-2.495109	-1.826613	0.377969
C	-4.069542	0.238200	-0.212179
H	-4.432161	-0.373810	-1.042469
H	-4.452161	-0.209432	0.709757
H	-4.489712	1.239191	-0.308936

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.291467 a.u.

C	1.745589	0.666350	-0.470304
C	0.403417	0.067423	-0.751033
C	2.871030	-0.060383	-0.057728
C	2.857913	-1.424534	0.096935
C	-2.958626	1.433708	0.221255
C	-2.945068	-0.073098	0.075869
C	-4.114878	-0.735276	-0.227317
C	-1.751999	-0.773771	0.258555
C	-0.423742	-0.148125	0.542420
H	0.507601	-0.893298	-1.265173
H	-0.164862	0.717899	-1.421569
H	1.970944	-2.015063	-0.093736
H	3.745533	-1.956811	0.413544
H	-3.934801	1.839089	-0.043941
H	-2.737436	1.729475	1.249933
H	-2.210015	1.902153	-0.422313
H	-4.132199	-1.813762	-0.326666
H	-5.045089	-0.202123	-0.373913
H	-1.777836	-1.853221	0.137928
H	0.159045	-0.783887	1.215592
H	-0.543771	0.816056	1.044240
H	1.840453	1.745349	-0.548412
C	4.139035	0.715565	0.231199
H	4.430624	1.315818	-0.633436
H	3.990850	1.397259	1.072019
H	4.964942	0.047912	0.476800

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.291499 a.u.

C	1.747340	-0.648124	0.530845
C	0.415052	-0.039449	0.801481
C	2.860783	0.059269	0.050905
C	2.839708	1.413048	-0.167654
C	-2.953131	-1.435353	-0.273657
C	-2.939747	0.066386	-0.085055
C	-4.108398	0.721300	0.227156
C	-1.741751	0.771471	-0.239486
C	-0.414852	0.155769	-0.510850
H	0.519412	0.934318	1.288920
H	-0.162285	-0.672618	1.479228
H	1.958830	2.012003	0.025339
H	3.715715	1.930618	-0.536898
H	-3.937080	-1.844739	-0.046099
H	-2.704288	-1.703277	-1.303570
H	-2.223222	-1.923212	0.377218
H	-4.123429	1.796001	0.362273
H	-5.042775	0.187623	0.342529
H	-1.766882	1.845204	-0.073779
H	0.175161	0.788256	-1.180754
H	-0.520764	-0.816448	-0.997806
H	1.840667	-1.724673	0.638993

C	4.119853	-0.730003	-0.239502
H	4.424838	-1.307245	0.636082
H	3.953155	-1.434424	-1.057942
H	4.943802	-0.073262	-0.518829

Combination: 1t-1t

TS

State: T_1

Imaginary frequency: -502.0692

Absolute Gibbs free energy at 298 K: -390.233463 a.u.

C	2.216511	1.406800	-0.405296
C	2.055377	-0.035306	-0.025950
C	0.687919	-0.572281	0.168163
C	3.142551	-0.907048	0.105209
C	4.475350	-0.618529	-0.061443
C	-2.686869	-0.040920	1.579955
C	-2.133016	0.385757	0.251078
C	-0.964993	1.079017	0.164710
C	-2.807804	-0.046926	-0.962342
C	-3.914165	-0.798657	-1.008855
H	1.760567	1.600618	-1.382981
H	1.709920	2.058293	0.312551
H	3.260807	1.709250	-0.457001
H	0.420623	-0.938108	1.155801
H	0.244462	-1.139928	-0.647023
H	2.893410	-1.931311	0.374586
H	4.832820	0.365185	-0.334329
H	5.221899	-1.387632	0.081696
H	-2.694842	-1.132951	1.665009
H	-2.092022	0.362987	2.399461
H	-3.719420	0.298281	1.703472
H	-0.515710	1.515128	1.049193
H	-0.625121	1.458917	-0.792175
H	-2.355759	0.280201	-1.896075
H	-4.405757	-1.151500	-0.109416
H	-4.361048	-1.078865	-1.954152

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.297711 a.u.

C	-2.242311	-1.657557	-0.046267
C	-1.896445	-0.215345	-0.274442
C	-0.472399	0.119743	-0.601047
C	-2.856516	0.785957	-0.133877
C	-4.169498	0.591697	0.222191
C	2.242440	1.657542	0.046295
C	1.896398	0.215342	0.274361
C	0.472341	-0.119677	0.600890
C	2.856443	-0.785971	0.133908
C	4.169493	-0.591716	-0.222034
H	-3.137463	-1.942599	-0.606828
H	-1.426604	-2.313451	-0.355479
H	-2.450560	-1.857524	1.011298
H	-0.394722	1.163663	-0.918293
H	-0.120018	-0.500033	-1.435257
H	-2.529471	1.806342	-0.321143
H	-4.564093	-0.394392	0.432777
H	-4.852402	1.425703	0.307445
H	2.451333	1.857414	-1.011158
H	1.426610	2.313501	0.355009
H	3.137297	1.942554	0.607354
H	0.119956	0.500081	1.435112
H	0.394614	-1.163604	0.918113
H	2.529376	-1.806376	0.321016
H	4.564111	0.394384	-0.432516
H	4.852356	-1.425750	-0.307314

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.297632 a.u.

C	-2.254105	1.665128	0.031437
C	-1.887722	0.234657	0.296269
C	-0.462944	-0.074431	0.622916
C	-2.827453	-0.787467	0.148634
C	-4.137009	-0.621238	-0.227184
C	2.254104	-1.665128	-0.031440
C	1.887721	-0.234655	-0.296266
C	0.462943	0.074434	-0.622912
C	2.827453	0.787466	-0.148632
C	4.137011	0.621233	0.227180
H	-3.149654	1.953573	0.589850
H	-1.445245	2.339868	0.316949
H	-2.472726	1.832760	-1.029848
H	-0.372740	-1.092900	1.011237
H	-0.090624	0.607088	1.395950
H	-2.484189	-1.799230	0.353598
H	-4.545843	0.355371	-0.454598
H	-4.805309	-1.467534	-0.307606
H	2.472747	-1.832758	1.029841
H	1.445235	-2.339865	-0.316933
H	3.149639	-1.953577	-0.589872
H	0.090622	-0.607083	-1.395946
H	0.372740	1.092904	-1.011232
H	2.484192	1.799231	-0.353592
H	4.545845	-0.355376	0.454588
H	4.805312	1.467529	0.307601

<u>Combination: 2c-2c</u>

TS

State: T_1

Imaginary frequency: -550.6615

Absolute Gibbs free energy at 298 K: -390.230312 a.u.

C	-1.959104	-1.000457	-0.222121
C	-0.663294	-1.151981	-0.592102
C	-2.661351	0.280695	-0.148471
C	-2.014232	1.453792	-0.106117
C	3.602141	1.211727	-0.495597
C	2.674140	0.139647	0.013228
C	2.993847	-1.216917	-0.325738
C	1.585941	0.452718	0.763602
C	0.623173	-0.517210	1.288128
H	-0.126608	-0.356636	-1.096521
H	-0.228217	-2.141593	-0.658438
H	-0.931140	1.507022	-0.111281
H	-2.557346	2.390568	-0.065358
H	3.668422	1.178229	-1.586874
H	3.262258	2.204880	-0.201628
H	4.613305	1.063868	-0.105634
H	2.403629	-2.048214	0.030104
H	3.852138	-1.437144	-0.946304
H	1.396592	1.500251	0.981918
H	-0.216864	-0.140200	1.855691
H	0.953937	-1.515680	1.544893
H	-2.519124	-1.875415	0.098860
C	-4.166257	0.205555	-0.092695
H	-4.560599	-0.287021	-0.985587
H	-4.487476	-0.385164	0.770210
H	-4.612929	1.196836	-0.016753

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.292446 a.u.

C	1.750461	-0.721956	0.357316
C	0.382354	-0.190246	0.646944
C	2.874048	0.073318	0.092157
C	2.833268	1.445487	0.113964
C	-4.172173	0.633965	0.236345
C	-2.874041	-0.073304	-0.092158

C	-2.833292	-1.445486	-0.113998
C	-1.750439	0.721948	-0.357231
C	-0.382319	0.190236	-0.646845
H	0.438398	0.691684	1.293025
H	-0.205507	-0.935963	1.187775
H	1.924661	1.988405	0.340965
H	3.719604	2.031704	-0.091528
H	-4.079187	1.198017	1.167408
H	-4.438012	1.340707	-0.552818
H	-4.992316	-0.075145	0.349376
H	-1.924697	-1.988426	-0.340991
H	-3.719653	-2.031684	0.091440
H	-1.869948	1.800106	-0.304600
H	0.205537	0.935966	-1.187666
H	-0.438356	-0.691695	-1.292925
H	1.869997	-1.800111	0.304699
C	4.172146	-0.633960	-0.236453
H	4.437759	-1.341119	0.552411
H	4.079245	-1.197556	-1.167803
H	4.992403	0.075095	-0.349010

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.291955 a.u.

C	1.746067	0.717365	-0.365737
C	0.386560	0.182272	-0.654454
C	2.873286	-0.074728	-0.094899
C	2.836573	-1.445499	-0.109237
C	-4.166770	-0.639408	-0.236021
C	-2.873285	0.074731	0.094889
C	-2.836569	1.445500	0.109217
C	-1.746062	-0.717364	0.365717
C	-0.386555	-0.182272	0.654434
H	0.442565	-0.711617	-1.281925
H	-0.206908	0.918850	-1.201479
H	1.930089	-1.992972	-0.333836
H	3.724062	-2.027887	0.102377
H	-4.067669	-1.205762	-1.165153
H	-4.431743	-1.345358	0.554144
H	-4.989919	0.065415	-0.353795
H	-1.930082	1.992972	0.333810
H	-3.724057	2.027889	-0.102398
H	-1.854866	-1.794948	0.282898
H	0.206913	-0.918852	1.201457
H	-0.442558	0.711616	1.281906
H	1.854871	1.794949	-0.282923
C	4.166759	0.639405	0.236072
H	4.431527	1.345705	-0.553848
H	4.067761	1.205368	1.165454
H	4.989997	-0.065385	0.353418

Combination: 2t-1c

TS

State: T_1

Imaginary frequency: -527.9047

Absolute Gibbs free energy at 298 K: -390.235354 a.u.

C	2.457154	1.297558	-0.464049
C	2.713956	-0.128901	-0.054545
C	3.883205	-0.502531	0.485890
C	1.650733	-1.103406	-0.255828
C	0.418481	-0.809919	-0.738994
C	-1.912687	2.027676	0.072596
C	-2.027973	0.547851	0.279386
C	-0.943891	-0.081314	1.056494
C	-3.055846	-0.172937	-0.250010
C	-3.234581	-1.572803	-0.108165
H	1.592673	1.704068	0.069576
H	2.237349	1.361049	-1.533294
H	3.321011	1.926390	-0.250868
H	4.060208	-1.531050	0.779856

H	4.688033	0.205622	0.642971
H	1.865358	-2.119886	0.062254
H	-0.302804	-1.592281	-0.937984
H	0.200985	0.154096	-1.185167
H	-2.719623	2.413613	-0.550497
H	-1.930376	2.554041	1.033283
H	-0.956485	2.278124	-0.402672
H	-1.097772	-1.041826	1.528144
H	-0.217706	0.564320	1.535091
H	-3.801817	0.366648	-0.826586
H	-2.552477	-2.182633	0.466667
H	-4.077864	-2.067941	-0.567412

Min

State: T_1

Absolute Gibbs free energy at 298 K: -390.294044 a.u.

C	-2.602561	1.312959	0.342442
C	-2.674103	-0.167346	0.032785
C	-3.865238	-0.714770	-0.390902
C	-1.535593	-0.959675	0.189995
C	-0.190153	-0.444480	0.589928
C	2.064327	1.999359	-0.137679
C	1.999245	0.507074	-0.227907
C	0.681575	-0.083986	-0.639768
C	3.088434	-0.290234	0.112542
C	3.127046	-1.666374	0.090486
H	-1.786231	1.795285	-0.201327
H	-2.429850	1.480983	1.408656
H	-3.532447	1.810965	0.068811
H	-3.943276	-1.773138	-0.607828
H	-4.752774	-0.108862	-0.518310
H	-1.618151	-2.016419	-0.047242
H	0.346702	-1.193395	1.178964
H	-0.287275	0.443513	1.221763
H	3.013296	2.343183	0.275523
H	1.934758	2.455156	-1.126504
H	1.254438	2.389199	0.490969
H	0.823698	-0.981172	-1.249051
H	0.131740	0.631548	-1.259903
H	3.989709	0.228875	0.430904
H	2.273870	-2.261237	-0.210530
H	4.023919	-2.199645	0.373575

Min

State: Open shell S_0

Absolute Gibbs free energy at 298 K: -390.293842 a.u.

C	-2.603193	1.304290	0.393324
C	-2.669433	-0.165529	0.037307
C	-3.855355	-0.704021	-0.404951
C	-1.525838	-0.959228	0.173319
C	-0.184621	-0.451436	0.571940
C	2.064061	2.000636	-0.154268
C	1.999236	0.508717	-0.252448
C	0.689686	-0.081096	-0.668845
C	3.076647	-0.291556	0.125545
C	3.103125	-1.666363	0.129039
H	-1.799396	1.809390	-0.148805
H	-2.413061	1.439778	1.461147
H	-3.540922	1.803827	0.151153
H	-3.927353	-1.754625	-0.658893
H	-4.747393	-0.100080	-0.508578
H	-1.602779	-2.005742	-0.107952
H	0.360608	-1.204598	1.147658
H	-0.273674	0.434833	1.206159
H	3.016510	2.342841	0.252205
H	1.922386	2.464028	-1.137452
H	1.260874	2.384468	0.487341
H	0.830344	-0.979014	-1.276242
H	0.132487	0.634100	-1.281298
H	3.974861	0.226186	0.454477
H	2.251737	-2.259279	-0.181119
H	3.988875	-2.202588	0.440424

Cycloadduct formation

Prod. 2

TS

State: Open shell S_0

Imaginary frequency: -543.7762

Absolute Gibbs free energy at 298 K: -390.289406 a.u.

C	-1.266534	0.024385	1.656650
C	-1.190164	0.410012	0.209737
C	-0.756238	1.821167	-0.135457
C	-1.690544	-0.461363	-0.779779
C	-2.088043	-1.747634	-0.574283
C	1.266525	0.024376	-1.656649
C	1.190161	0.410017	-0.209739
C	0.756229	1.821172	0.135446
C	1.690551	-0.461348	0.779781
C	2.088058	-1.747618	0.574293
H	-2.312533	-0.042948	1.978437
H	-0.803019	-0.950885	1.834037
H	-0.765747	0.756151	2.293274
H	-1.293754	2.579848	0.444396
H	-0.956174	2.017183	-1.191858
H	-1.711451	-0.079490	-1.798396
H	-2.089820	-2.195994	0.411346
H	-2.424437	-2.363384	-1.397842
H	0.803003	-0.950893	-1.834025
H	0.765741	0.756140	-2.293278
H	2.312522	-0.042967	-1.978438
H	1.293741	2.579851	-0.444413
H	0.956163	2.017196	1.191845
H	1.711463	-0.079466	1.798395
H	2.089832	-2.195985	-0.411334
H	2.424460	-2.363359	1.397854

TS

State: T_1

Imaginary frequency: -776.5710

Absolute Gibbs free energy at 298 K: -390.233021 a.u.

C	-1.107816	-0.017750	1.662411
C	-1.011937	0.343015	0.192108
C	-0.825852	1.836354	-0.092493
C	-1.686697	-0.475199	-0.719635
C	-2.035566	-1.870350	-0.456726
C	1.092926	0.064367	-1.670387
C	0.928415	0.384651	-0.205795
C	0.696229	1.862368	0.104530
C	1.675616	-0.436825	0.731543
C	2.241132	-1.624378	0.462788
H	-2.138622	0.120344	2.002808
H	-0.827483	-1.058442	1.834752
H	-0.466428	0.618315	2.275369
H	-1.405954	2.485616	0.568618
H	-1.102736	2.065781	-1.123661
H	-1.851641	-0.088978	-1.725778
H	-1.313731	-2.668775	-0.597700
H	-3.044590	-2.159824	-0.183655
H	0.807624	-0.966018	-1.894060
H	0.477035	0.719550	-2.289401
H	2.138908	0.202362	-1.965856
H	1.247748	2.546608	-0.546195
H	0.964377	2.090737	1.138214
H	1.744374	-0.058205	1.749157
H	2.221858	-2.061125	-0.528745
H	2.750559	-2.185463	1.236069

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.340339 a.u.

C	-1.026579	-0.005298	1.661064
C	-0.777146	0.280925	0.183965
C	-0.766963	1.812786	-0.081986
C	-1.655859	-0.537212	-0.714773
C	-2.430684	-1.554969	-0.354370
C	1.026579	-0.005298	-1.661064
C	0.777146	0.280925	-0.183965
C	0.766963	1.812786	0.081986
C	1.655859	-0.537212	0.714773
C	2.430684	-1.554969	0.354370
H	-2.080335	0.163420	1.895909
H	-0.771923	-1.036097	1.918248
H	-0.433086	0.655717	2.296284
H	-1.351585	2.420699	0.610253
H	-1.072404	2.051679	-1.102286
H	-1.641412	-0.251832	-1.764539
H	-2.501872	-1.895378	0.672169
H	-3.027727	-2.085603	-1.086514
H	0.771923	-1.036097	-1.918248
H	0.433086	0.655717	-2.296284
H	2.080335	0.163420	-1.895909
H	1.351585	2.420699	-0.610253
H	1.072404	2.051679	1.102286
H	1.641412	-0.251832	1.764539
H	2.501872	-1.895378	-0.672169
H	3.027727	-2.085603	1.086514

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.245159 a.u.

C	1.125979	-0.038861	1.666047
C	0.893671	-0.246936	0.166845
C	1.062660	-1.736155	-0.218578
C	1.647263	0.763662	-0.630867
C	1.550766	2.188635	-0.343117
C	-0.947146	-0.023674	-1.642438
C	-0.665785	-0.397968	-0.191722
C	-0.459329	-1.932186	-0.052922
C	-1.625543	0.232697	0.768640
C	-2.530486	1.165705	0.488077
H	2.195797	-0.107790	1.879295
H	0.772232	0.944025	1.986029
H	0.614663	-0.799628	2.261220
H	1.718642	-2.326288	0.423429
H	1.383536	-1.855586	-1.255253
H	2.133042	0.434821	-1.547480
H	0.731707	2.791124	-0.725570
H	2.292634	2.700455	0.261002
H	-0.846303	1.051555	-1.808470
H	-0.251988	-0.528037	-2.316640
H	-1.962757	-0.322564	-1.914822
H	-0.974377	-2.548208	-0.791854
H	-0.720814	-2.288511	0.945098
H	-1.556851	-0.120714	1.795402
H	-2.663717	1.562535	-0.511854
H	-3.177739	1.563303	1.260675

Prod. 3

TS

State: Open shell S_0

Imaginary frequency: -547.4121

Absolute Gibbs free energy at 298 K: -390.285048 a.u.

C	0.792970	-0.639003	0.731693
C	-0.051067	0.200742	1.652434
C	-1.721381	-1.757744	-0.788550
C	-1.427786	-0.406368	-0.211457
C	-1.485984	-0.205591	1.290367
C	-1.380949	0.716541	-1.077870
C	-1.482144	2.020661	-0.712070
H	0.097776	1.258841	1.430029
H	0.192274	0.052024	2.711226

H	-1.302905	-1.855266	-1.792867
H	-1.322368	-2.562112	-0.166918
H	-2.805366	-1.918116	-0.864735
H	-1.741979	-1.151958	1.774049
H	-2.237431	0.530621	1.594933
H	-1.258314	0.495199	-2.136237
H	-1.645567	2.319917	0.316502
H	-1.426439	2.810005	-1.450174
H	0.641811	-1.713494	0.792605
C	1.899936	-0.193468	-0.034127
C	2.649421	-1.079724	-0.746885
H	3.482246	-0.754093	-1.357274
H	2.429839	-2.140910	-0.723566
C	2.212254	1.283754	-0.079968
H	1.355756	1.844238	-0.463750
H	2.438639	1.668328	0.918008
H	3.070411	1.477976	-0.723238

TS

State: T_1

Imaginary frequency: -759.1973

Absolute Gibbs free energy at 298 K: -390.232913 a.u.

C	0.548726	-0.543541	0.796110
C	-0.291639	0.296159	1.750021
C	-1.472026	-1.786585	-0.829781
C	-1.160440	-0.443704	-0.223707
C	-1.654768	-0.128844	1.183232
C	-1.039030	0.661124	-1.165302
C	-1.311613	1.951721	-0.930825
H	-0.124279	1.360074	1.583510
H	-0.117918	0.079821	2.806331
H	-0.825035	-1.984762	-1.688893
H	-1.334946	-2.592684	-0.105343
H	-2.511301	-1.827314	-1.178923
H	-2.006681	-1.043644	1.665819
H	-2.454224	0.614206	1.240386
H	-0.651632	0.389515	-2.146920
H	-1.711621	2.295039	0.016693
H	-1.152476	2.702123	-1.695043
H	0.468896	-1.614710	0.981492
C	1.720809	-0.159248	0.149167
C	2.486715	-1.167528	-0.598697
H	2.247648	-1.394205	-1.633920
H	3.409609	-1.578637	-0.203477
C	2.158531	1.267326	-0.026313
H	2.014380	1.587165	-1.066108
H	1.610517	1.959890	0.611861
H	3.227476	1.366841	0.189106

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.345297 a.u.

C	0.418975	-0.032091	-0.848419
C	-0.346190	-1.298228	-1.274238
C	-1.241351	1.951067	-0.300394
C	-0.906957	0.471702	-0.150561
C	-1.657604	-0.505723	-1.086066
C	-0.925522	0.079625	1.302000
C	-1.608050	-0.908800	1.866303
H	-0.258688	-2.081358	-0.519770
H	-0.128841	-1.712215	-2.258406
H	-0.568876	2.574839	0.295320
H	-1.155902	2.260301	-1.345204
H	-2.263904	2.145588	0.034340
H	-1.941926	0.009655	-2.006258
H	-2.530874	-1.026949	-0.694705
H	-0.289759	0.692980	1.939958
H	-2.255966	-1.567451	1.299501
H	-1.535115	-1.095665	2.930921
H	0.572648	0.609318	-1.725915
C	1.699370	-0.098442	-0.071422
C	2.299214	-1.245670	0.232650

H	3.230839	-1.261344	0.787445
H	1.886393	-2.201800	-0.065673
C	2.270263	1.235089	0.334029
H	3.226932	1.122740	0.844935
H	2.415304	1.874651	-0.542154
H	1.584840	1.765537	1.002367

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.250194 a.u.

C	0.238320	0.033182	-0.891942
C	-0.401876	-1.322277	-1.244098
C	-1.599936	1.790556	-0.215060
C	-1.039003	0.388738	-0.021465
C	-1.766187	-0.752415	-0.801982
C	-0.872450	0.079391	1.434514
C	-0.526736	-1.237552	1.951827
H	-0.068050	-2.111656	-0.569000
H	-0.306001	-1.665188	-2.274319
H	-0.937153	2.541861	0.224512
H	-1.716345	2.019847	-1.276764
H	-2.579192	1.880883	0.263504
H	-2.330122	-0.340704	-1.641748
H	-2.415721	-1.403885	-0.216422
H	-1.000174	0.901810	2.136403
H	0.507309	-1.524496	2.113527
H	-1.292057	-1.935833	2.276731
H	0.212547	0.691687	-1.769837
C	1.599841	0.126120	-0.271186
C	2.426849	-0.913248	-0.191189
H	3.415560	-0.811798	0.242739
H	2.148334	-1.891953	-0.564666
C	1.972841	1.491730	0.240569
H	3.000153	1.516731	0.605077
H	1.863247	2.242417	-0.548540
H	1.307680	1.784936	1.058877

Prod. 4

TS

State: Open shell S_0

Imaginary frequency: -469.4671

Absolute Gibbs free energy at 298 K: -390.284774 a.u.

C	1.060654	0.501564	0.628300
C	0.750471	1.875203	0.099216
C	-0.994065	0.449426	-0.677908
C	-0.768855	1.820792	-0.096742
H	1.233670	2.028600	-0.867998
H	1.078939	2.681095	0.764003
H	-1.265858	1.909774	0.872574
H	-1.155493	2.624021	-0.735015
H	0.511275	0.205565	1.518576
C	2.066154	-0.382070	0.162377
C	2.958865	-0.059266	-0.812447
H	2.979769	0.918019	-1.276504
H	3.698624	-0.776775	-1.144443
C	2.083086	-1.758034	0.790125
H	2.236280	-1.688532	1.870038
H	1.125012	-2.257919	0.624120
H	2.875278	-2.378231	0.370800
H	-0.416175	0.211560	-1.567147
C	-1.995945	-0.473193	-0.291417
C	-2.163922	-1.642268	-0.972822
H	-2.909184	-2.368957	-0.675008
H	-1.550973	-1.876113	-1.835338
C	-2.861773	-0.163561	0.908186
H	-2.253586	-0.044908	1.809434
H	-3.417378	0.766444	0.764855
H	-3.578225	-0.965194	1.085839

TS

State: T_1

Imaginary frequency: -795.2452

Absolute Gibbs free energy at 298 K: -390.235162 a.u.

C	-0.791092	0.493384	-0.604775
C	-0.707643	1.964135	-0.214293
C	0.756342	0.472240	0.638134
C	0.766150	1.929961	0.211461
H	-1.355005	2.154459	0.645014
H	-0.971708	2.663221	-1.010996
H	1.414258	2.075616	-0.655630
H	1.065022	2.640116	0.986173
H	-0.243989	0.244352	-1.513918
C	-1.813294	-0.378358	-0.256480
C	-2.758343	-0.073634	0.826054
H	-3.752413	0.306357	0.617663
H	-2.555903	-0.389290	1.845986
C	-1.858621	-1.772254	-0.820427
H	-2.853737	-2.006102	-1.213682
H	-1.126559	-1.901261	-1.619761
H	-1.644194	-2.514146	-0.041990
H	0.237444	0.296528	1.579020
C	1.766018	-0.514487	0.309225
C	1.822343	-1.686979	0.970219
H	2.532705	-2.458357	0.698081
H	1.156677	-1.891775	1.801389
C	2.698410	-0.229045	-0.841488
H	2.140439	-0.002711	-1.755411
H	3.330559	0.637096	-0.628119
H	3.344783	-1.083873	-1.039599

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.349297 a.u.

C	0.727677	0.408290	0.418342
C	0.969450	1.906891	0.147076
C	-0.545896	0.506115	-0.479030
C	-0.532514	2.031134	-0.191230
H	1.578654	2.044720	-0.748601
H	1.371668	2.515420	0.956487
H	-1.119557	2.270179	0.697878
H	-0.829387	2.691523	-1.005242
H	0.408261	0.280426	1.460077
C	1.743002	-0.639149	0.076608
C	2.986793	-0.344839	-0.291389
H	3.335438	0.679740	-0.350350
H	3.699049	-1.124708	-0.536909
C	1.236072	-2.052832	0.175719
H	0.912168	-2.270754	1.198860
H	0.363056	-2.194485	-0.469153
H	2.002390	-2.775934	-0.104535
H	-0.241066	0.343443	-1.517734
C	-1.774794	-0.303655	-0.180546
C	-2.463959	-0.887406	-1.159754
H	-3.366662	-1.454049	-0.959525
H	-2.145376	-0.811318	-2.193806
C	-2.193346	-0.426642	1.260480
H	-1.472063	-1.030685	1.819580
H	-2.240483	0.550088	1.750038
H	-3.171004	-0.901046	1.345285

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.251808 a.u.

C	0.739124	0.437183	0.398220
C	1.043134	1.900888	0.024826
C	-0.531526	0.514255	-0.521454
C	-0.443293	2.061132	-0.361083
H	1.681991	1.947366	-0.859663
H	1.448283	2.552740	0.798409
H	-1.041003	2.399741	0.487554
H	-0.689107	2.663317	-1.235303
H	0.396898	0.384404	1.439636

C	1.713967	-0.668551	0.137896
C	2.995137	-0.447215	-0.143163
H	3.399667	0.557388	-0.191543
H	3.681040	-1.266987	-0.325815
C	1.122631	-2.051062	0.203607
H	0.608468	-2.206474	1.157738
H	0.374061	-2.179619	-0.585065
H	1.885343	-2.821452	0.087553
H	-0.229024	0.247056	-1.539056
C	-1.770651	-0.222197	-0.147516
C	-2.362849	-1.199041	-1.058846
H	-2.086583	-2.250277	-1.026791
H	-3.167815	-0.927734	-1.735367
C	-2.316847	-0.121890	1.245940
H	-2.012499	-0.984448	1.856367
H	-1.972090	0.778482	1.760338
H	-3.410597	-0.114521	1.240437

Prod. 5

TS

State: Open shell S_0

Imaginary frequency: -231.2256

Absolute Gibbs free energy at 298 K: -390.291882 a.u.

C	-1.959610	1.102466	0.993039
C	-1.195499	0.516995	-0.156872
C	0.005122	1.267680	-0.629029
C	-1.783858	-0.487424	-0.971269
C	-3.029228	-1.004125	-0.828100
C	3.159773	-0.197665	-0.791573
C	1.956780	-0.139880	0.098889
C	1.289843	1.180548	0.274318
C	1.348376	-1.273957	0.585595
C	0.211360	-1.256748	1.387507
H	-2.734699	1.790413	0.631755
H	-2.456417	0.331763	1.586424
H	-1.302751	1.673426	1.654828
H	-0.261889	2.330337	-0.687462
H	0.281387	0.951144	-1.638031
H	-1.167166	-0.854502	-1.789050
H	-3.704645	-0.668924	-0.050170
H	-3.392799	-1.771137	-1.498770
H	3.487242	-1.224537	-0.959596
H	2.948127	0.259776	-1.765985
H	3.997453	0.361420	-0.360474
H	1.962770	1.988501	-0.021758
H	1.001151	1.368102	1.313017
H	1.735839	-2.238932	0.266953
H	-0.084987	-0.375048	1.936073
H	-0.326962	-2.169153	1.607225

TS

State: T_1

Imaginary frequency: -646.4546

Absolute Gibbs free energy at 298 K: -390.245272 a.u.

C	-2.195509	0.992761	0.978522
C	-1.143760	0.406975	0.076624
C	-0.086233	1.390785	-0.389224
C	-1.564188	-0.631893	-0.845644
C	-2.796087	-1.153708	-0.943163
C	3.432247	-0.255688	-0.121255
C	1.958266	-0.066904	0.019740
C	1.216984	0.801532	-0.960807
C	1.130474	-1.069156	0.702305
C	0.078882	-0.658226	1.475939
H	-2.925448	1.574012	0.400273
H	-2.744845	0.213333	1.512397
H	-1.749022	1.663105	1.716468
H	0.175551	2.040633	0.453811
H	-0.534859	2.043584	-1.150752
H	-0.788556	-1.038821	-1.490823

H	-3.624758	-0.796399	-0.343062
H	-3.007097	-1.952607	-1.642831
H	3.873766	-0.619687	0.809163
H	3.666361	-0.998924	-0.899496
H	3.930498	0.674142	-0.406490
H	0.990038	0.231943	-1.876623
H	1.861711	1.627297	-1.278067
H	1.157358	-2.099195	0.342435
H	0.157257	0.280308	2.018959
H	-0.624411	-1.381584	1.876410

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.381632 a.u.

C	1.007793	-0.212115	1.510362
C	0.947858	0.027289	0.000842
C	0.176752	-1.113170	-0.696288
C	2.322938	0.104196	-0.616413
C	3.490784	-0.023816	0.001527
C	-3.447016	0.021935	0.146897
C	-1.959237	0.083245	-0.055780
C	-1.254923	-1.245427	-0.178522
C	-1.289892	1.234207	-0.111440
C	0.201805	1.345924	-0.290877
H	1.445449	-1.188680	1.735524
H	1.613398	0.555677	1.997787
H	0.008315	-0.171748	1.946625
H	0.719822	-2.053607	-0.565128
H	0.150421	-0.902768	-1.771501
H	2.319975	0.274443	-1.693288
H	3.565916	-0.198343	1.068642
H	4.421427	0.041438	-0.549410
H	-3.876662	1.016136	0.275126
H	-3.934550	-0.459356	-0.706694
H	-3.690945	-0.576313	1.030834
H	-1.830741	-1.895202	-0.846615
H	-1.266562	-1.745009	0.798984
H	-1.842380	2.166937	-0.026182
H	0.597826	2.132583	0.360495
H	0.418113	1.670201	-1.317043

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.278757 a.u.

C	1.365021	-0.114980	1.501647
C	0.889847	0.006954	0.053597
C	0.010821	-1.204848	-0.338689
C	2.046131	0.070572	-0.914135
C	3.340914	0.017888	-0.625617
C	-3.099129	0.147810	-0.822277
C	-2.068890	0.032269	0.261510
C	-1.331567	-1.270432	0.425239
C	-1.257522	1.206345	0.608786
C	0.049234	1.314271	-0.117780
H	1.925126	-1.041729	1.651706
H	2.013453	0.724326	1.765727
H	0.521541	-0.110929	2.193586
H	0.584016	-2.123759	-0.179158
H	-0.203230	-1.145577	-1.412672
H	1.749692	0.170084	-1.958469
H	3.705745	-0.082452	0.390061
H	4.087303	0.073127	-1.409050
H	-2.635111	0.176438	-1.820823
H	-3.781725	-0.706099	-0.810574
H	-3.683318	1.063944	-0.715655
H	-1.925582	-2.107299	0.047442
H	-1.134165	-1.467577	1.484922
H	-1.395618	1.724537	1.552934
H	0.640614	2.169662	0.218894
H	-0.137907	1.448213	-1.192552

Prod. 6

TS

State: Open shell S_0

Imaginary frequency: -248.0910

Absolute Gibbs free energy at 298 K: -390.290197

C	0.908389	-0.073938	0.828365
C	-0.044729	-1.200954	0.634447
C	2.194397	-0.013479	0.218882
C	3.083243	0.961062	0.545495
C	-3.412560	-0.355685	0.342704
C	-2.078619	0.044524	-0.208094
C	-1.109652	-1.037486	-0.524631
C	-1.661125	1.356388	-0.238351
C	-0.405087	1.759230	-0.680402
H	-0.605668	-1.377746	1.555450
H	0.508317	-2.118433	0.414799
H	2.836311	1.714959	1.284156
H	4.060144	1.014848	0.081833
H	-3.992776	0.510475	0.663725
H	-3.999950	-0.904015	-0.401641
H	-3.293256	-1.027253	1.202286
H	-0.573467	-0.851001	-1.458193
H	-1.624587	-1.995336	-0.630110
H	-2.320940	2.111034	0.183742
H	-0.064409	2.775803	-0.532371
H	0.214051	1.133156	-1.305359
H	0.692371	0.653590	1.600975
C	2.559844	-1.051317	-0.818321
H	3.513498	-0.810228	-1.287182
H	2.645063	-2.044873	-0.369703
H	1.800693	-1.115051	-1.602964

TS

State: T_1

Imaginary frequency: -658.2505

Absolute Gibbs free energy at 298 K: -390.247143

C	-0.865435	-0.097120	-0.580491
C	0.000882	-1.283077	-0.238435
C	-2.234229	-0.004176	-0.126958
C	-3.130479	0.777402	-0.767458
C	3.622053	0.047938	0.299348
C	2.143370	0.047707	0.096084
C	1.483788	-1.104876	-0.611227
C	1.388959	1.306479	0.046401
C	0.139790	1.364786	0.602584
H	-0.382504	-2.169372	-0.761819
H	-0.071095	-1.504919	0.832279
H	-2.857480	1.320969	-1.664995
H	-4.148193	0.880015	-0.411283
H	3.913262	0.758560	1.076032
H	3.989015	-0.943795	0.575039
H	4.150626	0.343198	-0.620630
H	2.026009	-2.030505	-0.395437
H	1.547449	-0.957052	-1.703129
H	1.684342	2.062769	-0.682957
H	-0.489368	2.237546	0.464484
H	-0.076176	0.760983	1.480030
H	-0.677333	0.343333	-1.557227
C	-2.623758	-0.759659	1.119577
H	-3.658352	-0.553122	1.392701
H	-2.514350	-1.838136	0.975616
H	-1.985491	-0.482889	1.964758

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.383942 a.u.

C	0.707579	0.059733	0.376085
C	0.016384	-1.229307	-0.083955
C	2.206465	0.035085	0.173737
C	3.036540	0.395893	1.149078

C	-3.639853	0.072779	0.060309
C	-2.138255	0.088496	0.003518
C	-1.454097	-1.218701	0.328781
C	-1.445158	1.182928	-0.309159
C	0.058962	1.257395	-0.335179
H	0.525075	-2.103144	0.333171
H	0.081885	-1.302416	-1.175387
H	2.663989	0.698600	2.121875
H	4.111689	0.400521	1.006769
H	-4.060377	1.059829	-0.135433
H	-4.048242	-0.630339	-0.672427
H	-3.983572	-0.259778	1.045207
H	-1.991657	-2.035370	-0.165539
H	-1.546222	-1.408929	1.406166
H	-1.985561	2.094460	-0.553440
H	0.393138	2.183114	0.143322
H	0.405508	1.313156	-1.374995
H	0.515292	0.175595	1.449354
C	2.716124	-0.409666	-1.172648
H	3.795267	-0.274200	-1.246026
H	2.492220	-1.467219	-1.340241
H	2.243421	0.148316	-1.985778

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.281966 a.u.

C	-0.738789	-0.143653	0.431705
C	0.032106	1.184197	0.359977
C	-2.186309	-0.005229	0.014268
C	-3.167630	-0.455913	0.792295
C	3.476995	0.063896	-0.601583
C	2.150551	-0.078530	0.064485
C	1.491916	1.027653	0.835548
C	1.403216	-1.343048	0.083315
C	-0.008187	-1.237553	-0.405893
H	-0.485821	1.937221	0.962374
H	0.043065	1.542420	-0.675355
H	-2.959971	-0.913032	1.753791
H	-4.207485	-0.381729	0.493252
H	3.538114	-0.567898	-1.492085
H	3.671847	1.099921	-0.891327
H	4.300687	-0.245451	0.059195
H	2.033293	1.969976	0.713649
H	1.481906	0.798057	1.912625
H	1.599139	-2.063794	0.879697
H	-0.550039	-2.181947	-0.318882
H	-0.014463	-0.933167	-1.459678
H	-0.725766	-0.482925	1.474686
C	-2.470882	0.647596	-1.313558
H	-3.527880	0.567036	-1.567810
H	-2.206448	1.708557	-1.289645
H	-1.888100	0.190250	-2.117846

Prod. 7

TS

State: Open shell S_0

Imaginary frequency: -482.1900

Absolute Gibbs free energy at 298 K: -390.279140

C	-1.053524	-1.339059	-0.049543
C	0.302809	-1.842085	0.384621
C	-1.688915	-0.188262	0.312857
C	-1.139114	0.808158	1.165024
C	2.559243	0.514641	0.688974
C	1.629455	0.086293	-0.406487
C	1.434904	-1.396899	-0.579904
C	0.741451	0.941661	-1.004841
C	0.315124	2.159641	-0.460496
H	0.276520	-2.935271	0.429529
H	0.537882	-1.493753	1.395243
H	-0.217150	0.637472	1.704230

H	-1.765010	1.620623	1.512620
H	2.722060	1.592092	0.693733
H	2.185712	0.221992	1.679300
H	3.530994	0.026428	0.568159
H	2.352033	-1.950362	-0.355137
H	1.140484	-1.633631	-1.607522
H	0.147010	0.539053	-1.821673
H	0.817673	2.613623	0.383209
H	-0.419598	2.766141	-0.973273
H	-1.572338	-1.981172	-0.757887
C	-3.034470	0.136579	-0.298239
H	-2.955711	1.025063	-0.932516
H	-3.409091	-0.686675	-0.906795
H	-3.773258	0.354378	0.476986

TS

State: T_1

Imaginary frequency: -689.9569

Absolute Gibbs free energy at 298 K:

C	1.151171	1.310565	-0.131624
C	-0.097839	1.749766	0.577307
C	1.866757	0.193308	0.119344
C	1.459634	-0.777428	1.102826
C	-3.218715	-0.452916	-0.112776
C	-1.766852	-0.081976	-0.132096
C	-1.404050	1.377168	-0.167444
C	-0.797405	-1.075443	-0.626866
C	-0.128037	-1.946127	0.189570
H	-0.076188	2.838722	0.681904
H	-0.146601	1.339303	1.588559
H	0.850899	-0.454940	1.937644
H	2.137046	-1.596380	1.322742
H	-3.354264	-1.494811	0.184445
H	-3.783590	0.185849	0.571655
H	-3.674330	-0.340303	-1.108832
H	-2.229639	1.954873	0.260993
H	-1.306910	1.710816	-1.213448
H	-0.511067	-1.020885	-1.678770
H	-0.519877	-2.154243	1.179413
H	0.494569	-2.718383	-0.249199
H	1.481209	1.953717	-0.944802
C	3.038904	-0.184232	-0.751858
H	2.816806	-1.105434	-1.301631
H	3.266984	0.598019	-1.476481
H	3.933543	-0.372038	-0.152493

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.349971

C	-0.862550	1.432677	-0.129077
C	0.577083	1.774689	-0.459152
C	-1.529145	0.278518	-0.275587
C	-0.952148	-1.030816	-0.801824
C	2.390737	-0.830886	-0.656108
C	1.576600	-0.233969	0.459440
C	1.626671	1.264121	0.585739
C	0.561132	-0.859937	1.059029
C	-0.295844	-1.869865	0.337811
H	0.663526	2.860643	-0.547738
H	0.845248	1.365240	-1.438187
H	-0.178125	-0.823277	-1.545760
H	-1.741114	-1.603378	-1.300451
H	2.155523	-1.881604	-0.825924
H	2.258248	-0.290293	-1.599224
H	3.453949	-0.763714	-0.404487
H	2.607986	1.687177	0.352082
H	1.334486	1.594901	1.585504
H	0.057961	-0.327763	1.861294
H	0.259539	-2.703839	-0.095058
H	-1.056809	-2.291940	0.997610
H	-1.425626	2.251464	0.315548
C	-2.963351	0.167930	0.175713
H	-3.071302	-0.630354	0.918358

H	-3.326057	1.097171	0.615934
H	-3.612541	-0.095203	-0.665408

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.284944

C	-1.107197	1.415994	-0.001394
C	0.277173	1.862659	-0.393470
C	-1.645496	0.215107	-0.220144
C	-0.901031	-0.904174	-0.904514
C	2.748653	-0.519578	-0.567398
C	1.689667	-0.111881	0.415821
C	1.373590	1.346786	0.579213
C	0.806816	-1.148099	0.962384
C	-0.219059	-1.841769	0.109947
H	0.306962	2.955176	-0.400563
H	0.525659	1.538269	-1.409019
H	-0.141492	-0.503586	-1.580849
H	-1.596431	-1.489585	-1.514082
H	3.180201	-1.489153	-0.303659
H	2.343927	-0.623633	-1.586584
H	3.555179	0.217081	-0.618189
H	2.286067	1.930072	0.414827
H	1.037127	1.541860	1.602925
H	1.096221	-1.643268	1.887572
H	0.256017	-2.664292	-0.447940
H	-0.971031	-2.314667	0.750395
H	-1.700115	2.142521	0.550401
C	-3.026565	-0.131675	0.267227
H	-2.999119	-0.997088	0.937134
H	-3.483319	0.700157	0.804366
H	-3.675161	-0.400088	-0.572766

Prod. 8

TS I

State: Open shell S_0

Imaginary frequency: -521.2344

Absolute Gibbs free energy at 298 K: -390.280538 a.u.

C	2.868782	-0.260707	0.564086
C	1.614272	0.042370	-0.205181
C	0.880335	-1.185537	-0.711403
C	1.227736	1.338878	-0.407817
C	0.052555	1.815725	-1.028616
C	-2.385724	-0.990906	-0.620109
C	-1.294456	-0.789589	0.388491
C	-0.132915	-1.746975	0.319561
C	-1.153573	0.360632	1.115707
C	-1.724492	1.597365	0.781664
H	3.602572	-0.764778	-0.075641
H	3.327815	0.641554	0.969411
H	2.664086	-0.943427	1.396770
H	1.620624	-1.957232	-0.951557
H	0.351773	-0.957018	-1.641895
H	1.878371	2.100480	0.017405
H	-0.601453	1.148976	-1.575570
H	-0.056931	2.873395	-1.227012
H	-3.224216	-0.313492	-0.460937
H	-2.024748	-0.851186	-1.647542
H	-2.764665	-2.015978	-0.562043
H	-0.455393	-2.747057	0.013453
H	0.354295	-1.837792	1.295744
H	-0.349414	0.381132	1.847693
H	-2.503568	1.682094	0.035670
H	-1.534276	2.472799	1.387749

TS I

State: T_1

Imaginary frequency: -677.5744

Absolute Gibbs free energy at 298 K: -390.248837 a.u.

C	1.581281	-0.438690	-0.001192
C	0.706270	-0.828180	1.159497
H	1.204815	-1.610737	1.742317
H	0.550254	0.019605	1.829799
C	1.776030	0.848495	-0.375492
H	2.354088	1.019821	-1.281335
C	1.206949	2.009514	0.245111
H	0.984775	1.999608	1.304233
H	1.506341	2.978446	-0.139611
C	-0.669736	-1.366742	0.716558
H	-1.214386	-1.682368	1.622465
H	-0.541956	-2.278341	0.121621
C	-0.863059	2.011418	-0.375749
H	-1.030765	3.052174	-0.118413
H	-0.560714	1.813147	-1.397659
C	-1.511116	1.032398	0.328489
C	-1.516834	-0.391177	-0.054419
C	2.180615	-1.574285	-0.780042
H	1.401354	-2.211344	-1.212932
H	2.810578	-1.213581	-1.593886
H	2.787669	-2.214618	-0.131034
C	-2.734930	-0.929888	-0.741198
H	-3.080224	-0.248805	-1.522001
H	-2.539875	-1.908217	-1.188748
H	-3.569473	-1.056837	-0.034184
H	-1.995304	1.304862	1.269984

TS II

State: Open shell S_0

Imaginary frequency: -438.4956

Absolute Gibbs free energy at 298 K: -390.277190

C	-0.651815	1.408174	0.338471
C	0.602184	1.993425	-0.266396
C	-1.481866	0.450414	-0.174639
C	-1.274884	-0.235445	-1.398260
C	1.766566	-0.144418	-0.433083
C	1.876636	1.223965	0.170487
C	1.058920	-1.189571	0.089012
C	0.430465	-2.092847	-0.796787
H	0.687266	3.043141	0.032426
H	0.543667	1.978096	-1.359527
H	-0.493108	0.064234	-2.081902
H	-2.057815	-0.870395	-1.794413
H	2.765358	1.750538	-0.188496
H	1.926715	1.196209	1.261429
H	0.699260	-2.115548	-1.845070
H	-0.178765	-2.906677	-0.422524
H	1.973544	-0.183642	-1.502130
H	-0.913051	1.802918	1.317963
C	-2.686613	0.011929	0.632059
H	-2.732429	0.520405	1.595700
H	-3.613059	0.221319	0.091248
H	-2.652605	-1.066835	0.812864
C	0.720179	-1.316482	1.554173
H	-0.348325	-1.156951	1.721008
H	0.964381	-2.324378	1.900314
H	1.270330	-0.607290	2.170889

TS II

State: T_1

Imaginary frequency: -645.9797

Absolute Gibbs free energy at 298 K: -390.247918

C	3.047496	-0.402934	0.507861
C	1.775005	-0.070547	-0.234812
C	1.086742	-1.181428	-0.841372
C	1.286616	1.191078	-0.226222
C	-0.031005	1.625017	-0.793312
C	-2.602198	-0.978334	-0.582590
C	-1.489537	-0.746457	0.405098
C	-0.489868	-1.664723	0.580726
C	-1.449543	0.574884	1.061921
C	-1.103980	1.821125	0.299462

H	3.794919	-0.830924	-0.165312
H	3.475348	0.479921	0.983610
H	2.849733	-1.147656	1.285964
H	1.599522	-2.138395	-0.855282
H	0.423474	-1.015700	-1.680548
H	1.856078	1.957742	0.294486
H	-0.396562	0.900148	-1.524944
H	0.087872	2.574807	-1.323772
H	-3.578608	-0.839372	-0.107164
H	-2.552246	-0.254953	-1.406596
H	-2.562032	-1.983596	-1.006231
H	-0.624346	-2.674202	0.203442
H	0.197650	-1.547778	1.410568
H	-1.967445	0.695320	2.009675
H	-2.009378	2.225941	-0.181294
H	-0.772349	2.592604	1.002834

Product

State: S_0

Absolute Gibbs free energy at 298 K: -390.349250 a.u.

C	2.947099	-0.112827	0.281203
C	1.549039	0.077737	-0.253270
C	0.863465	-1.227934	-0.634255
C	1.020601	1.307969	-0.321056
C	-0.381856	1.727157	-0.721857
C	-2.309492	-1.018881	-0.596949
C	-1.259741	-0.813327	0.460886
C	-0.112580	-1.787963	0.452926
C	-1.072884	0.335974	1.113475
C	-1.370266	1.674401	0.485781
H	3.596103	-0.561308	-0.477517
H	3.392638	0.828220	0.605000
H	2.937335	-0.800836	1.134011
H	1.634375	-1.976247	-0.841364
H	0.302522	-1.096688	-1.564065
H	1.657250	2.123724	0.018651
H	-0.767025	1.050393	-1.490564
H	-0.355977	2.730401	-1.156566
H	-2.990874	-0.171625	-0.674247
H	-1.872098	-1.201716	-1.584127
H	-2.904522	-1.903897	-0.349942
H	-0.409726	-2.805806	0.184413
H	0.396063	-1.820555	1.420323
H	-0.288706	0.352886	1.864942
H	-2.395585	1.786774	0.128393
H	-1.172083	2.492433	1.181353

Product

State: T_1

Absolute Gibbs free energy at 298 K: -390.284865 a.u.

C	1.592828	-0.225172	-0.008907
C	0.826626	-0.782259	1.165789
H	1.452830	-1.496683	1.709252
H	0.560825	0.012889	1.866381
C	1.458462	1.032400	-0.434096
H	2.007016	1.324088	-1.327346
C	0.580018	2.096150	0.172587
H	0.649217	2.087134	1.264393
H	0.934646	3.076572	-0.155622
C	-0.462022	-1.492591	0.710452
H	-0.963261	-1.909862	1.599179
H	-0.211679	-2.353259	0.079425
C	-0.914279	1.960232	-0.228178
H	-1.433274	2.883511	0.044108
H	-0.963306	1.863553	-1.319528
C	-1.599686	0.792008	0.413253
C	-1.408346	-0.590660	-0.033948
C	2.473753	-1.210131	-0.729378
H	1.897219	-2.078789	-1.063458
H	2.949133	-0.760893	-1.601934
H	3.256591	-1.585610	-0.062695
C	-2.479172	-1.224632	-0.869869

H	-2.882671	-0.517350	-1.598468	H	-2.237110	0.985708	1.276150
H	-2.101375	-2.099881	-1.405689				
H	-3.323890	-1.563214	-0.250370				

10. References

[S1] E. Englund, K. Shabestary, E. P. Hudson and P. Lindberg, *Metab. Eng*., 2018, **49**, 164-177.

[S2] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, I A. F. zmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A., Jr. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 16*, 2016.

[S3] C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1988, **37**, 785–789.

[S4] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys*., 2010, **132**, 154104.

[S5] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.

[S6] S. Hoz, M. Ben-Tzion and D. Major, *Sustainable Energy Fuels*, 2019, **3**, 457–466.

[S7] A. V. Marenich, C. J. Cramera and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378–6396.

[S8] G. D. Purvis III and R. J. Bartlett, J. *Chem. Phys*. 1982, **76**, 1910– 1918.

[S9] J. A. Pople, M. Head-Gordon and K. Raghavachari, J. *Chem. Phys*. 1987, **87**, 5968– 5975.

[S10] X. Wang, F-D. Liu, H-Y. Tu and A-D. Zhang, *J. Org. Chem*., 2014, **79**, 6554-6562.

[S11] M. Haddach and J. R. McCarthy, *Tetrahedron Lett*., 1999, **40**, 3109-3112.

[S12] S. K. Rajagopal, N. K, S. Deb, V. Bhat, D. sasikumar, E. Sebastian and M. Hariharan, *Phys. Chem. Chem. Phys.* 2018, **20**, 19120-19128.

[S13] A. Rérat, C. Michon, F. Agbossou-Niedercorn, and C. Gosmini, *Eur. J. Org. Chem*., 2016, 4554-4560.

[S14] X-J. Zhang, S-F. Ye, Y. Zhang, H-Y. Meng, M-Q. Zhang, W-L. Gao and Q-D. You, *Synth. Commun*., 2012, **42**, 2952-2958.

[S15] D. H.Guerra, A. Hlavackova, C. Pramthaisong, I. Vespoli, R. Pohl, T. Slanina, and U. Jahn, *Angew. Chem. Int. Ed.*, 2019, **58**, 12440 –12445

[S16] P. Klán and J. Wirz, Photochemistry of Organic Compounds: From Concepts to Practice, Wiley-Blackwell, Chichester, 2009.

[S17] H. J. Kuhn, S. E. Braslavsky and R. Schmidt, *Pure Appl.chem.*, 2004, **76**, 2105-2146.

[S18] S. K. Bengtsson, E. Fridell and K. E. Andersson, *Proc IMechE Part M: J Engineering for the Maritime Environment*, 2014, **228**, 44–54.

[S19] L. Benini, L. Mancini, S. Sala, S. Manfredi, E. M. Schau and R. Pant. Normalisation method and data for Environmental Footprints. European Commission, Joint Research Center, Institute for Environment and Sustainability, Publications Office of the European Union, Luxemburg. 2014, ISBN: 978-92-79-40847-2.

[S20] R. Y. Stanier, R. Kunisawa, M. Mandel and G. Cohen-Bazire, *Bacteriol. Rev*., 1971, **35**, 171-205.

[S21] E. Sierra, F. G. Acién, J. M. Fernández, J. L. García, C. González and E. Molina, *Chem. Eng. J*. 2008, **138**, 136-147.

[S22] N. R. Baral, M. Yang, B. G. Harvey, B. A. Simmons, A. Mukhopadhyay, T. S. Lee and C. D. Scown, *ACS Sustainable Chem. Eng*., 2021, **9**, 11872-11882.

[S23] N. R. Baral, O. Kavvada, D. Mendez-Perez, A. Muhopadhyay, T. S. Lee, B. A. Simmons and C. D. Scown, *Energy Environ. Sci*., 2019, **12**, 807-824.

[S24] X. Liu, A. Elgowainy and M. Wang, *Green. Chem*., 2020, **22**, 5751-5761.

[S25] International Energy Agency (IEA), *Energy Policies of IEA Countries: Sweden 2019 Review*, 2019.

[S26] Swedish Energy Agency, *Energy in Sweden 2022 – An overview*, 2022.

[S27] European Commission - Joint Research Centre - Institute for Environment and Sustainability: International Reference Life Cycle Data System (ILCD) Handbook - General guide for Life Cycle Assessment - Detailed guidance. First edition March 2010. EUR 24708 EN. Luxembourg. Publications Office of the European Union; 2010.