Supporting information

Aminoboranes as Rationally Tuned Organic Photosensitizers for Energy Transfer Catalysis

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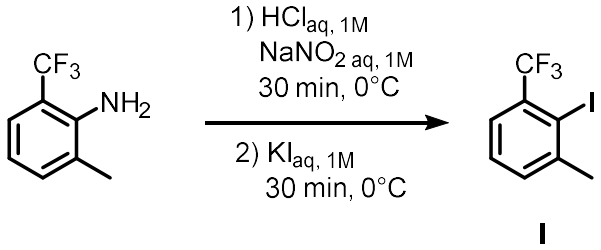
1. General Experimental Details

The NMR spectra were recorded at 400 MHz and 600 MHz for ^{1}H, 150 MHz for ^{13}C and 376 MHz and 565 MHz for ^{19}F. The chemical shift (δ) for ^{1}H and ^{13}C are given in ppm relative to residual signals of the solvents ($CHCl_3$ @ 7.26 ppm ^{1}H NMR and 77.16 ppm ^{13}C NMR). Coupling constants are given in Hertz. The following abbreviations are used to indicate the multiplicity: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad signal. High Resolution Mass Spectra (HRMS) were recorded on a Waters Synapt MALDI Q-Tof G2S spectrometer. UV-vis measurements were carried out on a Cary 3500 Multicell UV-vis spectrophotometer. Fluorescence measurements were carried out on an Edinburgh FLSP920 spectrometer equipped with a 450 W xenon arc lamp, double excitation and single emission monochromators, and a Peltier-cooled Hamamatsu R928P photomultiplier tube (185−850 nm). HPLC-MS analysis for mechanistic investigations were conducted with an Agilent 1260 infinity II analytical instrument with quaternary pump (800 bar) and MS module Infinity Lab LC/MSD iQ series with single quadrupole, equipped with a reverse phase column Agilent Infinity Lab Poroshell 120 EC-C18, 4.6 x 150 mm, 2.7 µm. Dry THF was obtained through SPS distillation system Pure Process Technology model PPT-SPS-5-CM. Solvents dryness was measured with a Karl-Fischer system, model Metrohm Eco Coulometer w/ gen. Electrode. The chemicals used for the reactions are commercial, provided by BLD pharm, Fluorochem, TCI, Thermo-Fischer, Sigma-Aldrich, unless otherwise stated. When referring to experimental procedures involving water, deionized water was exclusively employed. Yields refer to isolated materials of > 95% purity as determined by ^{1}H NMR analysis. When specified, yields were determined by ^{1}H NMR analysis of the crude mixture using dibromomethane (CH_2Br_2) as internal standard. General Procedures: all reactions were set up under an argon atmosphere in oven-dried glassware. Chromatographic purification of products was accomplished using forced-flow chromatography (FC) on silica gel (230-400 mesh). For thin layer chromatography (TLC) analysis throughout this work, Merck pre-coated TLC plates (silica gel 60 GF254, 0.25 mm) were employed, using UV light as the visualizing agent and an acidic mixture of vanillin or basic aqueous potassium permanganate ($KMnO_4$) stain solutions, and heat as developing agents. Organic solutions were concentrated under reduced pressure on a Büchi rotatory evaporator.

2. Synthesis and characterization of Substrates

2.1 Synthesis of intermediates I-III for the synthesis of C1-C6

2.1.1 Synthesis and characterization of 2-iodo-1-methyl-3-(trifluoromethyl)benzene (I):



1.42 g (8.11 mmol, 1.0 eq.) of 2-Methyl-6-(trifluoromethyl)aniline was added to a 3-necked 100 mL round bottom flask (RBF) and diluted in 10 mL of water at 0 °C under vigorous stirring. 8.5 mL (8.5 mmol, 1.05 eq.) of a 1 M HCl aqueous solution were slowly added via a dropping funnel at the same temperature. Then, a solution of 727 mg (10.5 mmol, 1.3 eq.) of $NaNO_2$ in 10 mL of water was slowly added at 0 °C. The solution was stirred at 0 °C for 30 minutes (full conversion to the intermediate diazo can be assessed in HPLC-MS – a single peak is visible at 230 nm with ESI+ ionization of 159 m/z [aryl+]). Consequently, a solution of 2.69 g (16.2 mmol, 2.00 eq.) of KI in 10 mL of water was slowly added at 0°C keeping the stirring high. Upon full addition the solution turned brown. After stirring for 30 minutes at RT, the reaction was quenched with a saturated aqueous solution of $Na_2S_2O_3$. The product was extracted with EtOAc (3 x 30 mL), and the combined organic layers were washed with water and brine, dried with Na_2SO_4, filtered and concentrated under reduced pressure.

The product was purified by flash column chromatography with an isocratic phase of pure *n*-hexane.

2-iodo-1-methyl-3-(trifluoromethyl)benzene (I): colorless oil; 52 % y*ield (1.2 g, 4.22 mmol)*.

TLC *Rf: 0.70 (hexane)* – *the product is difficult to spot even under 254 nm lamp*!

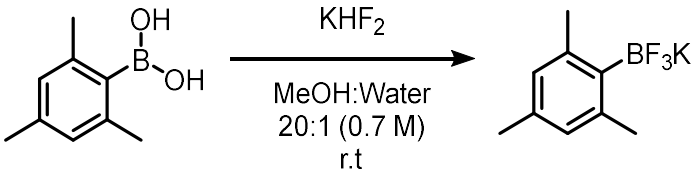
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.41 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.32 (t, *J* = 7.7 Hz, 1H), 2.55 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 144.6, 134.3 (q, *J* = 30.0 Hz, **C_q**-CF_3), 132.6, 127.8, 125.1 (q, *J* = 6.0 Hz), 123.1 (q, *J* = 273.0 Hz, **CF_3**), 98.5, 30.2.

^{19}F NMR (565 MHz, $CDCl_3$) δ -62.23.

GCMS (EI) m/z calculated for [$C_8H_6F_3I$]: 285.9; found 285.9.

2.1.2 Synthesis of trifluoro(mesityl)-λ⁴-borane, potassium salt (MesBF₃K) (II):



II

Trifluoro(mesityl)-λ⁴-borane, potassium salt (MesBF₃K) (II) was synthesized using a slightly modified reported procedure.[34]

To a 1 neck 100 mL RBF 2.28 g (13.9 mmol, 1.0 eq.) of 2,4,6-trimethylphenylboronic acid and 3.58 g (45.9 mmol, 3.30 eq.) of potassium hydrogen difluoride were sequentially added to a solution of 28 mL of methanol and 1.4 mL of water (20:1 / MeOH:H_2O). The colourless mixture was stirred for 4h at room temperature. The solvent was removed via rotary evaporation, and any residual water was dried under vacuum overnight. Acetone was then added until most of the precipitate dissolved, and the solution was further dried with anhydrous magnesium sulfate. After Buchner filtration, the filtrate was concentrated by rotary evaporation to reach a saturation point, and Et_2O was added to induce precipitation of the product. The resulting product was collected by filtration, washed with cold Et_2O/H_2O (1% water). An additional Soxhlet extraction with ACN as solvent was performed to remove all the KHF_2 which is scarcely soluble in ACN and will remain in the filter cake. The filtrate is concentrated under reduced pressure and dried under a high vacuum overnight.

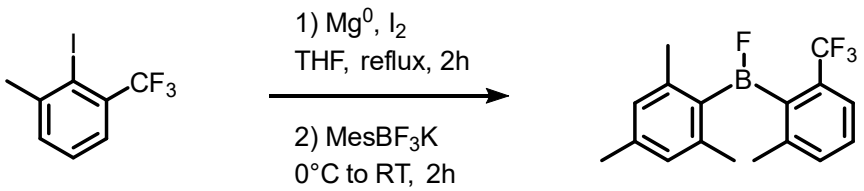
trifluoro(mesityl)-λ⁴-borane, potassium salt: white flaky solid; 62 % y*ield (1.95g, 8.62 mmol)*[i]
The NMR spectra agree with the reported data[34]:

^{1}H NMR (400 MHz, CD_3CN) δ 6.60 (s, 2H), 2.32 (s, 6H), 2.15 (s, 3H).

^{19}F NMR (376 MHz, CD_3CN) δ -131.23.

[i] The lower yield compared to literature procedures is due to an excess of Et_2O/H_2O mixture used during washing, and Soxhlet extraction with acetonitrile needed for removing residual traces of KHF_2 which has been noted to diminish the yields of the organometallic steps.

2.1.3 Synthesis and characterization of fluoro(mesityl)(2-methyl-6-(trifluoromethyl)phenyl) borane (III):



III
Detected at ^{19}FNMR

In a heat-vacuum dried 3 neck 50 mL RBF equipped with a water condenser and a pressure equalized dropping funnel under argon atmosphere 40 mg (1.65 mmol, 1.5 eq.) of previously activated magnesium turnings[ii] are added along with 5 mL of dry THF. To the suspension, a small crystal of sublimated iodine was added at room temperature to further activate the Mg^0. Heating is turned on and the suspension refluxed for 20 minutes. The heating is subsequently stopped, and the reaction mixture is stirred at room temperature. After this additional activation step, 315 mg (1.1 mmol, 1.0 eq.) of 2-iodo-1-methyl-3-(trifluoromethyl)benzene (**I**) dissolved in 6 mL of dry THF are slowly added with the dropping funnel. When 1/3 of the solution is added (≅ 2 mL), the heating is turned on and the addition continued, until all the iodo-aryl solution has been added. The reaction mixture is refluxed for 2 hours and then cooled down to 0 °C. Finally, 271 mg (1.2 mmol, 1.1 eq.) of dry $MesBF_3K$ (**II**) are added in one portion trough a funnel for solids. The reaction is stirred for an additional 2 hours at room temperature.

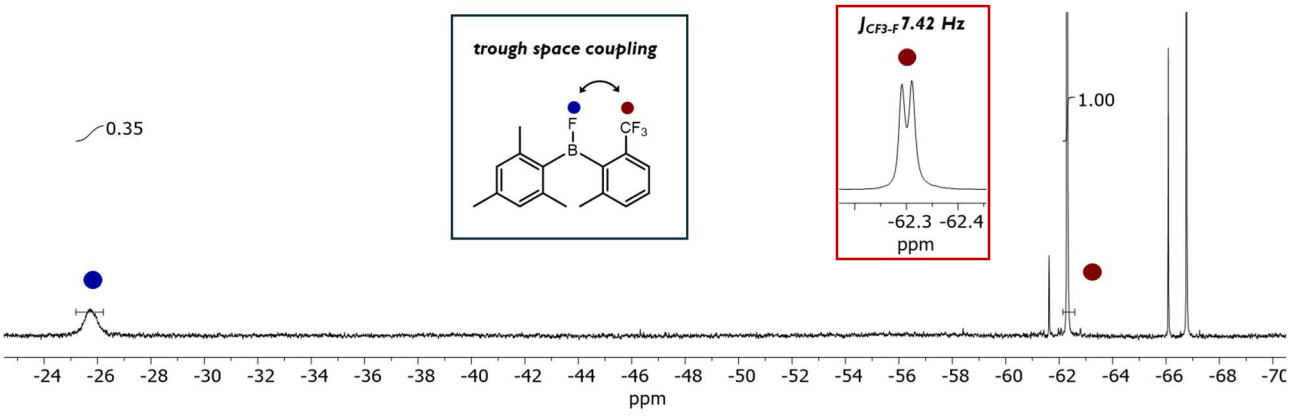


Figure S1 ^{19}F NMR spectra of **III;** To evaluate the formation of **III**, 50 µL of crude solution were taken and diluted with 600 µL of dry THF into a previously dried 5mm NMR tube under argon atmosphere.

The reaction crude could be monitored to check for the formation of **III** formed with ^{19}F NMR experiment in dry THF. The formation of **III** is evident through its fluorine peaks shown in Figure S1. The Aryl-**CF_3** signal of **III (-62.3 ppm**) shows a distinct coupling (d, J = 7.42 Hz) due to a through-space coupling with the fluorine connected to the boron atom[35]. Moreover, the Ar_2**B-F** signal (**-25.7 ppm**) shows broadening due to the coupling with the quadrupolar boron atom and the -CF_3 group.

[ii] The magnesium turnings were first washed with a 0.1M HCl_{aq} solution, followed by *i*PrOH and Et_2O. The last step is a thorough removal of any trace of solvents under strong vacuum overnight.

2.2 Synthesis of heterocyclic aromatic compounds Het2-3 for the synthesis of C2-C3

Most of the heterocyclic compounds used for the synthesis of **C1-C6** were commercially available (**Het1; Het4-6**). **Het2-3** were prepared using reported procedures (Figure S2).

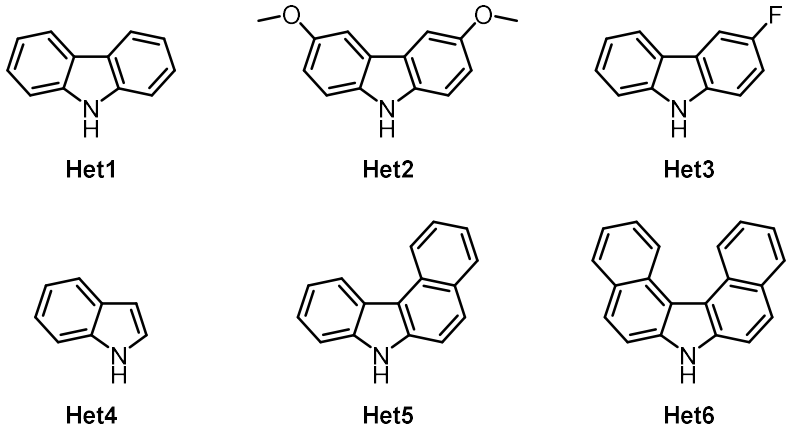
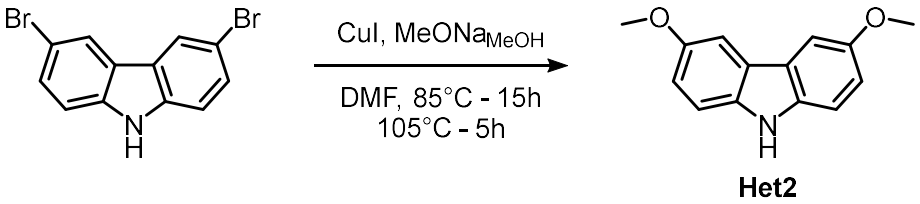


Figure S2 Selected N-heterocyclic aromatic compounds for the synthesis of **C1-C6**.

2.2.1 Synthesis and characterization of 3,6-dimethoxy-9H-carbazole (Het2):



3,6-dimethoxy-9H-carbazole (**Het2**) was synthesized using a slightly modified reported procedure.[36]

In a 100 mL 2 neck RBF equipped with a water condenser were placed 5.00 g (15.4 mmol, 1.0 eq.) of 3,6-Dibromocarbazole, 5.86 g (30.8 mmol, 2.0 eq.) of copper(I) iodide under a nitrogen atmosphere. DMF (30.8 mL) sodium methoxide in MeOH (28.1 mL of a 25% w/w solution; 123 mmol, 8.0 eq.). The solution was heated at 85 °C for 15 h, then at 105 °C for 5 h. The crude mixture was diluted in ethyl acetate (EtOAc) and filtered over a silica pad, then concentrated under vacuum. The solid precipitate was dissolved in the minimum amount of hot $CHCl_3$. After cooling to room temperature cold *n*-hexane was added while vigorous stirring. A white precipitate forms, and *n*-hexane is added until no more precipitate formation is observed. The supernatant was removed and the solid cake was washed with additional 30 mL of cold *n*-hexane. The solid was dried under vacuum to obtain pure 3,6-dimethoxy-9H-carbazole (**Het2**) as a flaky white solid.

3,6-dimethoxy-9H-carbazole (Het2): flaky white solid; 60 % y*ield (2.1 g, 9.24 mmol)*.

Rf (*n*-hexane/dichloromethane[iii] 1:1): 0.6. The NMR spectrum agrees with the reported data[36]:

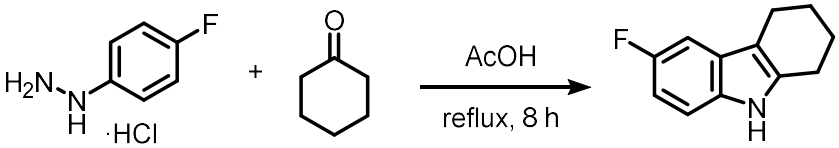
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (bs, 1H, -NH), 7.51 (d, *J* = 2.5Hz, 2H, ArH), 7.29 (d, *J* = 8.8 Hz, 2H, ArH), 7.06 (dd, *J* = 8.8, 2.5 Hz, 2H, ArH), 3.94 (s, 6H, -OMe).

[iii] dichloromethane: DCM

2.2.2 Synthesis and characterization of 3-fluoro-9H-carbazole (Het3):

The synthesis of **3-fluoro-9H-carbazole (Het3)** involves a two-step reported procedure.[37]

Step 1

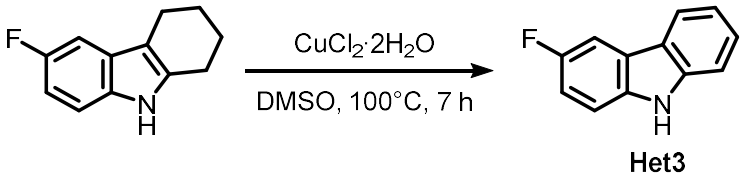


In a 100 mL 2 neck RBF equipped with a water condenser, were placed 1.34 mL of cyclohexanone (12.9 mmol, 1.00 eq.) and 41.8 mL of acetic acid. Subsequently, 2.00 g (12.3 mmol, 0.95 eq.) of 4-fluorophenylhydrazine hydrochloride was added in portions over a period of 30 min and the reaction mixture was refluxed for 8 h. After TLC monitoring confirming the disappearance of starting material, the crude was cooled to room temperature and poured into crushed ice. The white solid was collected by filtration, dried, and purified by recrystallization from methanol.

3,6- 3-Fluoro-6, 7, 8, 9-tetrahydro-5H-carbazole: white solid; 93 % y*ield (2.27 g, 12.0 mmol)*.

The NMR spectrum of the intermediate agrees with the reported data:[37]

Step 2



Het3

3-fluoro-9H-carbazole (**Het3**) was synthesized using a reported procedure.[3]

In a 50 mL 2 neck RBF equipped with a water condenser were placed 2.27 g (12.0 mmol, 1.0 eq.) of 3-fluoro-6, 7, 8, 9-tetrahydro-5H-carbazole and 204.6 mg (1.20 mmol, 0.1 eq.) of $CuCl_2{\cdot}2H_2O$ in 21 mL of DMSO. The reaction mixture was stirred at 100 °C, and its progress was monitored by TLC. Upon disappearance of the starting material, the mixture was poured into ice-cold water. The crude product was then purified by column chromatography using EtOAc and *n*-hexane as eluents, yielding **Het3**.

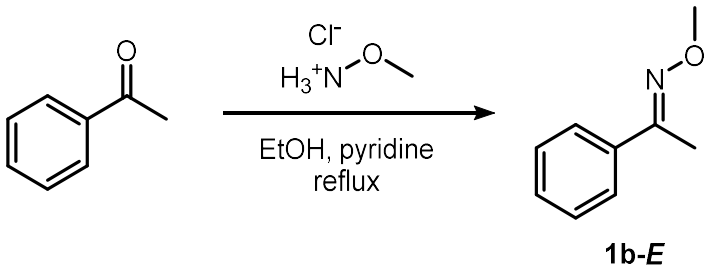
3-fluoro-9H-carbazole Het3: white solid; 94% y*ield (2.09 g, 11.28 mmol)*.

The NMR spectrum agrees with the reported data:[37]

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.27 (s, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.94 (dd, *J* = 9.5, 2.7 Hz, 1H), 7.53 – 7.44 (m, 2H), 7.40 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 1H), 7.22 (ddd, *J* = 9.6, 8.8, 2.7 Hz, 1H), 7.15 (ddd, *J* = 8.0, 7.0, 1.1 Hz, 1H).

2.3 Synthesis of starting materials for photochemical procedures

2.3.1 Synthesis of (E)-1-phenylethan-1-one O-methyl oxime **1b-*E***



1b-*E*

(*E*)-1-phenylethan-1-one O-methyl oxime 1b-*E* was synthesized using a reported procedure.[38]

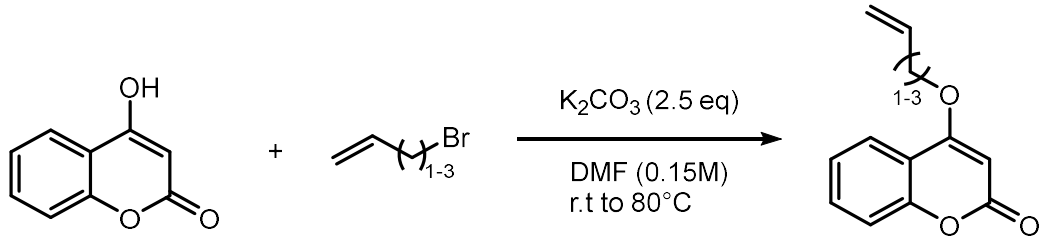
In a 100 mL 2 neck RBF equipped with a water condenser were placed 2.05 mL (16.6 mmol, 1.0 eq.) of acetophenone, 1.94 g (19.9 mmol, 1.2 eq.) of $MeONH_2 \cdot HCl$, 6.95 ml (86.3 mmol, 5.2 eq.) of pyridine and 42 ml of EtOH. The reaction mixture was stirred under reflux overnight. The reaction crude was quenched by the addition of water, and the organic components were extracted twice with EtOAc. The combined organic layers were washed with 1 M aqueous HCl and brine, dried over $MgSO_4$, and concentrated under reduced pressure to afford acetophenone oxime **1b-*E***.

(*E*)-1-phenylethan-1-one O-methyl oxime (1b-*E*): colorless oil; 88 % y*ield (2.18 g, 14.6 mmol)*.

The NMR spectrum agrees with the reported data:[38]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 – 7.62 (m, 2H), 7.37 (m, 3H), 4.00 (s, 3H), 2.23 (s, 3H).

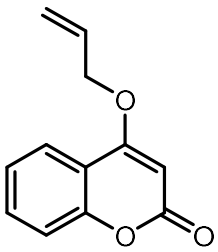
2.3.2 General procedure for the synthesis of coumarins for intramolecular [2+2] reactions 3a-c



3a-c

Coumarins **3a-c** were synthesized following a reported procedure.[39]

To a stirred solution of 4-hydroxycoumarin (1.0 mmol, 1.0 eq.) in DMF (6 mL) were added 345 mg (2.5 mmol, 2.5 eq.) of potassium carbonate (K_2CO_3) and the relative alkenyl-bromide (1.5 mmol, 1.5 eq.) at room temperature. The reaction mixture was heated at 80 °C, stirred for 1 h, and then quenched with ice-cold water. The resulting precipitate was collected by filtration, washed sequentially with water followed by petroleum ether, and then dried to afford **3a-c** as off-white solids. No further purification was necessary unless otherwise noted.



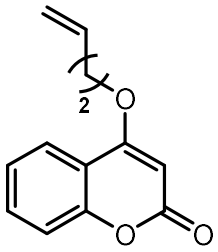
3a

4-(allyloxy)-2H-chromen-2-one (**3a**) was synthesized using allyl bromide (130 µL, 1.5 mmol, 1.5 eq.) as alkenylating agent.

4-(allyloxy)-2H-chromen-2-one (**3a**):
white solid; 51 % y*ield (103 mg, 0.51 mmol)*.

For **3a** a further purification step via column chromatography was necessary (gradient of *n*-hexane / EtOAc). The NMR spectrum agrees with the reported data:[39]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.53 (ddd, *J* = 8.6, 7.3, 1.7 Hz, 1H), 7.30 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.24 (ddd, *J* = 8.1, 7.3, 1.0 Hz, 1H), 6.07 (ddt, *J* = 17.2, 10.7, 5.5 Hz, 1H), 5.69 (s, 1H) 5.49 (dq, *J* = 17.2, 1.5 Hz, 1H), 5.40 (dq, *J* = 10.5, 1.3 Hz, 1H), 4.68 (dt, *J* = 5.5, 1.5 Hz, 2H).



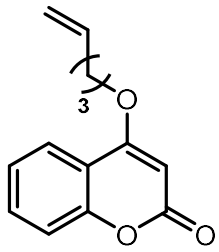
3b

4-(but-3-en-1-yloxy)-2H-chromen-2-one (**3b**) was synthesized using But-3-en-1-yl bromide (152 µL, 1.5 mmol, 1.5 eq.) as alkenylating agent.

4-(but-3-en-1-yloxy)-2H-chromen-2-one (**3b**):
white solid; 65 % y*ield (141 mg, 0.65 mmol)*.
The NMR spectrum agrees with the reported data:[40]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.55 (ddd, *J* = 8.4, 7.3, 1.7 Hz, 1H), 7.32 (dd, *J* = 8.3, 0.7 Hz, 1H), 7.30 – 7.25 (ddd, *J* = 8.1, 7.3, 1.0 Hz, 1H), 5.91 (ddt, *J* = 17.0, 10.2,

6.8 Hz, 1H), 5.68 (s, 1H), 5.24 (dq, *J* = 17.2, 1.6 Hz, 1H), 5.18 (dq, *J* = 10.3, 1.3 Hz, 1H), 4.19 (t, *J* = 6.5 Hz, 2H), 2.67 (qt, *J* = 6.6, 1.4 Hz, 2H).



3c

4-(pent-4-en-1-yloxy)-2H-chromen-2-one (**3c**) was synthesized according to 2.3.2 General procedure for the synthesis of coumarins for intramolecular [2+2] reactions **3a-c** using 4-Pentenyl bromide (177 µL, 1.5 mmol, 1.5 eq.) as alkenylating agent.

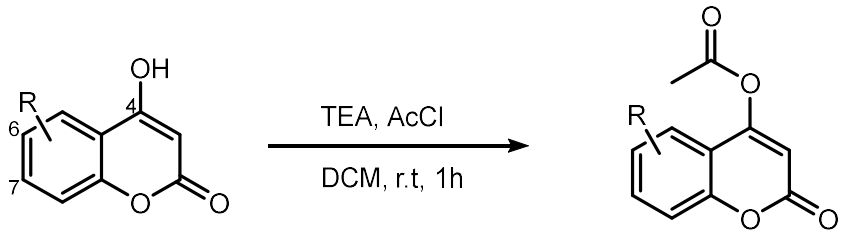
4-(pent-4-en-1-yloxy)-2H-chromen-2-one (**3c**):

white solid; 75 % y*ield (173 mg, 0.75 mmol)*.

The NMR spectrum agrees with the reported data:[41]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.55 (ddd, *J* = 8.7, 7.3, 1.6 Hz, 1H), 7.32 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.28 (ddd, *J* = 8.3, 7.3, 1.1 Hz, 1H), 5.86 (ddt, *J* = 16.9, 10.2, 6.7 Hz, 1H), 5.67 (s, 1H), 5.09 (dq, *J* = 17.1, 1.6 Hz, 1H), 5.06 (dt, *J* = 10.1, 1.4 Hz, 1H), 4.15 (t, *J* = 6.3 Hz, 2H), 2.30 (dtd, *J* = 7.7, 6.7, 1.4 Hz, 2H), 2.03 (dt, *J* = 7.7, 6.4 Hz, 2H).

2.3.3 General procedure for the synthesis of coumarins for interamolecular [2+2] reactions 5a-c

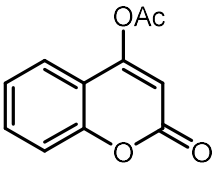


5a' R= -H
5b' R= 7 -OMe
5c' R= 6 -F

5a R= -H
5b R= 7 -OMe
5c R= 6 -F

Coumarins **5a-c** were synthesized following a reported procedure.[42]

To a stirred solution of 4-hydroxycoumarin **5a'-c'** (1.0 mmol, 1.0 eq.) in DCM (10 mL) were added 209 µL (1.5 mmol, 1.5 eq.) of triethylamine (TEA) and 107 µL (107 µL, 1.5 mmol, 1.5 eq.) of acetyl chloride (AcCl) at room temperature. The reaction mixture stirred for 1 h at the same temperature. The reaction was poured into water (30 mL), and the mixture was stirred vigorously for 30 min. The aqueous phase was extracted with EtOAc (3 x 30 mL). The combined organic phases were washed with 1 M aq. HCl (20 mL), saturated aq. $NaHCO_3$ (1 x 20 mL), water (1 x 20 mL) and brine (1 x 20 mL), and dried over anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure. No further purification was necessary.



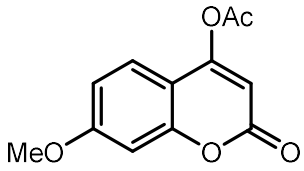
5a

2-oxo-2H-chromen-4-yl acetate (**5a**):

white solid; 95 % y*ield (194 mg, 0.95 mmol)*.

The NMR spectrum agrees with the reported data:[42]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.59 (ddd, *J* = 8.8, 7.4, 1.6 Hz, 1H), 7.37 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.31 (ddd, *J* = 8.3, 7.3, 1.1 Hz, 1H), 6.52 (s, 1H), 2.45 (s, 3H).



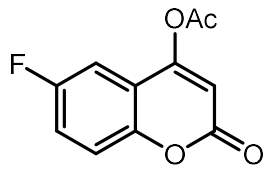
5b

7-methoxy-2-oxo-2H-chromen-4-yl acetate (5b):

white solid; 93 % y*ield (218 mg, 0.93 mmol)*.

The NMR spectrum agrees with the reported data:[43]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 8.5, 0.6 Hz, 1H), 6.90 – 6.81 (m, 2H), 6.34 (s, 1H), 3.88 (s, 3H), 2.43 (s, 3H).



5c

6-fluoro-2-oxo-2H-chromen-4-yl acetate (**5c**):

pale yellow solid; 90 % y*ield (200 mg, 0.90 mmol)*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.37 – 7.27 (m, 3H), 6.60 (d, *J* = 0.8 Hz, 1H), 2.45 (s, 3H).

^{19}F NMR (376 MHz, $CDCl_3$) δ -116.62 (td, *J* = 7.8, 4.3 Hz).

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.49, 161.20, 158.87 (d, *J* = 244.7 Hz), 157.40 (d, *J* = 2.7 Hz), 149.85 (d, *J* = 2.0 Hz), 120.42 (d, *J* = 24.5 Hz), 118.92 (d, *J* = 8.2 Hz), 116.45 (d, *J* = 9.0 Hz), 108.75 (d, *J* = 25.6 Hz), 106.00, 21.44.

HRMS (MALDI-TOF) = calculated for $C_{11}H_7FO_4$; $[M]^{\cdot+}$: 222.0328; found 222.0325

3. Synthesis and Characterization of Photocatalysts C1-C6

3.1 General procedure for the synthesis of Photocatalysts C1-C6

All photocatalysts studied consist in fully heteroleptic tris-aryl boranes and were obtained using the following general procedure in Figure S3 (a slightly modified procedure of a previous report).[44]

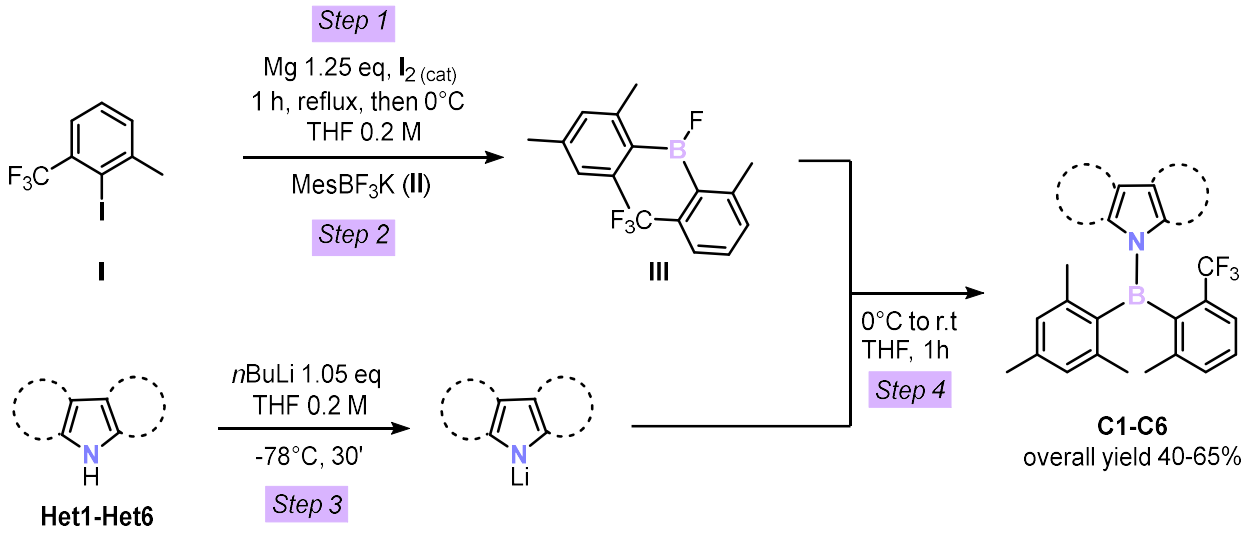
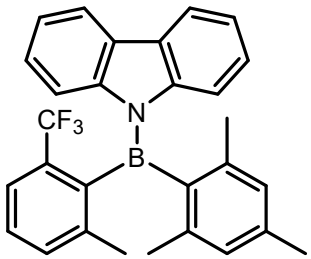


Figure S3 Scheme for the synthesis of photocatalysts **C1-C6** starting from intermediates **I-III** and metalated **Het1-6.**

In a heat-vacuum dried Schlenk tube under argon atmosphere 1.0 mmol (1.0 eq.) of aromatic heterocyclic compound (**Het1-Het6**) were dissolved in 2.5 mL of dry THF (0.4 M). The solution was cooled to -78 °C with a liquid nitrogen – acetone bath and 656 µL (1.05 mmol, 1.05 eq.) of a 1.6 M solution of *n*-BuLi were slowly added with an airtight syringe trough a rubber septum. The solution was stirred for 30 minutes at the same temperature. Consecutively, a solution of 339 mg (1.1 mmol, 1.1 eq.) of fluoro(mesityl)(2-methyl-6-(trifluoromethyl)phenyl) borane (**III**) dissolved in 11 mL of dry THF (0.1 M) was slowly added trough a pressure equalized fritted dropping funnel while keeping the temperature at -78 °C under argon atmosphere. 5 mL of dry THF were added to wash the filter. The cooling bath was removed after 30 minutes, and the solution was stirred for an additional 90 minutes at room temperature. The reaction was quenched by the addition of 5 mL of DCM and transferred to a 1 neck 50 mL RBF washing the tube with additional 5 mL of DCM. 2 g of flash silica (60 µm) were added and the solvent removed under reduced pressure. The reaction crude was dry loaded for flash chromatography as is (eluent: hexane/DCM) to yield pure **C1-C6**.

3.1.1 Synthesis and characterization of 9-(mesityl(2-methyl-6-(trifluoromethyl)phenyl)boraneyl)-9H-carbazole (C1):



C1

The product was purified by flash column chromatography with a gradient of *n*-hexane : DCM 100:0 to 95:5 v/v.

White powder; 60% y*ield (273 mg, 0.6 mmol)*.

TLC *Rf: 0.35 (n*-hexane : DCM = 95:5). *A vanillin stain was used for these compounds as the azole was slowly released upon strong heating and a purple stain is observed.*

Single crystals suitable for X-Ray analysis (see 9.1.1 X-Ray Crystallography of **C1**) were obtained by dissolving ≈ 5 mg of **C1** in the minimum amount of DCM, and diluting with *n*-hexane. The solution was slowly evaporated into a 2 mL vial capped with a punctured HPLC septa.

HRMS (MALDI-qTOF) = calculated for $C_{29}H_{25}BF_3NNa^+$ ($[M+Na]^+$): 478.1924; found 478.1912.

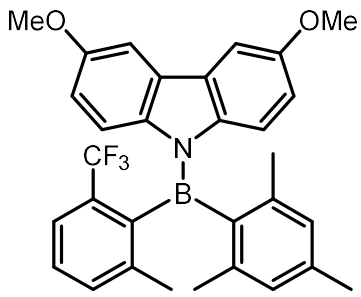
Note for the NMR spectra: Certain resonances in the ^1H and ^{13}C NMR spectra appear broadened or split as a consequence of slow B–C bond rotation on the NMR timescale. The ^{13}C resonances corresponding to the two quaternary carbons bonded to boron are not observed, likely due to signal broadening arising from coupling to the boron nucleus.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.8 Hz, 2H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.32 – 7.26 (m, 2H), 7.23 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.11 (ddd, *J* = 8.4, 7.1, 1.3 Hz, 1H), 7.04 (m, 2H), 6.85 (s, 1H), 6.81 (s, 1H), 6.68 (s, 1H), 2.32 (s, 3H), 1.99 (bs, 6H), 1.90 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.53 (br), 143.00, 142.95, 142.51, 142.02, 140.31, 133.90, 133.24 (q, $^2J_{C-F}$ = 30.5 Hz), 129.64, 129.41, 129.21, 128.34, 128.18, 126.55, 126.26, 125.00 (q, $^1J_{C-F}$ = 276.1 Hz), 124.12, 122.98, 122.82, 119.79, 119.69, 115.50, 22.30, 22.24, 21.91(br), 21.47.

^{19}F NMR (376 MHz, $CDCl_3$) δ -57.20.

3.1.2 Synthesis and characterization of 9-(mesityl(2-methyl-6-(trifluoromethyl)phenyl) boraneyl) -3,6-dimethoxy-9H-carbazole (C2):



C2

The product was purified by flash column chromatography with a gradient of *n*-hexane:DCM 100:0 to 95:5.

White powder; 60 % y*ield (309 mg, 0.6 mmol)*.

TLC *Rf: 0.25 (n*-hexane:DCM = 95:5). *A vanillin stain is used for these compounds as the azole is slowly released upon strong heating and a purple stain is observed.*

Single crystals suitable for X-Ray analysis (see 9.1.2 X-Ray Crystallography of C2). were obtained by dissolving ≈ 5 mg of **C1** in the minimum amount of DCM, and diluting with acetonitrile. The solution was slowly evaporated into a 8 mL vial capped with a punctured HPLC septa.

HRMS (MALDI-qTOF) = calculated for $C_{31}H_{29}BF_3KNO_2^+$; $[M+K]^+$: 554.1875; found 554.1886.

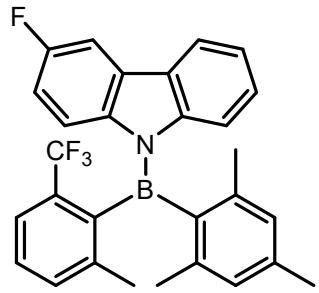
Note for the NMR spectra: Certain resonances in the ^1H and ^{13}C NMR spectra appear broadened or split as a consequence of slow B–C bond rotation on the NMR timescale. The ^{13}C resonances corresponding to the two quaternary carbons bonded to boron are not observed, likely due to signal broadening arising from coupling to the boron nucleus.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.9 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.37 (dd, *J* = 2.7, 1.5 Hz, 2H), 7.29 (d, *J* = 7.6 Hz, 1H), 6.90 (dd, *J* = 9.0, 0.5 Hz, 1H), 6.84 (s, 1H), 6.81 (s , 1H), 6.70 (dd, *J* = 9.1, 2.7 Hz, 1H), 6.63 (dd, *J* = 9.0, 2.7 Hz, 1H), 6.53 (d, *J* = 9.1 Hz, 1H), 3.89 (s, 3H), 3.87 (s, 3H), 2.32 (s, 3H), 2.00 (2 singlets overlapping, 6H), 1.90 (s, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 155.94, 155.83, 142.81, 142.26, 139.86, 137.80, 133.70, 129.41, 129.10, 128.95, 128.93, 116.41, 116.33, 114.68, 114.32, 102.54, 102.32, 55.70, 22.13, 22.04, 21.70, 21.32.

^{19}F NMR (376 MHz, $CDCl_3$) δ -57.48 (broad).

3.1.3 Synthesis and characterization of 3-fluoro-9-(mesityl(2-methyl-6-(trifluoromethyl) phenyl)boraneyl)-9H-carbazole (C3):



C3

The product was purified by flash column chromatography with a gradient of *n*-hexane : DCM 100:0 to 95:5 v/v.

White powder; 52 % y*ield (246 mg, 0.52 mmol)*.

TLC *Rf: 0.35 (n*-hexane:DCM = 95:5). *A vanillin stain is used for these compounds as the azole is slowly released upon strong heating and a purple stain is observed.*

Due to the high rotational barrier around the B-N bond, a mixture of *E:Z* isomers (B=N) were obtained in a ratio ≈ 1:1. The mixture of isomers was not separated and used as is.

HRMS (MALDI-qTOF) = calculated for $C_{29}H_{24}BF_4NNa^+$([M+Na]$^+$): 496.1830; found 496.1819.

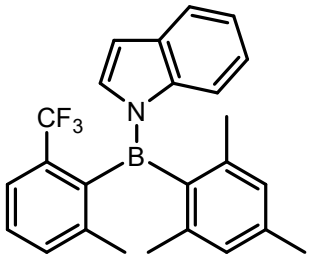
Note for the NMR spectra: The presence of *E* and *Z* isomers results in a doubling of the number of observed signals. Furthermore, certain resonances in the ^{1}H and ^{13}C NMR spectra appear broadened or split as a consequence of slow B–C bond rotation on the NMR timescale. The ^{13}C resonances corresponding to the two quaternary carbons bonded to boron are not observed, likely due to signal broadening arising from coupling to the boron nucleus.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (dtd, *J* = 7.7, 1.5, 0.7 Hz, 1H), 7.61 (dd, *J* = 8.3, 2.5 Hz, 2H), 7.47 (t, *J* = 7.8 Hz, 1H), 7.31 (d, *J* = 7.7 Hz, 1H), 7.29 – 7.27 (m, 0.5H), 7.24 (d, *J* = 7.5 Hz, 0.5H), 7.14 (ddd, *J* = 8.5, 7.2, 1.3 Hz, 0.5H), 7.09 – 7.06 (m, 0.5H), 7.04 (dt, *J* = 8.5, 0.8 Hz, 0.5H), 6.96 (dd, *J* = 9.1, 4.5 Hz, 0.5H), 6.85 (s, 1H), 6.83 (dd, *J* = 9.0, 2.7 Hz, 0.5H), 6.81 (d, *J* = 1.6 Hz, 1H), 6.76 (td, *J* = 9.0, 2.7 Hz, 0.5H), 6.66 (s, 1H), 6.59 (s, 1H), 2.32 (s, 3H), 2.00 – 1.97 (m, 6H), 1.89 (d, *J* = 2.2 Hz, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 160.29, 158.70, 158.57, 143.76, 142.94, 142.50, 141.95, 140.49, 140.44, 139.59, 139.02, 133.97, 133.95, 133.33, 133.13, 129.73, 129.68, 129.55, 129.52, 129.34, 129.30, 129.26, 127.74, 127.61, 127.59, 127.18, 126.89, 125.80, 124.19, 123.98, 123.06, 122.89, 120.03, 119.92, 116.51, 116.45, 116.38, 116.32, 115.67, 115.64, 114.06, 113.90, 113.79, 113.63, 105.78, 105.62, 105.46, 32.38, 32.08, 29.85, 29.81, 29.52, 22.85, 22.29, 22.27, 22.20, 22.18, 21.87, 21.47, 14.28.

^{19}F NMR (565 MHz, $CDCl_3$) δ -57.32, -120.43.

3.1.4 Synthesis and characterization of 1-(mesityl(2-methyl-6-(trifluoromethyl)phenyl) boraneyl)-1H-indole (C4):



C4

The product was purified by flash column chromatography with a gradient of *n*-hexane:DCM 100:0 to 95:5.

white powder; 55 % y*ield (223 mg, 0.55 mmol)*.

TLC *Rf: 0.30 (n*-hexane:DCM = 95:5). *A vanillin stain is used for these compounds as the azole is slowly released upon strong heating and a purple stain is observed.*

Due to the high rotational barrier around the B-N bond, a mixture of *E:Z* isomers (B=N) were obtained in a ratio ≈ 1:1. The mixture of isomers was not separated and used as is.

1-(mesityl(2-methyl-6-(trifluoromethyl)phenyl) boraneyl)-1H-indole (**C4**):
white powder; 55 % y*ield (223 mg, 0.55 mmol)*.

HRMS (MALDI-qTOF) = calculated for $C_{25}H_{23}BF_3NNa^+([M+Na])^+$: 428.1768; found 428.1778.

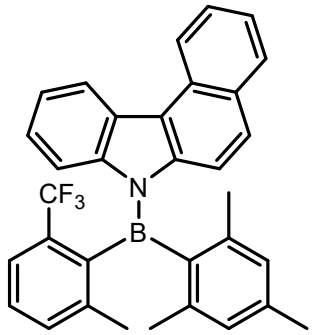
Note for the NMR spectra: The presence of *E* and *Z* isomers results in a doubling of the number of observed signals. Furthermore, certain resonances in the ^{1}H and ^{13}C NMR spectra appear broadened or split as a consequence of slow B–C bond rotation on the NMR timescale. The ^{13}C resonances corresponding to the two quaternary carbons bonded to boron are not observed, likely due to signal broadening arising from coupling to the boron nucleus.

^{1}H NMR (600 MHz, $CDCl_3$) *Sum of isomers* δ 7.60 (d, *J* = 7.9 Hz, 1H), 7.56 – 7.52 (m, 2.6H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 0.8H), 7.35 (d, *J* = 7.7 Hz, 0.8H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.19 – 7.11 (m, 2.8H), 7.03 (dq, *J* = 8.3, 0.9 Hz, 0.8H), 6.99 (ddd, *J* = 8.3, 7.0, 1.3 Hz, 0.8H), 6.92 – 6.84 (m, 3.6H), 6.81 (s, 0.8H), 6.78 (s, 1H), 6.70 (dd, *J* = 3.5, 0.8 Hz, 1H), 6.66 (dd, *J* = 3.5, 0.8 Hz, 0.8H), 6.53 (d, *J* = 8.4 Hz, 1H), 2.32 (s, 2.4H), 2.30 (s, 3H), 2.11 (s, 5.4H), 1.97 (s, 2.4H), 1.96 (s, 3H), 1.95 (s, 3.0H), 1.94 (s, 2.4H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.49, 143.14, 143.01, 142.48, 142.32, 141.92, 140.29, 139.81, 139.75, 133.71, 133.48, 133.37, 133.24, 133.18, 133.10, 132.96, 132.76, 131.85, 129.33, 129.18, 128.99, 128.81, 128.63, 125.68, 125.65, 123.86, 123.84, 123.67 (4C), 123.34 (2C), 123.27, 123.03, 122.92, 122.83, 120.58, 120.50, 115.05, 114.85, 110.49, 110.40, 29.71, 22.62, 22.61, 22.56, 22.35, 22.09, 21.79, 21.77, 21.31, 21.20.

^{19}F NMR (376 MHz, $CDCl_3$) δ -57.14.

3.1.5 Synthesis and characterization of 7-(mesityl(2-methyl-6-(trifluoromethyl)phenyl) boraneyl)-7H-benzo[c]carbazole (C5):



C5

The product was purified by flash column chromatography with a gradient of *n*-hexane:DCM 100:0 to 95:5.

White powder; 58 % y*ield (293 mg, 0.58 mmol)*.

TLC *Rf: 0.45 (n*-hexane:DCM = 95:5). *A vanillin stain is used for these compounds as the azole is slowly released upon strong heating and a purple stain is observed.*

Due to the high rotational barrier around the B-N bond, a mixture of *E:Z* isomers (B=N) were obtained in a ratio ≈ 1:1. The mixture of isomers was not separated and used as is.

HRMS (MALDI-qTOF) = calculated for $C_{33}H_{27}BF_3NK^+$ ($[M+K]^+$): 544.1820; found 544.1812.

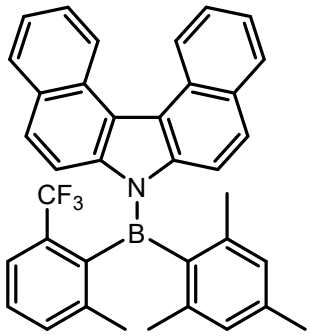
Note for the NMR spectra: The presence of *E* and *Z* isomers results in a doubling of the number of observed signals. Furthermore, certain resonances in the ^{1}H and ^{13}C NMR spectra appear broadened or split as a consequence of slow B–C bond rotation on the NMR timescale. The ^{13}C resonances corresponding to the two quaternary carbons bonded to boron are not observed, likely due to signal broadening arising from coupling to the boron nucleus.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.86 – 8.81 (m, 2H), 8.55 (dt, *J* = 8.1, 1.4 Hz, 2H), 7.90 (ddd, *J* = 15.3, 8.2, 1.3 Hz, 2H), 7.69 (dddd, *J* = 8.3, 6.8, 2.3, 1.3 Hz, 2H), 7.63 (t, *J* = 7.0 Hz, 2H), 7.56 (d, *J* = 9.1 Hz, 1H), 7.53 – 7.43 (m, 5H), 7.43 – 7.34 (m, 2H), 7.31 (d, *J* = 9.1 Hz, 1H), 7.25 – 7.20 (m, 1H), 7.15 (ddd, *J* = 8.4, 7.1, 1.2 Hz, 1H), 7.09 (ddd, *J* = 8.4, 7.1, 1.2 Hz, 1H), 7.03 – 6.97 (m, 1H), 6.87 – 6.81 (m, 4H), 2.33 (s, 5H), 1.52 (s, 1H), 1.32 – 1.22 (m, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 171.2, 143.0, 142.9, 142.6, 142.5, 142.3, 142.0, 141.9, 141.4, 140.7, 140.6, 140.5, 136.6, 133.9, 133.8, 133.2, 133.0, 132.8, 130.7, 130.5, 129.6, 129.6, 129.5, 129.5, 129.2, 129.1, 128.9, 128.9, 128.7, 128.6, 127.5, 127.3, 127.1, 126.9, 126.8, 125.7, 125.7, 125.1, 124.8, 124.2, 124.2, 124.1, 124.0, 123.9, 123.9, 123.8, 123.6, 123.2, 123.0, 122.1, 121.8, 121.7, 121.2, 121.0, 115.6, 115.5, 115.3, 77.2, 77.0, 76.8, 68.0, 60.4, 31.9, 31.6, 29.7, 25.6, 22.7, 22.2, 22.1, 22.1, 21.8, 21.4, 21.1, 14.2, 14.1, 1.0, -0.0.

^{19}F NMR (565 MHz, $CDCl_3$) δ -57.0

3.1.6 Synthesis and characterization of 7-(mesityl(2-methyl-6-(trifluoromethyl)phenyl) boraneyl)-7H-dibenzo[c,g]carbazole (C6):



C6

The product was purified by flash column chromatography with a gradient of *n*-hexane:DCM 100:0 to 95:5.

White powder; 55 % y*ield (305 mg, 0.55 mmol)*.

TLC *Rf: 0.5 (n*-hexane:DCM = 95:5). *A vanillin stain is used for these compounds as the azole is slowly released upon strong heating and a purple stain is observed.*

HRMS (MALDI-qTOF) = calculated for $C_{37}H_{29}BF_3KN^+$ ($[M+K]^+$): 594.1977; found 594.1967.

Note for the NMR spectra: Certain resonances in the ^1H and ^{13}C NMR spectra appear broadened or split as a consequence of slow B–C bond rotation on the NMR timescale. The ^{13}C resonances corresponding to the two quaternary carbons bonded to boron are not observed, likely due to signal broadening arising from coupling to the boron nucleus.

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.08 (dd, *J* = 8.5, 1.1 Hz, 2H), 7.94 (ddd, *J* = 14.7, 8.1, 1.5 Hz, 2H), 7.64 (ddt, *J* = 8.4, 6.8, 1.6 Hz, 2H; m, 1H), 7.59 (d, *J* = 9.0 Hz, 1H), 7.55 – 7.48 (m, 4H), 7.37 (d, *J* = 9.0 Hz, 1H), 7.32 (bs, 1H), 7.13 (bs, 1H), 6.87 (s, 2H), 2.35 (s, 3H), 1.91 (s, 9H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 143.18, 142.75, 140.84, 133.93, 131.18, 130.98, 129.69, 129.23, 128.66, 128.62, 128.29, 126.88, 126.65, 126.03, 125.68, 125.08, 125.05, 124.30, 124.09, 123.87, 123.04, 115.24, 22.18 (*broad signal, 4 methyls)*, 21.40.

^{19}F NMR (376 MHz, $CDCl_3$) δ -56.89.

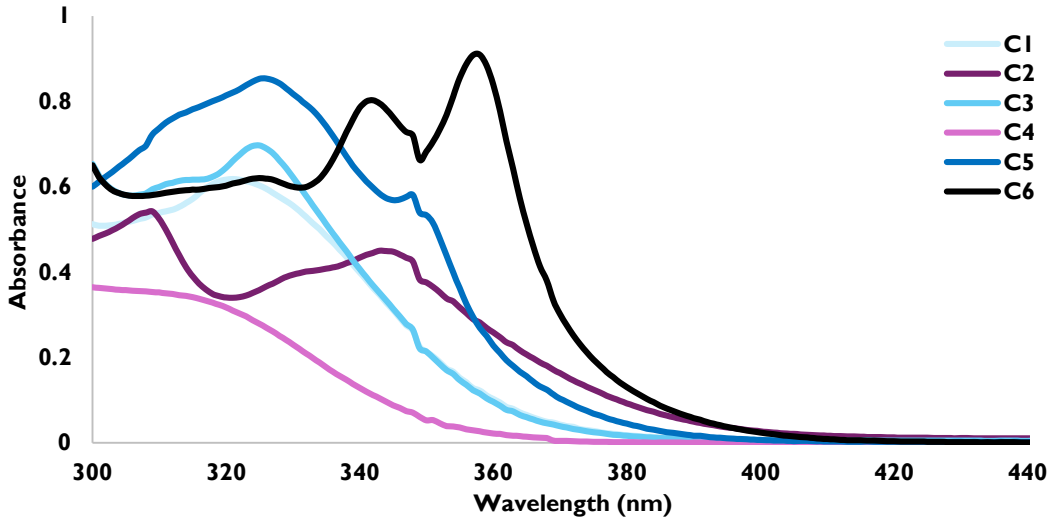
3.2 Photophysical measurements of Photocatalysts C1-C6

Sample Preparation: Six 25 mL glass vials, each containing one catalyst amongst **C1-C6** were sealed with a septum and degassed. Then, dry and degassed THF (20 mL) was added to each vial to prepare 0.1 M solutions of the catalysts. The 10^{-4} M solutions were prepared from the stock solutions by dilution. Then, 2.5 mL of each solution was transferred into an argon-filled quartz cuvette (10 x 10 mm light path) equipped with a septum.

3.2.1 Absorption spectra and ε of C1-C5

UV-Vis measurements were carried out on a Cary 3500 Multicell UV-Vis spectrophotometer equipped with two silicon diode detectors, double beam optics and Xenon pulse light (Figure S4-Figure S5).

The data shown in Figure S4 was used to derive the molar absorptivity coefficient and in particular the ε_{427} shown in the study (Figure 2e).



Wavelength / nm (Kessil® lamp)	C1 ε (M^{-1} cm^{-1})	C2 ε (M^{-1} cm^{-1})	C3 ε (M^{-1} cm^{-1})	C4 ε (M^{-1} cm^{-1})	C5 ε (M^{-1} cm^{-1})
370	430	1629	391	49	1035
390	94	492	88	5	165
427	61	113	55	3	16
440	55	99	49	1	14

Figure S4 Top: UV-Vis absorption spectra of **C1-C6** in 10^{-4} M degassed THF solutions recorded at 298K; **bottom:** Derived ε at different wavelengths.

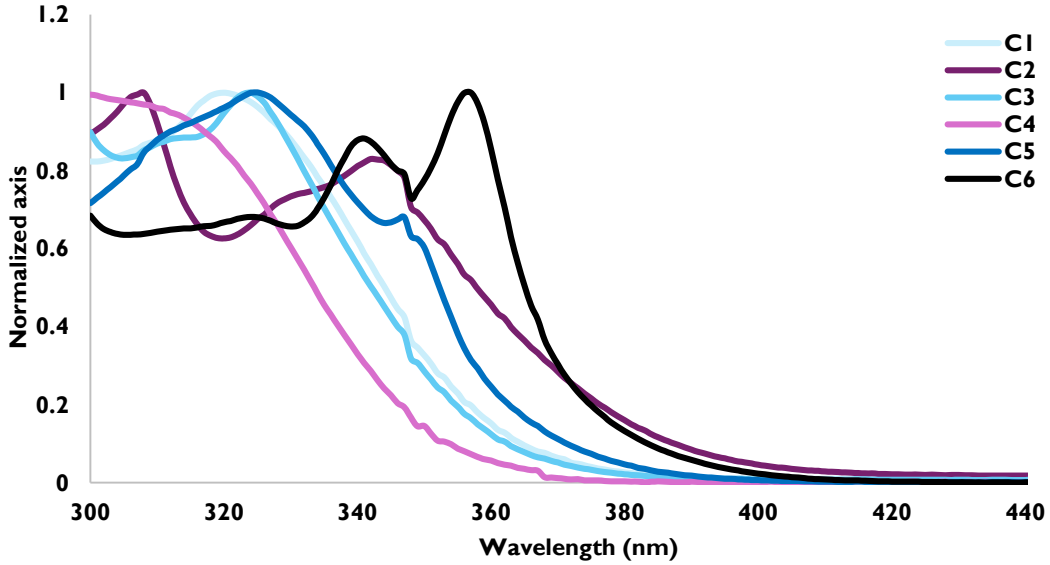


Figure S5 Normalized UV-Vis absorption spectra of **C1-C6** in 10^{-4} M degassed THF solutions recorded at 298K.

3.2.2 Excitation and emission spectra of C1-C6 at 298K and 77K: determination of E_T

Fluorescence measurements (excitation and emission profiles) were carried out on an Edinburgh FLSP920 spectrometer equipped with a 450 W xenon arc lamp, double excitation and single emission monochromators, and a Peltier-cooled Hamamatsu R928P photomultiplier tube (185−850 nm).

The normalized excitation profiles of photocatalysts **C1-C6** at 298K and 77K (Figure S6 and Figure S7, respectively) show broad excitation bands, typical of charge transfer (CT) complexes.[45]

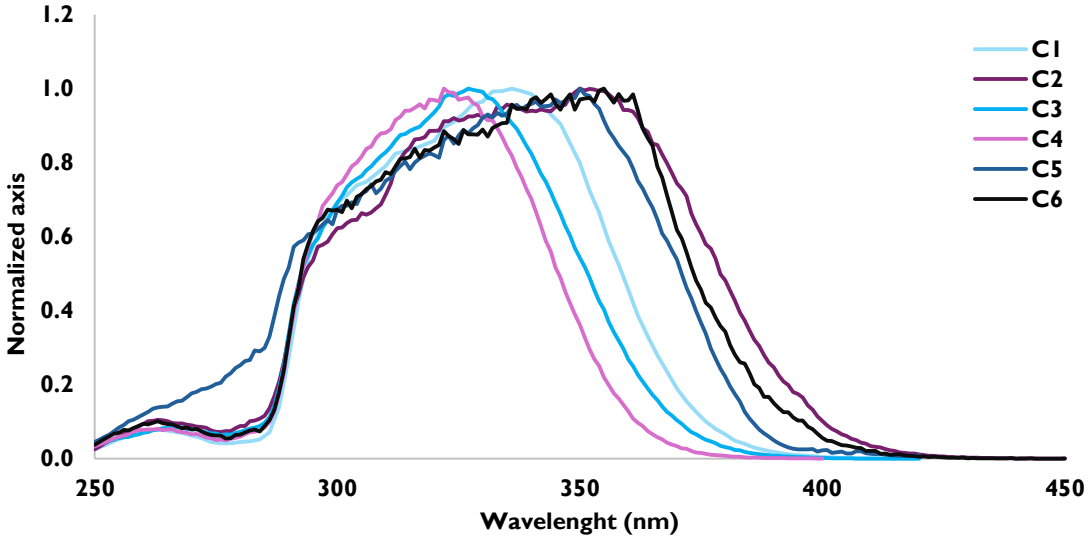


Figure S6 *Normalized* excitation profiles in the range of 250-450 nm for **C1-C6** in 10^{-4} M THF solutions at 298K. In all cases the emission maxima from Figure S8 were used as reference for studying excitation profiles.

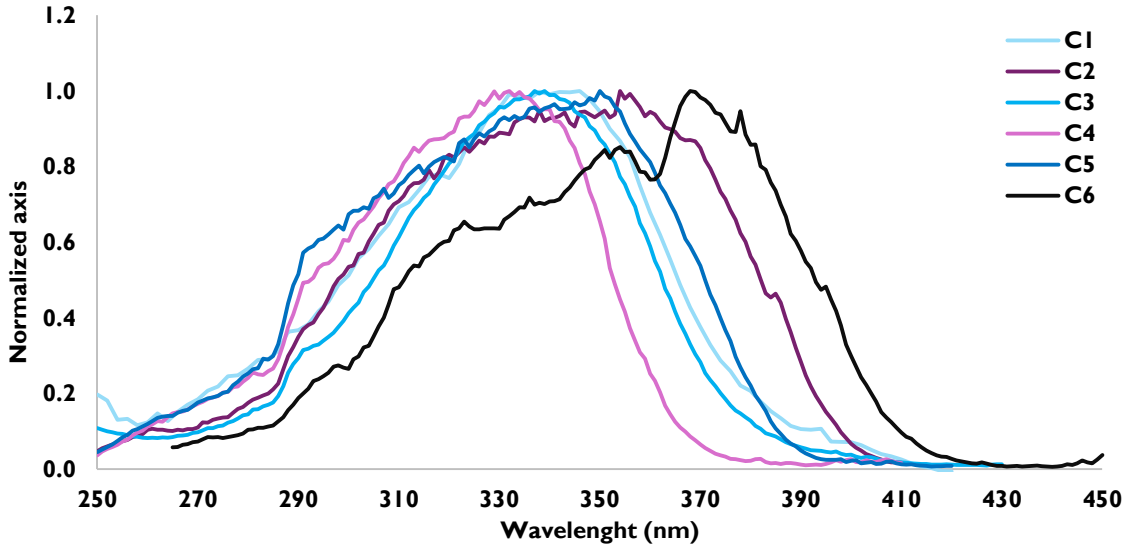


Figure S7 *Normalized* excitation profiles in the range of 250-450 nm for **C1-C6** in 10^{-4} M THF solutions at 77K (glass matrix). In all cases the emission maxima from Figure S8 were used as reference for studying excitation profiles.

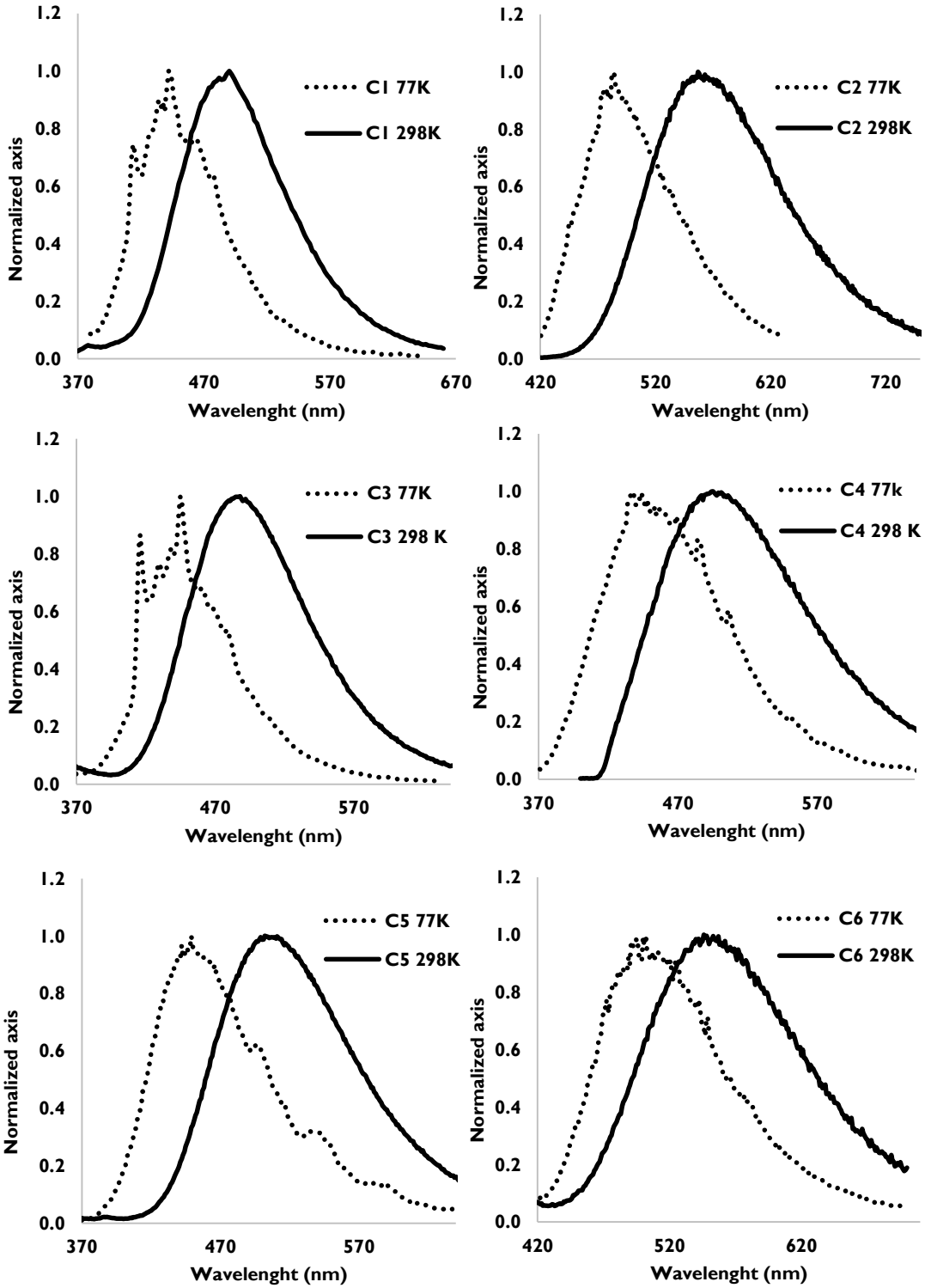


Figure S8 *Normalized* emission profiles for **C1-C6** in 10^{-4} M THF solutions at 298K (solid line) *vs* 77K (dotted line). In all cases the excitation maxima from Figure S6 and Figure S7 were used as reference for studying emission profiles.

The normalized emission profiles of photocatalysts **C1-C6** at 298K and 77K are shown in Figure S8.

Determination of triplet energies:

The triplet energies for the catalysts studied were determined via glassy matrix (77K) emission studies. Catalysts **C1** and **C3** show a clear vibro-electronic progression (Figure S8). The higher energy band was used for the determination of the triplet energy (E_T) for these two compounds.[46] A vibro-electronic progression was lacking in all the other catalysts, so the energy difference between the first vibro-electronic band and the maximum of emission of **C1** was used as a reference for determining the other E_T (**C2**; **C4-C6**). This approach was validated by the computational investigation of the triplets (3.3 DFT and TD-DFT calculations of Photocatalysts) which was in good agreement in most cases with the experimental values obtained as discussed above.

All the catalysts **C1-C6** show a blue-shifted emission upon recording the glassy matrix emission spectra (77K; Dotted lines in Figure S8).[iv] However, all the catalysts showed extremely prolonged lifetime at 77K (in most cases even on the seconds time scale) and μs lifetimes at room temperature (see Table S1 and Table S2). Moreover, due to the charge transfer nature of the excited state, we expected a strong destabilization effect in the absence of any solvent contribution which is lacking in the glassy matrix and could explain the higher energy emission.

[iv] The expected behavior arising from triplet emission at low temperature (phosphorescence) is a red shift compared to the room temperature (fluorescence) emission arising from singlet states. This is the case since triplets have lower energy compared to singlet states.

3.2.3 Overlap of normalized absorption and emission spectra for $E_{0\text{-}0}$ determination

The normalized absorption spectra (Figure S5) and normalized emission spectra at 298K (Figure S8; solid line) of catalysts **C1-C6** were overlapped to determine the experimental value for $E_{0\text{-}0}$ energy (Figure S9). The value is expressed in nanometres and a conversion to eV is presented in Table S1.

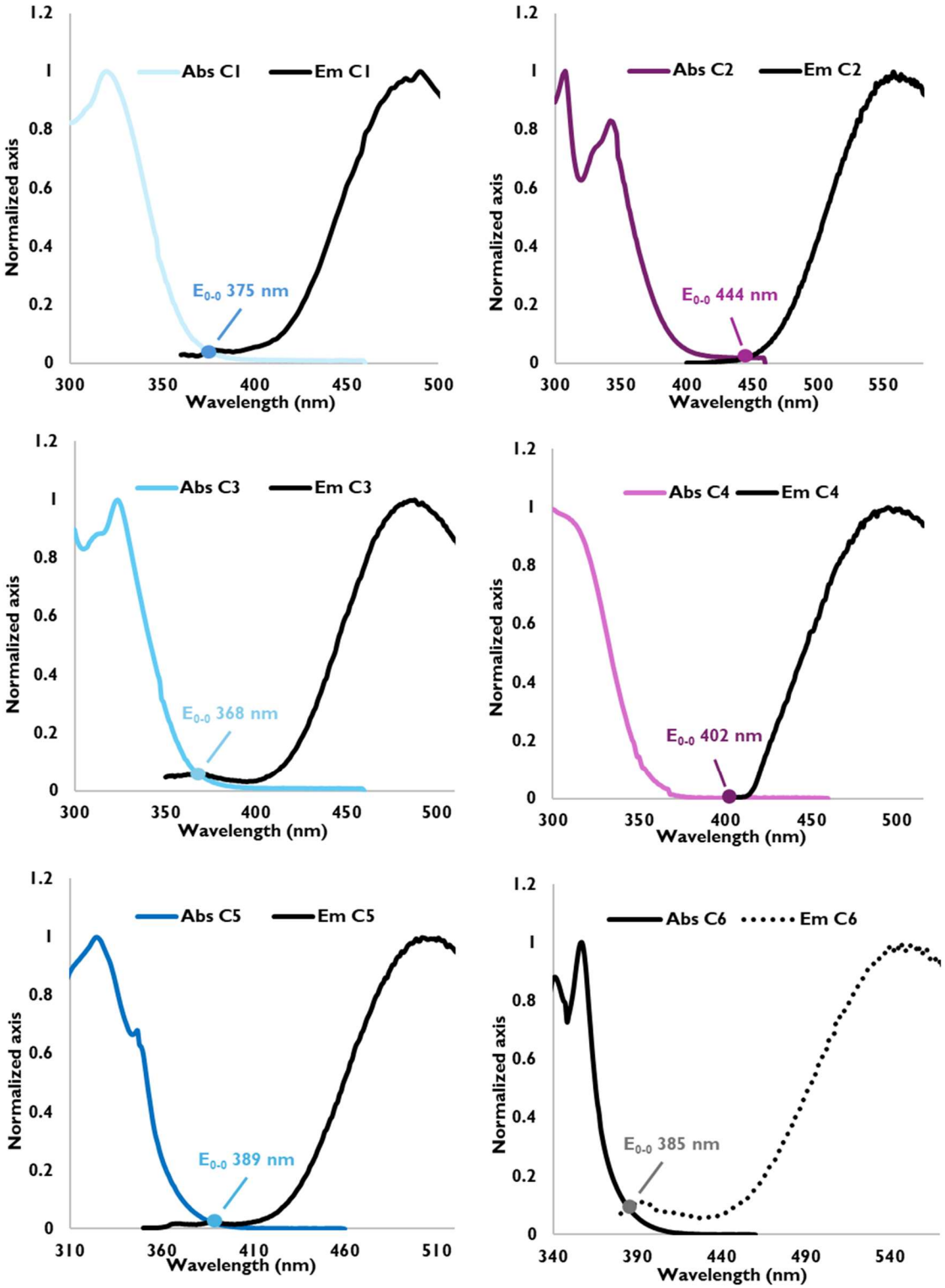


Figure S9 Overlap between *normalized* absorption and emission spectra of **C1-C6** at 298K; the crossing point between the two spectra was used as reference for $E_{0\text{-}0}$ determination.

3.2.4 Solvatochromism of C1-C2:

Three 10^{-4} M solutions of **C1** and **C2** were prepared in degassed HPLC-grade n-hexane, tetrahydrofuran (THF), and acetonitrile (ACN). Emission spectra of **C1** and **C2** were analyzed in these solvents, selected for their increasing polarity, to investigate charge-transfer (CT) states. As anticipated, in both cases, emission wavelengths shift to lower energy with increasing solvent polarity, consistently with greater stabilization of the CT excited states as evident from Figure S10 and Figure S11.

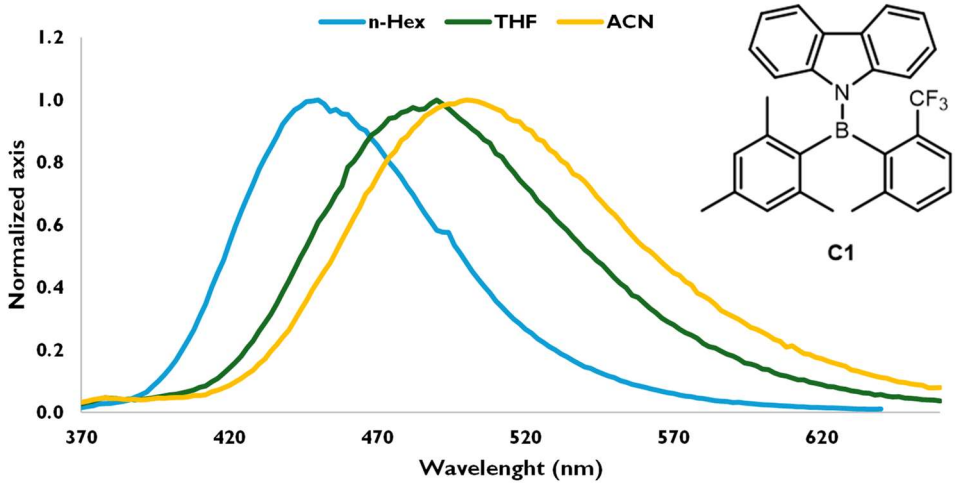


Figure S10 Normalized 298K emission spectra of **C1** in 10^{-4} M solutions of increasing polarity. *n*-hexane: light blue (λ_{exc}: 330 nm); THF: green (λ_{exc}: 336 nm); ACN: yellow (λ_{exc}: 336 nm).

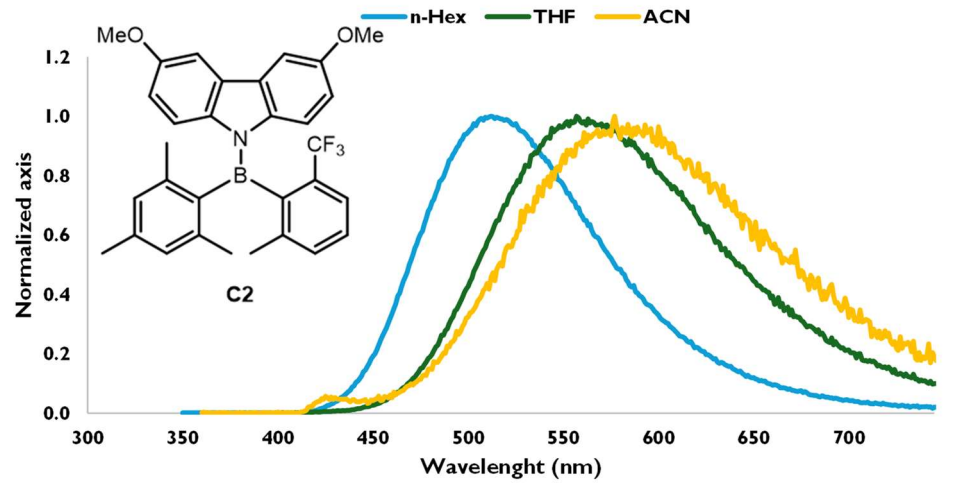


Figure S11 Normalized 298K emission spectra of **C2** in 10^{-4} M solutions of increasing polarity. *n*-hexane: light blue (λ_{exc}: 338 nm); THF: green (λ_{exc}: 352 nm); ACN: yellow (λ_{exc}: 338 nm).

3.2.5 Tables of important photophysical parameters

All the data derived from UV-Vis and emission studies at 298K and 77K are reported below in Table S1 and

Table **S2**, respectively.

Emission lifetimes (τ) in the nanoseconds range were determined via single photon counting technique (TCSPC) with Edinburgh FLSP920 spectrometer using pulsed picosecond LED (EPLED 365, FWHM < 800ps) as the excitation source. Lifetimes in the microseconds range were determined via single photon counting technique (TCSPC) with Edinburgh FLSP920 spectrometer using pulsed nF920 nanosecond flashlamp as the excitation source. Lifetimes in the seconds range were determined via single photon counting technique (TCSPC) with Edinburgh FLSP920 spectrometer using Kinetic Scan function in combination with 450 W continuous Xenon Arc Lamp light as source. The detector was the R928P PMT. The goodness of fit was assessed by minimizing the reduced χ^2 function and by visual inspection of the weighted residuals.

Table S1 Relevant photophysical parameters for **C1-C6** acquired in in 10^{-4} M THF solutions**.** Data acquired at **298K**. [a] **t** T_1 for **C2** was also determined in *n*-hexane and resulted to be 8.6 ms and in $CHCl_3$ to be 8.7 ms.

Cat	Abs λ_{max} / nm	Em λ_{max} / nm	τ S_1 / ns	τ T_1 / μs	$\Delta\lambda_{abs\text{-}em}$ / nm	S_1 / kcal/mol (eV)
C1	321	490	18.0	9.5	169	76.2 (3.30)
C2	309	557	6.2	66.0[a]	248	64.4 (2.79)
C3	325	488	13.0	10.2	163	77.7 (3.37)
C4	300	495	12.3	10.6	195	71.1 (3.08)
C5	326	502	13.5	13.2	176	73.5 (3.19)
C6	358	546	19.7	12.6	188	74.3 (3.22)

Table S2 Relevant photophysical parameters for **C1-C6** acquired in in 10^{-4} M THF solutions**.** Data acquired at **77K**.

Cat	Em λ_{max} / nm	τ S_1 / ns	τ T_1 / s	T_1 / kcal/mol (eV)	$\Delta E(S_1\text{-}T_1)$ / eV
C1	443	5.0	6.0	69.2 (3.00)	0.3
C2	484	5.5	1.9	63.0 (2.73)	0.06
C3	445	4.7	4.6	68.7 (2.98)	0.39
C4	437	12.3	**13 μs**	70.2 (3.04)	0.04
C5	449	13.5	**13.1 μs**	68.2 (2.96)	0.23
C6	502	74.7	1.3	60.8 (2.64)	0.58

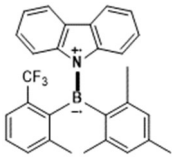
3.3 DFT and TD-DFT calculations of Photocatalysts

3.3.1 Ground state optimized geometries.

A: Cq-Cq-B-N dihedral (°)

B: Cq-B-N-Cq dihedral (°)

C: B-N bond lenght (Å)



		S_0			T_1			S_0 *vs* T_1		
		A	**B**	**C**	**A'**	**B'**	**C'**	**A'-A**	**B'-B**	**C'-C**
C1	GS1	-125.7	29.4	1.441	-137.5	54.4	1.549	-11.8	25.0	0.108
	GS2	-62.4	-31.4	1.441	-38.7	-57.3	1.547	23.7	-25.9	0.106
C2	GS1-conf1	-125.2	27.5	1.433	-137.2	53.6	1.546	-12.0	26.1	0.113
	GS1-conf2	-125.4	27.8	1.434	-137.2	54.1	1.546	-11.8	26.3	0.112
	GS1-conf3	-124.9	27.8	1.434	-137.9	53.8	1.546	-13.0	26.0	0.112
	GS1-conf4	-125.3	28.3	1.435	-137.3	53.0	1.545	-12.0	24.7	0.110
	GS2-conf1	-63.6	-29.2	1.433	-37.8	-56.3	1.544	25.8	-27.1	0.111
	GS2-conf2	-63.0	-29.2	1.434	-36.7	-56.0	1.543	26.3	-26.8	0.109
	GS2-conf3	-63.7	-29.0	1.434	-37.9	-56.8	1.543	25.8	-27.8	0.109
	GS2-conf4	-63.4	-29.6	1.435	-36.5	-55.5	1.542	26.9	-25.9	0.107
C3	GS1-E	-125.6	-144.5	1.441	-137.2	-127.4	1.548	-11.6	17.1	0.107
	GS2-E	-62.3	152.4	1.441	-39	127.7	1.546	23.3	-24.7	0.105
	GS1-Z	-125.5	28.8	1.441	-136.8	54.4	1.548	-11.3	25.6	0.107
	GS2-Z	-62.3	-30.9	1.441	-37.1	-55.9	1.546	25.2	-25.0	0.105
C4	GS1-E	-122.9	-153.9	1.440	-124.7	-155.8	1.442	-1.8	-1.9	0.002
	GS2-E	-65.9	161.6	1.439	-61.9	156.1	1.444	4.0	-5.5	0.005
	GS1-Z	-123.0	22.4	1.440	-125.3	22.8	1.440	-2.3	0.4	0.000
	GS2-Z	-66.2	-17.4	1.438	-61.0	-25.0	1.445	5.2	-7.6	0.007
C5	GS1-E	-126.1	-142.8	1.445	-125.7	-145.9	1.437	0.4	-3.1	-0.008
	GS2-E	-62	151.3	1.446	-63.2	153.7	1.437	-1.2	2.4	-0.009
	GS1-Z	-126.6	30.2	1.445	-126.7	27.1	1.437	-0.1	-3.1	-0.008
	GS2-Z	-61.6	-33	1.445	-62.2	-28.9	1.438	-0.6	4.1	-0.007

Figure S12 Optimized Singlet and Triplet geometries for **C1**-**C5**. DFT level: IEF-PCM(THF) wB97X-D/6-311G(d,p).

			H°	ΔH°	ΔH° (triplet)	pop %	Boltzmann-averaged energy
C1	Singlet	GS1	-1498.779385	**0.00**		53.0%	-1498.776546
	Singlet	GS2	-1498.779272	0.07		47.0%	
	Triplet	GS1	-1498.666349	70.93	1.44	8.0%	-1498.663629
	Triplet	GS2	-1498.668649	69.49	**0.00**	92.0%	
			Triplet-Singlet energy (kcal/mol)				**70.86**
C2	Singlet	GS1-conf1	-1727.743931	1.17		4.7%	-1727.743989
	Singlet	GS1-conf2	-1727.745048	0.47		15.2%	
	Singlet	GS1-conf3	-1727.744782	0.64		11.5%	
	Singlet	GS1-conf4	-1727.745794	**0.00**		33.6%	
	Singlet	GS2-conf1	-1727.743652	1.34		3.5%	
	Singlet	GS2-conf2	-1727.743897	1.19		4.5%	
	Singlet	GS2-conf3	-1727.743833	1.23		4.2%	
	Singlet	GS2-conf4	-1727.745431	0.23		22.9%	
	Triplet	GS1-conf1	-1727.644970	63.27	0.86	8.7%	-1727.644363
	Triplet	GS1-conf2	-1727.643971	63.89	1.49	3.0%	
	Triplet	GS1-conf3	-1727.644202	63.75	1.35	3.8%	
	Triplet	GS1-conf4	-1727.643954	63.90	1.50	3.0%	
	Triplet	GS2-conf1	-1727.646346	62.40	**0.00**	37.3%	
	Triplet	GS2-conf2	-1727.645578	62.89	0.48	16.5%	
	Triplet	GS2-conf3	-1727.645811	62.74	0.34	21.2%	
	Triplet	GS2-conf4	-1727.644704	63.43	1.03	6.5%	
			Triplet-Singlet energy (kcal/mol)				**62.52**
C3	Singlet	GS1-E	-1598.024817	**0.00**		37.8%	-1598.022709
	Singlet	GS2-E	-1598.023997	0.51		15.8%	
	Singlet	GS1-Z	-1598.024718	0.06		34.0%	
	Singlet	GS2-Z	-1598.023767	0.66		12.4%	
	Triplet	GS1-E	-1597.911769	70.94	1.68	3.4%	-1597.911360
	Triplet	GS2-E	-1597.914439	69.26	**0.00**	57.0%	
	Triplet	GS1-Z	-1597.911876	70.87	1.61	3.8%	
	Triplet	GS2-Z	-1597.914004	69.54	0.27	35.9%	
			Triplet-Singlet energy (kcal/mol)				**69.87**
C4	Singlet	GS1-E	-1345.196306	0.17		34.6%	-1345.194341
	Singlet	GS2-E	-1345.195243	0.84		11.2%	
	Singlet	GS1-Z	-1345.196574	**0.00**		45.9%	
	Singlet	GS2-Z	-1345.194964	1.01		8.3%	
	Triplet	GS1-E	-1345.088971	67.52	**0.00**	52.3%	-1345.086456
	Triplet	GS2-E	-1345.086752	68.91	1.39	5.0%	
	Triplet	GS1-Z	-1345.088557	67.78	0.26	33.7%	
	Triplet	GS2-Z	-1345.08731	68.56	1.04	9.0%	
			Triplet-Singlet energy (kcal/mol)				**67.70**
C5	Singlet	GS1-E	-1652.351824	**0.00**		43.0%	-1652.349253
	Singlet	GS2-E	-1652.350963	0.54		17.3%	
	Singlet	GS1-Z	-1652.351227	0.37		22.8%	
	Singlet	GS2-Z	-1652.350942	0.55		16.9%	
	Triplet	GS1-E	-1652.257228	59.36	0.36	19.2%	-1652.255764
	Triplet	GS2-E	-1652.257393	59.26	0.25	22.8%	
	Triplet	GS1-Z	-1652.257798	59.00	**0.00**	35.0%	
	Triplet	GS2-Z	-1652.257401	59.25	0.25	23.0%	
			Triplet-Singlet energy (kcal/mol)				**58.66**

Figure S13 Optimized Singlet and Triplet energies (as ΔH°). for **C1**-**C5**. DFT level: IEF-PCM(THF) ωB97X-D/6-311G(d,p).

3.3.2 Excited state analysis.

Fluorescence calculation for C1-C5

TD-DFT fluorescence cycle to calculate the fluorescence emission of **C1-C5** were run at the CAM-B3LYP/6-311G(d,p) level including solvent THF with IEF-PCM following the following calculation scheme, using Gaussian 16 rev A.03.

```
!step 1 - PEs optimization with standard grid set with threshold raised to 150% of the standard
%chk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-1.chk
%nprocshared=44
%mem=64gb
# cam-b3lyp/6-311g(d,p) Opt freq(savenormalmodes) SCRF=(Solvent=tetrahydrofuran)
iop(1/7=450)

C1-GS1-fluo-tetrahydrofuran

0 1
 N              0.61131200    0.14687200    0.01908400
……..

--link1--
!step 2 - UV absorption spectrum with TD-DFT and 3 states
%oldchk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-1.chk
%chk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-2.chk
%nprocshared=44
%mem=64gb
# cam-b3lyp/6-311g(d,p) TD(NStates=3) SCRF(solvent=tetrahydrofuran) Geom=allCheck Guess=Read


--link1--
!step 3 - Solvatation on GS of the PES with unquilibrated solvent
%oldchk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-1.chk
%chk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-3.chk
%nprocshared=44
%mem=64gb
# cam-b3lyp/6-311g(d,p) SCRF(Solvent=tetrahydrofuran,NonEquilibrium=Save) Geom=allCheck Guess=Read


--link1--
!Step 4 - Excitation on first state (Root=1) with solvent contribution out-of-equilibrium
!Excitation energy can be calculated as E4-E3
%oldchk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-3.chk
%chk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-4.chk
%nprocshared=44
%mem=64gb
# cam-b3lyp/6-311g(d,p) TD(NStates=1,Root=1) Geom=allCheck Guess=Read
SCRF(Solvent=tetrahydrofuran,ExternalIteration,NonEquilibrium=Read)
```

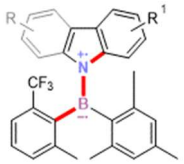
--link1--
!Step 5 - geometry optimization and 150% threshold values, frequency calc. on the S1 ES
%oldchk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-2.chk
%chk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-5.chk
%nprocshared=44
%mem=64gb
cam-b3lyp/6-311g(d,p) opt freq(savenormalmodes) TD(NStates=1,Root=1)
SCRF(Solvent=tetrahydrofuran) Geom=allCheck Guess=Read
iop(1/7=450)

--link1--
!step 6 TD calculation on the ES to evaluate solvent contribution out-of-equilibrium – equiv. to step 4
%oldchk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-5.chk
%chk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-6.chk
%nprocshared=44
%mem=64gb
# cam-b3lyp/6-311g(d,p) TD(NStates=1, Root=1) Geom=allCheck Guess=Read
SCRF(Solvent=tetrahydrofuran,ExternalIteration,NonEquilibrium=Save)

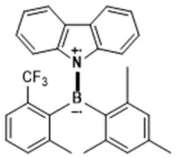
--link1--
!step 7 PES energy with geometry of the EES + solvent contribution from step 6
!emission energy = E6-E7
%oldchk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-6.chk
%chk=C2-GS1-cam-b3lyp-large-fluo-tetrahydrofuran-step-7.chk
%nprocshared=44
%mem=64gb
# cam-b3lyp/6-311g(d,p) SCRF(Solvent=tetrahydrofuran, NonEquilibrium=Read) Geom=allCheck
Guess=Read

A: Cq-Cq-B-N dihedral (°)

B: Cq-B-N-Cq dihedral (°)



C: B-N bond lenght (Å)



		S_0			S_1			λ S_0-S_1	*f*	HOMO-LUMO	S_1 *vs* S_0			Fluorescence		
		A	B	C	A'	B'	C'	nm		%	A'-A	B'-B	C'-C	S_1 energy (E6)	S_0 energy (E7)	Emis. (nm)
C1	GS1	-124.8	29.8	1.441	-133.95	57.8	1.534	292	0.3055	86	-9.1	28.0	0.093	-1498.871491	-1498.972005	454
	GS2	-62.7	-29.8	1.441	-40.06	-59.5	1.532	293	0.2762	87	22.6	-29.7	0.091	-1498.872238	-1498.969675	468
C2	GS1-conf1	-124.4	28.0	1.434	-134.8	59.0	1.539	313	0.3666	86	-10.4	31.0	0.105	-1727.900501	-1727.983759	548
	GS1-conf2	-124.6	28.3	1.434	-134.5	58.9	1.538	312	0.3913	84	-9.9	30.7	0.104	-1727.900140	-1727.984762	539
	GS1-conf3	-124.3	28.3	1.434	-135.0	59.3	1.538	312	0.4024	84	-10.7	31.0	0.104	-1727.900163	-1727.984645	540
	GS1-conf4	-124.5	28.5	1.436	-134.7	59.3	1.538	310	0.4127	84	-10.2	30.8	0.102	-1727.899420	-1727.985475	530
	GS2-conf1	-64.5	-27.1	1.433	-38.4	-60.2	1.536	306	0.3647	83	26.1	-33.1	0.103	-1727.900650	-1727.981520	564
	GS2-conf2	-64.0	-27.6	1.435	-38.9	-60.2	1.536	310	0.3751	85	25.1	-32.5	0.101	-1727.900391	-1727.982498	555
	GS2-conf3	-64.1	-27.7	1.435	-38.2	-60.4	1.536	310	0.3877	83	26.0	-32.7	0.101	-1727.900547	-1727.982341	557
	GS2-conf4	-64.0	-27.9	1.436	-38.6	-60.3	1.535	308	0.4024	83	25.4	-32.4	0.099	-1727.899892	-1727.983281	547
C3	GS1-E	-124.8	-146.1	1.442	-133.9	-122.0	1.535	292	0.3273	83	-9.2	24.2	0.093	-1598.118767	-1598.217941	460
	GS2-E	-62.8	151.6	1.442	-40.5	121.6	1.533	293	0.3036	83	22.3	-30.1	0.091	-1598.119591	-1598.215598	475
	GS1-Z	-124.6	29.4	1.441	-134.1	58.3	1.536	292	0.3206	83	-9.5	28.9	0.095	-1598.118587	-1598.217986	459
	GS2-Z	-62.9	-29.3	1.442	-39.0	-59.6	1.534	294	0.2843	84	23.9	-30.3	0.092	-1598.119584	-1598.215605	475
C4	GS1-E	-121.6	-155.9	1.439	-127.9	-132.9	1.530	283	0.2436	76	-6.4	23.0	0.091	-1345.275435	-1345.372738	469
	GS2-E	-66.4	160.8	1.438	-40.5	131.8	1.533	281	0.2030	79	25.9	-29.0	0.095	-1345.278761	-1345.367111	516
	GS1-Z	-122.3	22.7	1.439	-137.8	49.7	1.533	282	0.3025	79	-15.5	27.0	0.094	-1345.276838	-1345.370134	489
	GS2-Z	-67.1	-17.1	1.438	-38.6	-57.8	1.532	278	0.3119	79	28.5	-40.7	0.094	-1345.278745	-1345.365047	528
C5	GS1-E	-125.2	-144.2	1.445	-135.3	-123.3	1.533	302	0.2436	40	-10.1	20.9	0.088	-1652.461685	-1652.559235	467
	GS2-E	-62.3	150.5	1.446	-39.6	123.6	1.530	303	0.2030	40	22.7	-26.9	0.084	-1652.462718	-1652.556614	486
	GS1-Z	-125.9	30.8	1.446	-133.6	55.8	1.532	304	0.3025	60	-7.7	25.0	0.086	-1652.461108	-1652.560115	461
	GS2-Z	-62.2	-31.5	1.446	-39.1	-57.0	1.531	303	0.3119	54	23.1	-25.5	0.085	-1652.463111	-1652.556678	487

Figure S14. Summary of DFT and TD-DFT geometries for fluorescence calculations of **C1-C5**. DFT and TD-DFT level: IEFPCM(THF) CAM-B3LYP/6-311G(d,p).

DFT calculation of the S_1-T_1 energy gap in compound C2

In order to evaluate the S_1-T_1 gap of the most effective catalyst **C2,** we used the DeltaSCF[47] algorithm, based on the information gained from the TD-DFT calculations about the high coefficient of the HOMO-LUMO transition (≈ 85% as a mean value, see Figure S14).

ORCA[48] (v. 6.0.1) has been used and the 8 conformations of **C2** have been re-optimized at the r^{2}SCAN-3c[49] [CPCM(THF)] level for the S_0, S_1 and T_1 states.

The geometric parameters for S_0, S_1 and T_1 are reported in Table S3. They are in good agreement with those obtained with TD-DFT (for S_0 and S_1) at the IEF-PCM (THF) CAM-B3LYP[50]/6-311G(d,p) and with SCF procedure (for S_0 and T_1) at the IEF-PCM(THF) ω97X-D/6-311G(d,p).

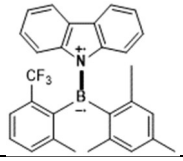
The electronic energies have been then recalculated as single point calculations at the CAM-B3LYP/def2-TZVPPD[51] [CPCM(THF)] level, and weighted using the Boltzmann distribution based on ΔE, $\Delta E_{el+ZVPE}$ (where ZPVE is the Zero Point Value Energy), and ΔG. The free energy has been calculated using the thermal correction obtained at the r^{2}SCAN-3c level.

A summary of data is reported below in Table S3. All the data are in good to very good agreement with the experimental values, even considering different contribution to the energy.

Figure S15 and Figure S16 report all the geometrical parameters and energy differences for the eight conformers of **C2.**

Table S3. Energy gaps considering different energetic contribution at CAM-B3LYP/def2-TZVPPD [CPCM(THF)]// r2SCAN-3c/def2-mTZVPP [CPCM(THF)].

	ΔE [kcal/mol]	**$\Delta E_{el+ZPVE}$ [kcal/mol]**	**ΔG° [kcal/mol]**	**Exp [kcal/mol]**
$S_0 \rightarrow S_1$	65.40	63.50	63.70	64.40
$T_1 \rightarrow S_1$	1.57	1.64	2.31	1.38
$S_0 \rightarrow T_1$	63.83	61.86	61.39	63.00

A: Cq-Cq-B-N dihedral (°)	B : Cq-B-N-Cq dihedral (°)	C : B-N bond length (Å)
		

	S_0			S_1			T_1		
	A	B	C	A'	B'	C'	A"	B"	C"
	°	°	Å	°	°	Å	°	°	Å
GS1-conf1	-126.8	28.4	1.439	-137.0	52.6	1.537	-136.9	50.2	1.532
GS1-conf2	-127.0	28.0	1.439	-136.9	53.2	1.537	-137.0	51.2	1.532
GS1-conf3	-126.8	29.0	1.439	-137.2	53.1	1.537	-137.1	50.8	1.533
GS1-conf4	-126.9	28.4	1.440	-137.0	52.9	1.537	-137.0	50.9	1.533
GS2-conf1	-61.5	-29.1	1.441	-38.3	-54.5	1.536	-38.9	-52.8	1.532
GS2-conf2	-61.1	-29.9	1.442	-38.4	-54.7	1.536	-38.9	-53.2	1.533
GS2-conf3	-61.8	-29.9	1.442	-38.1	-55.2	1.536	-38.5	-53.7	1.533
GS2-conf4	-60.9	-29.4	1.443	-38.1	-55.2	1.536	-38.4	-53.9	1.532

	S_0 *vs* S_1			S_1 *vs* T_1			S_0 *vs* T_1		
	A'-A	B'-B	C'-C	A"-A'	B"-B'	C"-C'	A"-A	B"-B	C"-C
	Δ°	Δ°	ΔÅ	Δ°	Δ°	ΔÅ	Δ°	Δ°	ΔÅ
GS1-conf1	-10.2	24.2	0.098	0.1	-2.4	-0.005	-10.1	21.8	0.093
GS1-conf2	-9.9	25.2	0.098	-0.1	-2.0	-0.005	-10	23.2	0.093
GS1-conf3	-10.4	24.1	0.098	0.1	-2.3	-0.004	-10.3	21.8	0.094
GS1-conf4	-10.1	24.5	0.097	0.0	-2.0	-0.004	-10.1	22.5	0.093
GS2-conf1	23.2	-25.4	0.095	-0.6	1.7	-0.004	22.6	-23.7	0.091
GS2-conf2	22.7	-24.8	0.094	-0.5	1.5	-0.003	22.2	-23.3	0.091
GS2-conf3	23.7	-25.3	0.094	-0.4	1.5	-0.003	23.3	-23.8	0.091
GS2-conf4	22.8	-25.8	0.093	-0.3	1.3	-0.004	22.5	-24.5	0.089

Figure S15 DeltaSCF Geometries for compound **C2**. DFT level: [CPCM(THF)] r^{2}SCAN-3c/def2-mTZVPP.

	Electronic Energies					
	S_0		**S_1**		**T_1**	
	Energy (a.u.)	**%**	**Energy (a.u.)**	**%**	**Energy (a.u.)**	**%**
GS1-conf1	-1728.25136	7%	-1728.14722	8%	-1728.14973	8%
GS1-conf2	-1728.25208	15%	-1728.14673	4%	-1728.14926	5%
GS1-conf3	-1728.25220	18%	-1728.14674	5%	-1728.14929	5%
GS1-conf4	-1728.25287	36%	-1728.14589	2%	-1728.14845	2%
GS2-conf1	-1728.25024	2%	-1728.14851	29%	-1728.15102	31%
GS2-conf2	-1728.25108	5%	-1728.14808	20%	-1728.15060	20%
GS2-conf3	-1728.25107	5%	-1728.14817	21%	-1728.15063	20%
GS2-conf4	-1728.25179	11%	-1728.14744	10%	-1728.14995	10%
Avg. Value	**-1727.72340**		**-1727.62220**		**-1727.62480**	
S_1-S_0 (kcal/mol)	**65.40**					
S_1-T_1 (kcal/mol)	**1.57**					
T_1-S_0 (kcal/mol)	**63.83**					
	ZPVE-corrected Electronic Energies					
	S_0		**S_1**		**T_1**	
	Energy (a.u.)	**%**	**Energy (a.u.)**	**%**	**Energy (a.u.)**	**%**
GS1-conf1	-1727.72273	7%	-1727.62153	9%	-1727.62415	8%
GS1-conf2	-1727.72335	14%	-1727.62091	4%	-1727.62358	4%
GS1-conf3	-1727.72349	16%	-1727.62108	5%	-1727.62375	5%
GS1-conf4	-1727.72409	30%	-1727.62031	2%	-1727.62299	2%
GS2-conf1	-1727.72197	3%	-1727.62277	28%	-1727.62543	30%
GS2-conf2	-1727.72284	8%	-1727.62243	21%	-1727.62505	20%
GS2-conf3	-1727.72278	8%	-1727.62247	21%	-1727.62502	20%
GS2-conf4	-1727.72331	13%	-1727.62178	10%	-1727.62439	10%
Avg. Value	**-1727.72340**		**-1727.62220**		**-1727.62480**	
S_1-S_0 (kcal/mol)	**63.50**					
S_1-T_1 (kcal/mol)	**1.64**					
T_1-S_0 (kcal/mol)	**61.86**					
	Gibbs Free Energies					
	S_0		**S_1**		**T_1**	
	Energy (a.u.)	**%**	**Energy (a.u.)**	**%**	**Energy (a.u.)**	**%**
GS1-conf1	-1727.78304	6%	-1727.68174	8%	-1727.68538	8%
GS1-conf2	-1727.78362	11%	-1727.68092	5%	-1727.68466	4%
GS1-conf3	-1727.78385	14%	-1727.68129	5%	-1727.68502	6%
GS1-conf4	-1727.78438	24%	-1727.68051	2%	-1727.68427	3%
GS2-conf1	-1727.78286	5%	-1727.68285	31%	-1727.68660	30%
GS2-conf2	-1727.78374	12%	-1727.68257	20%	-1727.68622	20%
GS2-conf3	-1727.78365	11%	-1727.68258	20%	-1727.68616	19%
GS2-conf4	-1727.78399	16%	-1727.68192	10%	-1727.68558	10%
Avg. Value	**-1727.78380**		**-1727.68230**		**-1727.68600**	
S_1-S_0 (kcal/mol)	**63.70**					
S_1-T_1 (kcal/mol)	**2.31**					
T_1-S_0 (kcal/mol)	**61.39**					

Figure S16. DeltaSCF Energies for compound **C2**.
DFT level: [CPCM(THF)] CAM-B3LYP/def2-TZVPPD // [CPCM(THF)] r2SCAN-3c/def2-mTZVPP

4. Optimization studies of known EnT benchmarks

Photochemical set-up 1:

- *Kessil® lamp setup* with PhotoRedOx Box TC™ (Figure S17)

The reactions were performed using a PhotoRedOx Box TC™ reactor under the illumination of a *Kessil*® lamp (positioned 2-3 cm away from the Schlenk tube), with a fan to maintain a stable temperature. Under these conditions, the reaction temperature within the vessel was measured to be between 25-30 ºC.

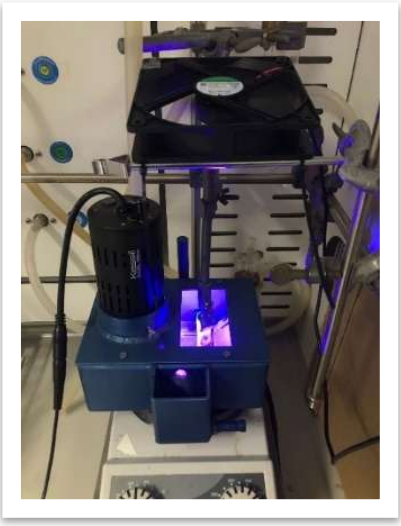


Figure S17 Photochemical set-up 1.

*4.1. Optimization of Dimethyl Fumarate (***1a-*E*)* Photo-isomerization*

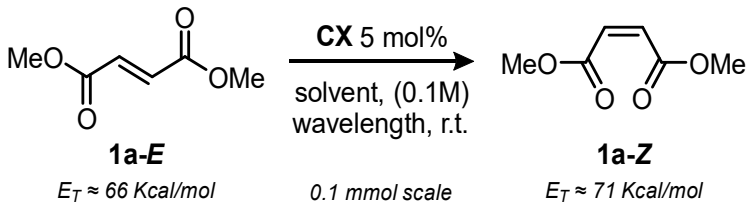


Figure S18 photo-isomerization of dimethyl fumarate **1a-*E***; E_T taken from literature.[52]

In a Schlenk tube, (*E*)-dimethyl fumarate **1a-*E*** (14.4 mg, 0.1 mmol) and **CX** (5 % mol) were dissolved in 1 mL of the solvent specified in Table S4 to Table S6. The reaction mixture was degassed by repeated freeze-pump-thaw cycles until gas evolution ceased. Subsequently, the tubes were backfilled with argon and irradiated using a Kessil® lamp at the wavelength and for the duration specified in Table S4 to Table S6.

For experiments in which a non-deuterated solvent was initially used, a solvent exchange was conducted prior to analysis: the original solvent was removed under reduced pressure, and the tubes were then refilled with $CDCl_3$. All the *E:Z* ratios in the tables below were determined via ^{1}HNMR analysis. Using dibromomethane as internal standard (0.1 mmol) ensured no conversion to byproducts.

Table S4 – Photocatalysts screening at 390 nm and 427 nm.

Catalyst	Wavelength (nm)	Time	Loading	Solvent (conc, temp °C)	*E*%	*Z*%
C1	**390**	**16h**	**5 % mol**	**$CDCl_3$ (0.1M, RT)**	**20**	**80**
C2	**390**	**16h**	**5 % mol**	**$CDCl_3$ (0.1M, RT)**	**21**	**79**
C3	**390**	**16h**	**5 % mol**	**$CDCl_3$ (0.1M, RT)**	**24**	**76**
C4	**390**	**16h**	**5 % mol**	**$CDCl_3$ (0.1M, RT)**	**29**	**71**
C5	**390**	**16h**	**5 % mol**	**$CDCl_3$ (0.1M, RT)**	**36**	**64**
C6	390	16h	5 % mol	$CDCl_3$ (0.1M, RT)	92	8
no PC	390	16h	0% mol	$CDCl_3$ (0.1M, RT)	99	1
C2	no light	16h	5 % mol	$CDCl_3$ (0.1M, RT)	99	1
C1	427	16h	5 % mol	$CDCl_3$ (0.1M, RT)	86	14
C2	**427**	**16h**	**5 % mol**	**$CDCl_3$ (0.1M, RT)**	**39**	**61**
C3	427	16h	5 % mol	$CDCl_3$ (0.1M, RT)	85	15
C4	427	16h	5 % mol	$CDCl_3$ (0.1M, RT)	98	2
C5	427	16h	5 % mol	$CDCl_3$ (0.1M, RT)	87	13

Table S4 summarizes the preliminary screening of our family of photocatalysts under irradiation at 390 nm to determine the most effective candidate (first section). Catalyst **C6** was excluded from further studies due to their poor catalytic activity in promoting the E/Z photo-isomerization. Subsequent experiments were conducted at 427 nm, where catalyst **C2** exhibited superior performance compared to the others (Table S4, second section).

Table S5 optimization with **C2**: solvent, wavelength and reaction time screening.

Catalyst	Wavelength (nm)	Time	Loading	Solvent (conc, temp °C)	*E*%	*Z*%
C2	427	16h	5 % mol	$CDCl_3$ (0.1M, RT)	39	61
C2	**427**	**16h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**4**	**96**
C2	427	16h	5 % mol	CD_3CN (0.1M, RT)	93	7
C2	**440**	**16h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**4**	**96**
C2	440	1h	5 % mol	*n*-hexane (0.1M, RT)	72	28
C2	440	2h	5 % mol	*n*-hexane (0.1M, RT)	57	43
C2	440	4h	5 % mol	*n*-hexane (0.1M, RT)	32	68
C2	440	6h	5 % mol	*n*-hexane (0.1M, RT)	21	79
C2	**440**	**8h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**4**	**96**
C2	**440**	**16h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**4**	**96**
C2	**440**	**24h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**4**	**96**

Catalyst **C2** was thus identified as the most efficient within the tested series and was selected for further optimization of the reaction conditions. In the first section of Table S5, *n*-hexane emerged as the most suitable solvent, while in the second section, the irradiation wavelength was increased to 440 nm, yielding comparable results to those obtained at 427 nm. Third section of Table S5 addresses the effect of reaction time: after 8 hours of irradiation, the ratio stabilized at 4:96 (*E:Z*), indicating that the photo stationary state had been reached. Results from the time experiments are summarized in Figure S19.

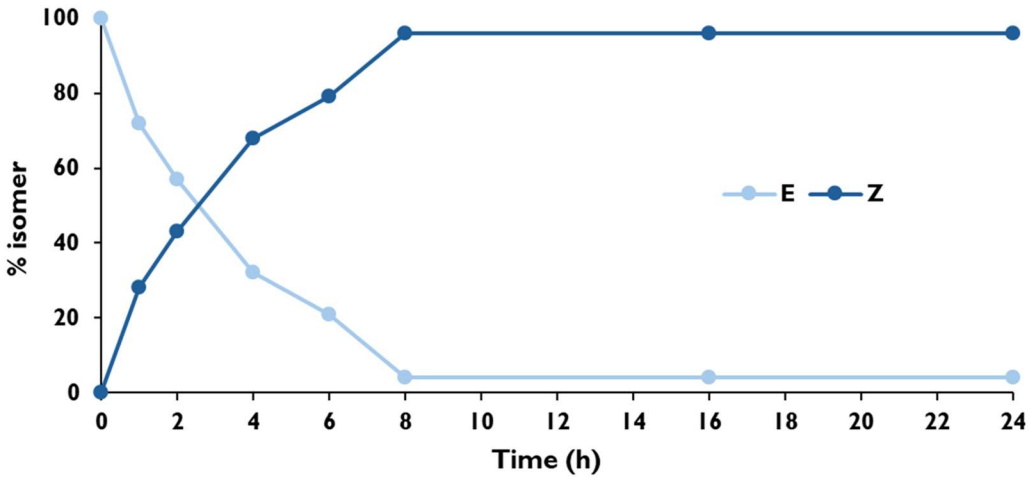


Figure S19 Time experiment for the photo-isomerization of (*E*)-dimethyl fumarate **1a-*E*** in the presence of **C2** (5 % mol) at 440 nm in *n*-hexane.

Table S6:Further control experiments for the photo-isomerization of **1a-*E***.

Catalyst	Wavelength (nm)	Time	Loading	Solvent (conc, temp °C)	*E*%	*Z*%
$(Ir[dF(CF_3)ppy]_2(dtbpy))PF_6$	440	16h	1 % mol	*n*-hexane (0.1M, RT)	77	23
Thioxanthone	440	16h	5 % mol	*n*-hexane (0.1M, RT)	99	1
C2	456	16h	5 % mol	*n*-hexane (0.1M, RT)	48	52
C2	456	24h	5 % mol	*n*-hexane (0.1M, RT)	40	60
C2	456	30h	5 % mol	*n*-hexane (0.1M, RT)	28	72
C2	**456**	**48h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**10**	**90**
C2	467	72h	5 % mol	*n*-hexane (0.1M, RT)	47	53
C2	**467**	**120h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**20**	**80**
C2	White led	1week	5 % mol	*n*-hexane (0.1M, RT)	50	50
C2	**White led**	**2weeks**	**5 % mol**	***n*-hexane (0.1M, RT)**	**9**	**91**

Upon establishing the optimal conditions for the **C2**-catalyzed E/Z photo-isomerization of (*E*)-dimethyl fumarate, we screened two commercially available photocatalysts (Table S6, section one). None demonstrated superior performance relative to catalyst **C2** under the reaction conditions.

In the second section of Table S6, further experiments were performed at longer irradiation wavelengths. While the photo-isomerization reaction proceeded more slowly under these conditions than at 440 nm, a final *E:Z* ratio of 10:90 was achieved after 48 hours of irradiation at 456 nm. Similarly, irradiation at 467 nm for 120 hours resulted in an *E:Z* ratio of 20:80. Moreover a *E:Z* ratio of 9:91 was achieved irradiating with a common white led strip for 2 weeks (set up is shown in Figure S20).

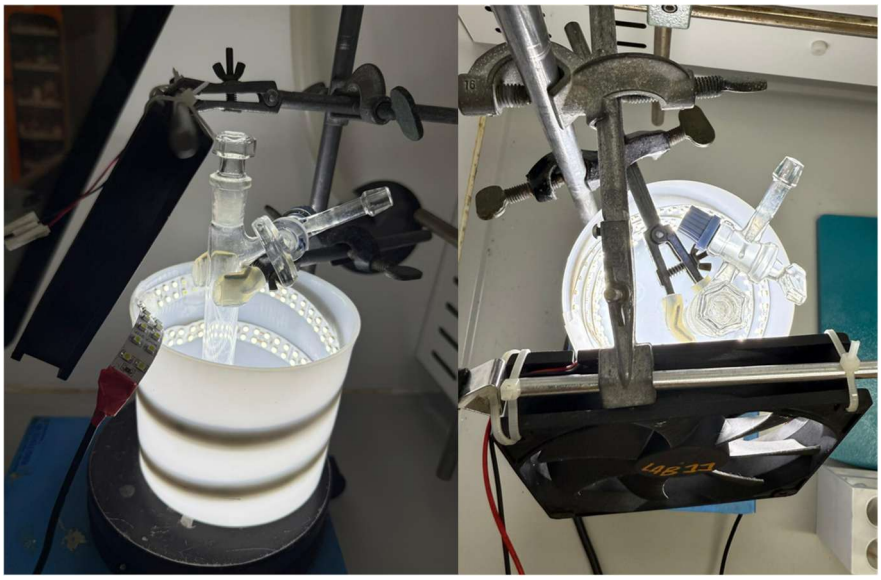


Figure S20 Experimental set-up for photoisomerization of **1a-*E*** with **C2** (5 % mol) under white led strip irradiation.

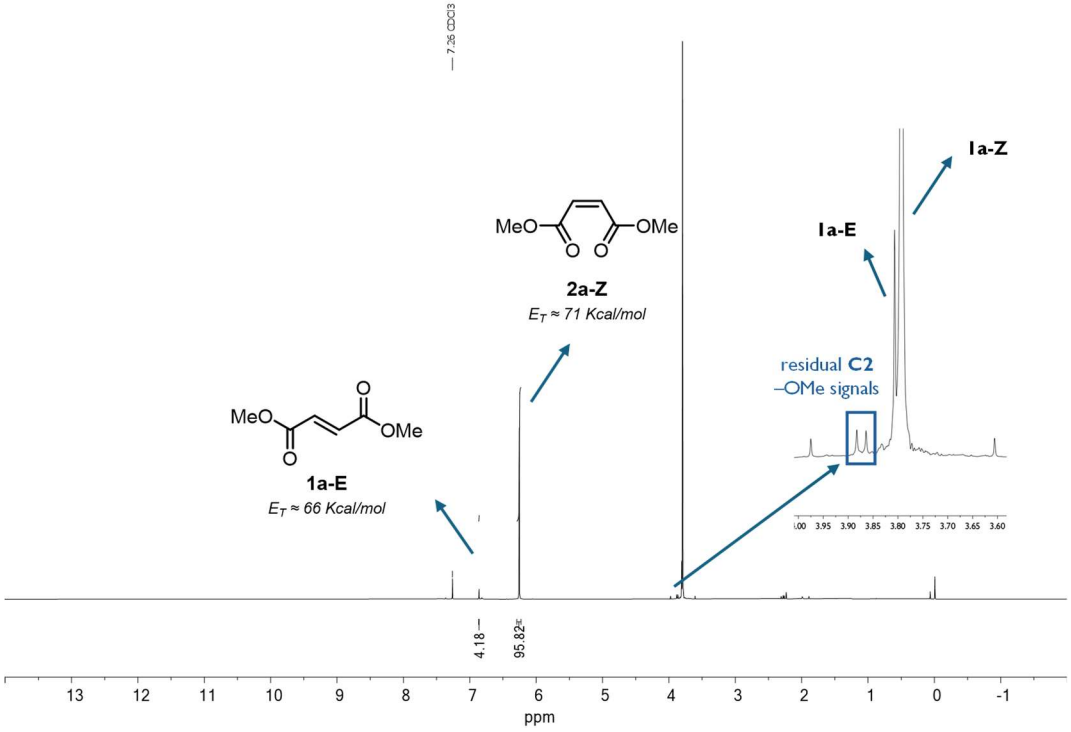


Figure S21 Reaction crude ^{1}H NMR for photo-isomerization of **1a-*E*** with **C2** at 440 nm.

*4.2 Optimization of Oxime (***1b-*E*) *Photo-isomerization***

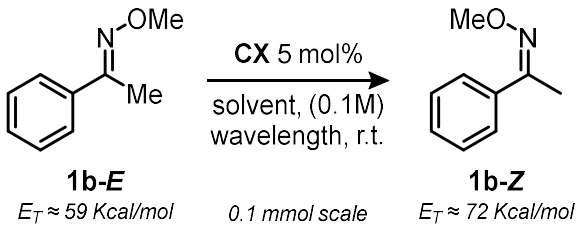


Figure S22: photo-isomerization of oxime **1b-*E***; E_T taken from literature.[52]

In a Schlenk tube, (*E*)-acetophenone O-methyloxime (**1b-*E***) (14.9 mg, 0.1 mmol) and **C2** (5 % mol) were dissolved in 1 mL of the solvent specified in Table S7. The reaction mixture was degassed by repeated freeze-pump-thaw cycles until gas evolution ceased. Subsequently, the tubes were backfilled with argon and irradiated using a Kessil® lamp at the wavelength and for the duration indicated in Table S7.

For experiments in which a non-deuterated solvent was initially used, a solvent exchange was conducted prior to analysis: the original solvent was removed under reduced pressure, and the tubes were then refilled with $CDCl_3$. All the *E:Z* ratios in the tables below were determined via ^{1}HNMR analysis.

Table S7: reaction condition screening for Oxime **1b** photo-isomerization.

Catalyst	Wavelength (nm)	Time	Loading	Solvent (conc, temp °C)	*E*%	*Z*%
C2	**440**	**16h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**25**	**75**
C2	440	16h	5 % mol	$CDCl_3$ (0.1M, RT)	47	53
C2	440	16h	5 % mol	CD_3CN (0.1M, RT)	62	38
C2	**440**	**24h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**19**	**81**
C2	440	30h	5 % mol	*n*-hexane (0.1M, RT)	20	80
No PC	440	24h	0% mol	*n*-hexane (0.1M, RT)	100	0

The first section of Table S7 shows a solvent screening for the photo-isomerization of **1b-*E*** using catalyst **C2** and 440 nm lamp. *n*-hexane emerged as the most suitable solvent, demonstrating a comparable trend with the *E:Z* photo-isomerization of dimethyl fumarate **1a-*E***. In the second section of Table S7, we were able to achieve 19:81 *E:Z* ratio after 24h of irradiation. Prolonged irradiation (30h) didn't improve the *E:Z* ratio.

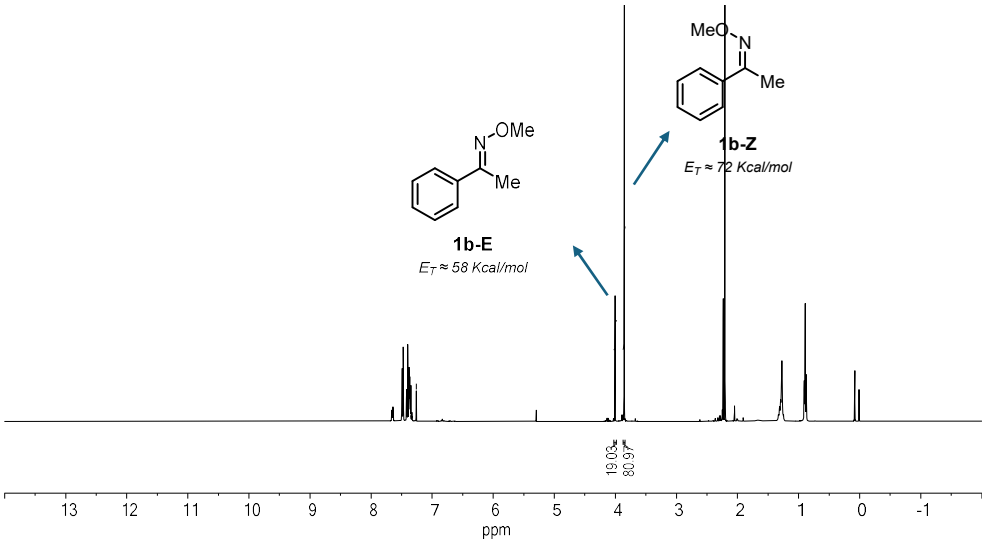


Figure S23 Reaction crude ^{1}H NMR for photo-isomerization of **1b-*E*** with **C2** at 440 nm.

4.3 Optimization of [2+2]-Cycloaddition of Norbornadiene (1c) to Quadricyclane (2c)

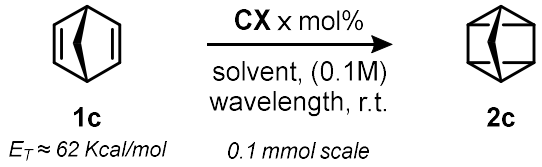


Figure S24: [2+2]-cycloaddition of norbornadiene (**1c**) to quadricyclane (**2c**); E_T taken from literature.[53]

In a Schlenk tube, norbornadiene (**1c**) (10.2 µL, 0.1 mmol) and **CX** (1 % mol) were dissolved in 1 mL of the solvent specified in the tables below. The reaction mixture was degassed by repeated freeze-pump-thaw cycles until gas evolution ceased. Subsequently, the tubes were backfilled with argon and irradiated using a Kessil® lamp at the wavelength and for the duration indicated in Table S8.

All the results in the tables below were determined via ^{1}HNMR analysis, using dibromomethane as internal standard (0.1 mmol) to quantify yield and conversion.

Table S8: photocatalyst and reaction condition screening for [2+2]-Cycloaddition of Norbornadiene **1c**

Entry	Catalyst	Wavelength (nm)	Time	Loading	Solvent (conc, temp °C)	yield%	conv%
1	**C1**	**370**	**3h**	**1 % mol**	**CD_3CN (0.1M, RT)**	**78**	**90**
2	**C1**	370	4h	1 % mol	CD_3CN (0.1M, RT)	64	98
3	**C2**	370	3h	1 % mol	CD_3CN (0.1M, RT)	traces	66
4	**C5**	370	3h	1 % mol	CD_3CN (0.1M, RT)	15	90
5	**C1**	390	3h	1 % mol	CD_3CN (0.1M, RT)	10	20
6	**C2**	390	3h	1 % mol	CD_3CN (0.1M, RT)	0	40
7	**C1**	390	6h	1 % mol	CD_3CN (0.1M, RT)	6	35
8	**C1**	390	16h	1 % mol	CD_3CN (0.1M, RT)	10	90
9	**C2**	390	16h	1 % mol	CD_3CN (0.1M, RT)	5	94
10	**C3**	390	16h	1 % mol	CD_3CN (0.1M, RT)	20	62
11	**C4**	390	16h	1 % mol	CD_3CN (0.1M, RT)	12	34
12	**C5**	**390**	**16h**	**1 % mol**	**CD_3CN (0.1M, RT)**	**57**	**57**
13	**C6**	390	16h	1 % mol	CD_3CN (0.1M, RT)	3	31
14	**C5**	390	60h	1 % mol	CD_3CN (0.1M, RT)	0	99
15	**C1**	427	16h	1 % mol	CD_3CN (0.1M, RT)	2	23
16	**C2**	427	16h	1 % mol	CD_3CN (0.1M, RT)	4	37
17	**C5**	427	16h	1 % mol	CD_3CN (0.1M, RT)	16	18
18	**C5**	**427**	**60h**	**1 % mol**	**CD_3CN (0.1M, RT)**	**32**	**85**
19	**C5**	427	60h	5 % mol	CD_3CN (0.1M, RT)	0	95

The optimization of this reaction was non-trivial due to an unexpected decrease in yield overtime probably caused by a degradation of the product **2c** in the reaction conditions (this side reactivity wasn't further investigated in this study). This was the case especially with **C2** which in all the reaction tried delivered high conversion with minimal yield of desired product **2c** (entries 3,6,9,16). Lower reaction times and lower catalyst loading were crucial for diminishing this effect (see comparison of entry 18 and 19).

The best result was obtained with **C1** after 3 hours of irradiation at 370 nm (entry 1) which furnished a 78% yield with marginal conversion to by-products. Notably, also **C5** was effective in catalyzing the reaction with a promising 57 % yield using 390 nm irradiation and 32 % yield with 427 nm irradiation but needed prolonged reaction times (entry 12 and 18).

The best results ^{1}H NMR crude is shown in Figure S25:

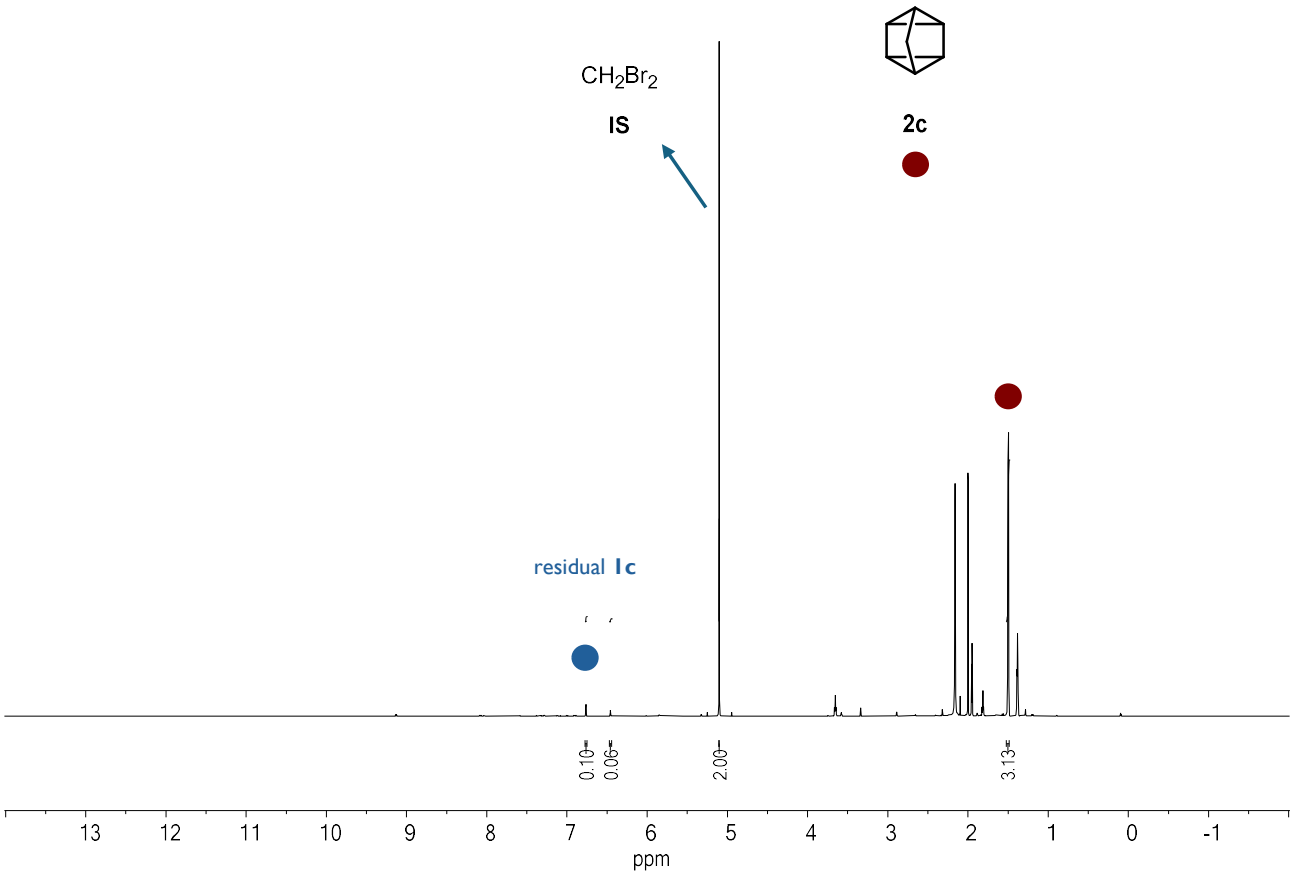


Figure S25 Reaction crude ^{1}H NMR for [2+2] photo-cycloaddition of norbornandiene (NBD, **1c**) to quadricyclane (QD, **2c**) with **C1** at 370 nm.

4.4 Optimization of [1,3]-Sigmatropic Shift of Verbenone (1d) to Chrysanthenone (2d)

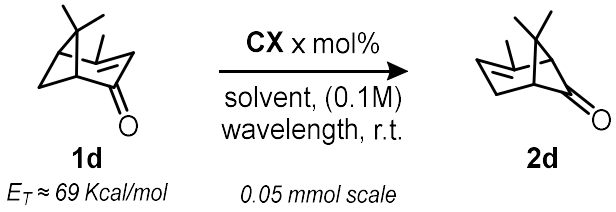


Figure S26: [1,3]-sigmatropic shift of verbenone (**1d**) to chrysanthenone (**2d**); E_T taken from literature.[53]

In a Schlenk tube, verbenone (**1d**) (7.2 µL, 0.05 mmol) and **CX** (5 % mol) were dissolved in 0.5 mL of the solvent specified in Table S9 below. The reaction mixture was degassed by repeated freeze-pump-thaw cycles until gas evolution ceased. Subsequently, the tubes were backfilled with argon and irradiated using a Kessil® lamp at the wavelength and for the duration indicated in Table S9.

For experiments in which a non-deuterated solvent was initially used, a solvent exchange was conducted prior to analysis: the original solvent was removed under reduced pressure, and the tubes were then refilled with CD_3CN. All the results in the tables below were determined via ^{1}HNMR analysis, using dibromomethane as internal standard (0.050 mmol) to observe yield and conversion.

Table S9: photocatalyst and reaction condition screening for [1,3]-Sigmatropic Shift of Verbenone **1d**.

Entry	Catalyst	Wavelength (nm)	Time	Loading	Solvent (conc, temp °C)	yield%	conv%
1	**no PC**	370	4h	0 % mol	CD_3CN (0.1M, RT)	77	93
2	**no PC**	390	4h	0 % mol	CD_3CN (0.1M, RT)	72	95
3	**no PC**	405	4h	0 % mol	CD_3CN (0.1M, RT)	49	51
4	**no PC**	427	16h	0 % mol	CD_3CN (0.1M, RT)	0	0
4	**no PC**	427	48h	0 % mol	CD_3CN (0.1M, RT)	0	0
5	**no PC**	427	48h	0 % mol	*n*-hexane (0.1M, RT)	8	8
6	**C5**	427	16h	1 % mol	CD_3CN (0.1M, RT)	6	8
7	**C2**	427	16h	1 % mol	CD_3CN (0.1M, RT)	25	28
8	**C2**	**427**	**48h**	**5 % mol**	**CD_3CN (0.1M, RT)**	**58**	**58**
9	**C1**	427	18h	1 % mol	CD_3CN (0.1M, RT)	2	5
10	**C2**	427	24h	5 % mol	*n*-hexane (0.1M, RT)	76	85
11	**C2**	**427**	**48h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**98%**	**quant.**
12	**C2**	440	48h	5 % mol	*n*-hexane (0.1M, RT)	31	40
13	**C2**	**440**	**120h**	**5 % mol**	***n*-hexane (0.1M, RT)**	**44**	**49**

Table S9 summarizes the experiments conducted on verbenone (**1d**) to identify the most effective photocatalyst and optimal reaction conditions. In the first section, various irradiation wavelengths were tested to assess the background reaction (entries 1-5). It was observed that background reactions proceeded up to 405 nm (entry 3). However, at 427 nm, background reactions were only marginally active for a prolonged reaction time (after 48 h of irradiation an 8% of product **2d** was noticed). In the second section, the most promising photocatalysts for 427 nm irradiation (**C1**, **C2**, and **C5**), identified from the dimethyl fumarate screening, were evaluated. Among these, **C2** emerged as the most efficient, affording a 58% yield after 48 hours of irradiation (entry 8). Using **C2**, a solvent effect was further investigated based on insights obtained from the dimethyl fumarate

experiments. A significant increase in both conversion and yield was observed at 427 nm when the solvent was switched to *n*-hexane (entries 10 and 11). In the final section of Table S9, the irradiation wavelength was increased to 440 nm. A 44% yield of **2d** was obtained after 120 hours of 440 nm irradiation in *n*-hexane (entries 12 and 13).

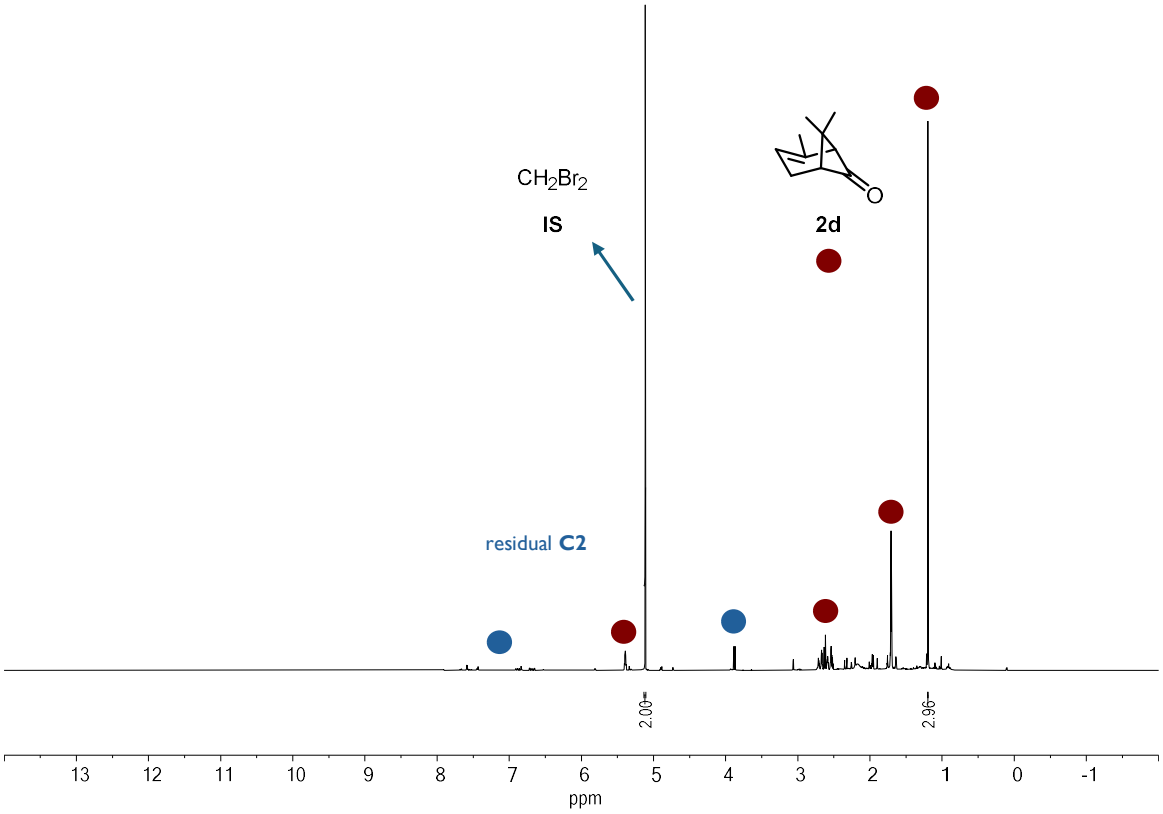


Figure S27 Reaction crude ^{1}H NMR for [1,3]-sigmatropic shift of verbernone (**1d**) to chrysanthenone (**2d**) with **C2** at 427 nm.

5. Photochemical Synthesis Procedures

All the experimental procedures reported in the current section were conducted in the photochemical set-up 1 depicted in Figure S17.

5.1 Poorly reactive or unsuccessful sensitizations

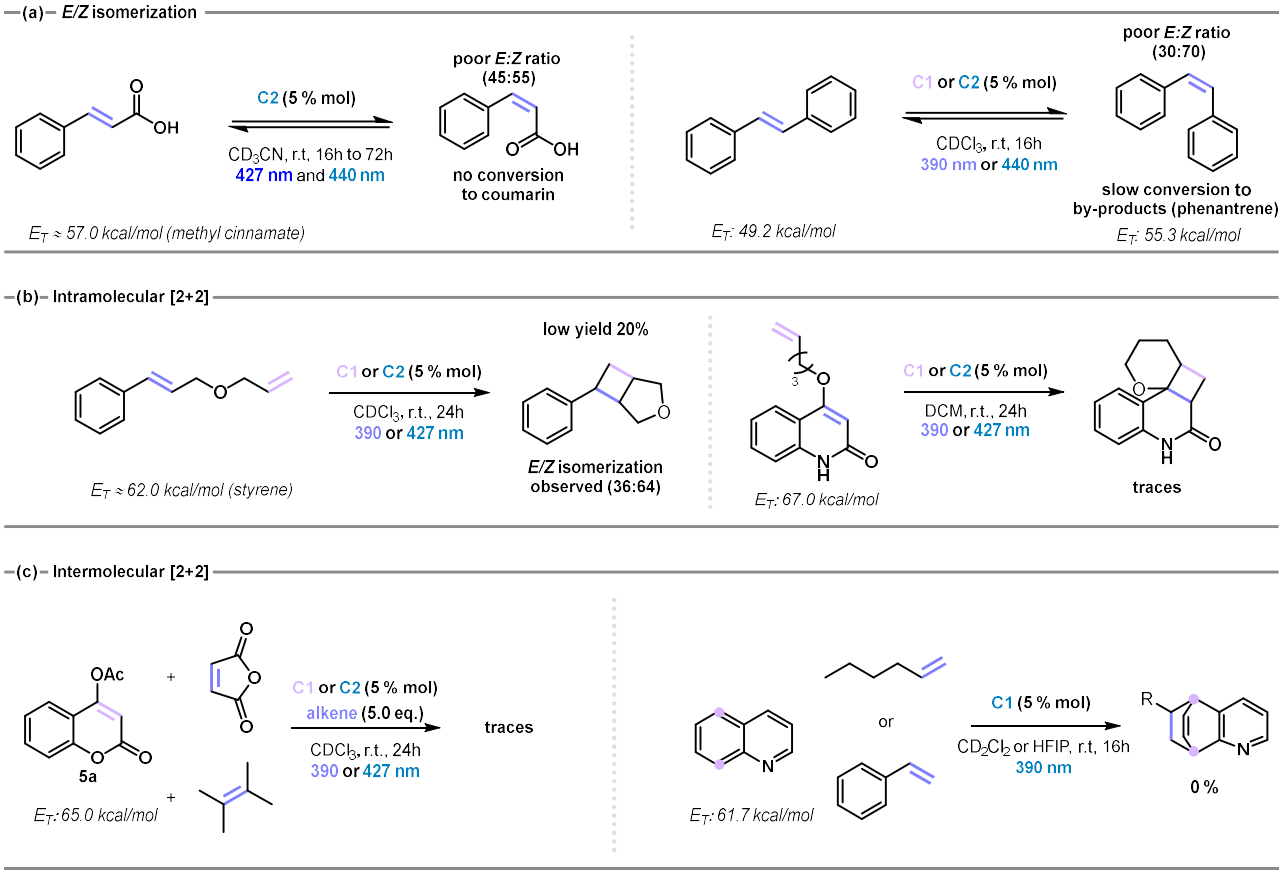


Figure S28 Unsuccessful transformations in the presence of **C1** or **C2**. Triplet energies (E_T) were taken from related literature.

A series of unsuccessful *E/Z* photo-isomerization or [2+2] photo-cycloadditions is reported in Figure S28.

5.2 Intramolecular cyclization of 3a-c

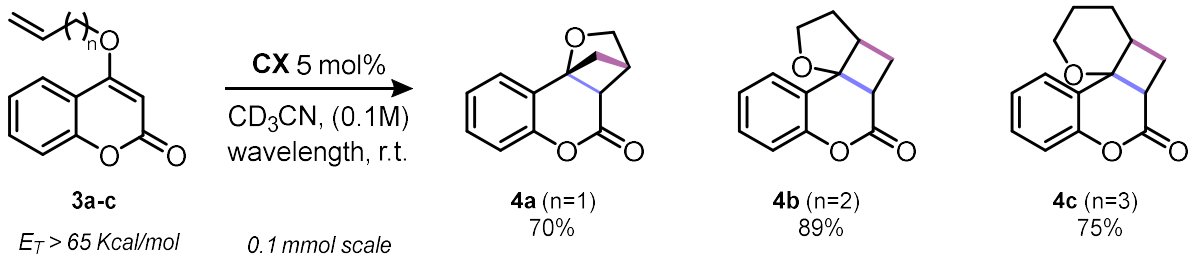


Figure S29: intramolecular cyclization of **3a-c** substrates;

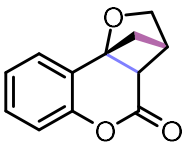
In a Schlenk tube, **coumarins 3a-c** (0.1 mmol) and **CX** (5 % mol) were dissolved in 1 mL of CD_3CN. The reaction mixture was degassed by repeated freeze-pump-thaw cycles until gas evolution ceased. Subsequently, the tubes were backfilled with argon and irradiated using a Kessil® lamp at the wavelength and for the duration indicated in the Table S10.

All the results in the tables below were determined via ^{1}H-NMR analysis, using dibromomethane as internal standard (0.1 mmol) to observe yield. For the highest yielding entries, the products were isolated by flash chromatography (gradient of *n*-hexane / EtOAc).

Table S10 photocatalyst and reaction condition screening for intramolecular [2+2] cycloaddition of substrates **3a-c**.

Substrate	Catalyst	Wavelength (nm)	Time	Loading	Solvent (conc, temp °C)	yield% (isolated)
3a	**C1**	**390**	**24h**	**5 % mol**	**CD_3CN (0.1M, RT)**	**80 (70)**
3a	**C2**	440	24h	5 % mol	CD_3CN (0.1M, RT)	<10
3b	**C1**	390	18h	5 % mol	CD_3CN (0.1M, RT)	75
3b	**C1**	**390**	**24h**	**5 % mol**	**CD_3CN (0.1M, RT)**	**98 (89)**
3b	**C1**	405	24h	5 % mol	CD_3CN (0.1M, RT)	40
3b	**C2**	440	24h	5 % mol	CD_3CN (0.1M, RT)	<10
3c	**C1**	**390**	**24h**	**5 % mol**	**CD_3CN (0.1M, RT)**	**90 (75)**
3c	**C2**	440	24h	5 % mol	CD_3CN (0.1M, RT)	<10

5.1.1 Characterization of products 4a-c



4a

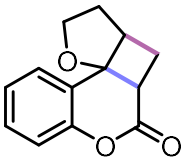
(3S,9bR)-3,3a-dihydro-3,9b-methanofuro[3,2-c]chromen-4(2H)-one (**4a**):

white powder; 70 % y*ield (14.1 mg, 0.07 mmol)*.

HRMS (MALDI-qTOF) = calculated for $C_{12}H_{10}Na\ O_3^+$ ([M+Na]$^+$): 225.0522; found: 225.0526

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.33 (ddd, *J* = 8.2, 7.5, 1.7 Hz, 1H), 7.20 (td, *J* = 7.5, 1.1 Hz, 1H), 7.11 (dd, *J* = 8.2, 1.1 Hz, 1H), 4.15 (dd, *J* = 6.5, 0.7 Hz, 1H), 4.13 (dt, *J* = 6.4, 0.9 Hz, 1H), 3.51 (dt, *J* = 3.1, 0.7 Hz, 1H), 2.78 (d, *J* = 9.9 Hz, 1H), 2.43 (ddd, *J* = 8.7, 3.1, 1.3 Hz, 1H), 1.86 (dd, *J* = 10.0, 8.7 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 167.89, 151.94, 129.97, 124.88, 124.22, 121.36, 116.82, 84.93, 71.59, 51.15, 43.23, 42.91.



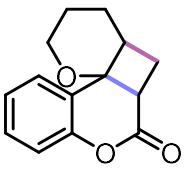
4b

3,3a,4,4a-tetrahydrofuro[2',3':2,3]cyclobuta[1,2-c]chromen-5(2H)-one (**4b**):

White powder; 89 % y*ield (19.2 mg, 0.089 mmol)*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.30 (m, 2H), 7.17 (td, *J* = 7.5, 1.2 Hz, 1H), 7.07 – 7.04 (m, 1H), 4.45 (ddd, *J* = 9.6, 7.9, 1.9 Hz, 1H), 4.21 (ddd, *J* = 10.7, 9.4, 5.9 Hz, 1H), 3.50 (ddd, *J* = 11.6, 7.2, 1.5 Hz, 1H), 2.98 – 2.91 (m, 1H), 2.43 (dddd, *J* = 13.2, 9.1, 7.1, 0.6 Hz, 1H), 2.27 – 2.14 (m, 2H), 1.90 (ddt, *J* = 12.9, 5.9, 1.7 Hz, 1H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 168.57, 150.72, 130.29, 126.48, 125.34, 122.41, 117.36, 82.00, 69.05, 46.38, 40.86, 32.33, 25.99.



4c

2,3,4,4a,5,5a-hexahydro-6H-pyrano[2',3':2,3]cyclobuta[1,2-c]chromen-6-one (**4c**):

White powder; 75 % y*ield (17.3 mg, 0.075 mmol)*.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.47 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.34 (ddd, *J* = 8.2, 7.3, 1.7 Hz, 1H), 7.23 (ddd, *J* = 7.7, 7.3, 1.2 Hz, 1H), 7.06 (ddd, *J* = 8.3, 1.2, 0.4 Hz, 1H), 4.02 (td, *J* = 9.8, 1.2 Hz, 1H), 4.01 – 3.95 (m, 1H), 3.85 – 3.76 (m, 1H), 2.51 – 2.44 (m, 1H), 2.32 (ddt, *J* = 12.7, 5.8, 2.3 Hz, 1H), 1.96 – 1.85 (m, 2H), 1.77 – 1.64 (m, 3H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.70, 150.69, 130.19, 128.75, 125.34, 125.16, 117.31, 71.66, 63.63, 40.53, 38.85, 27.39, 25.28, 23.32.

5.3 Intermolecular cyclization of 5a-c with cyclohexene

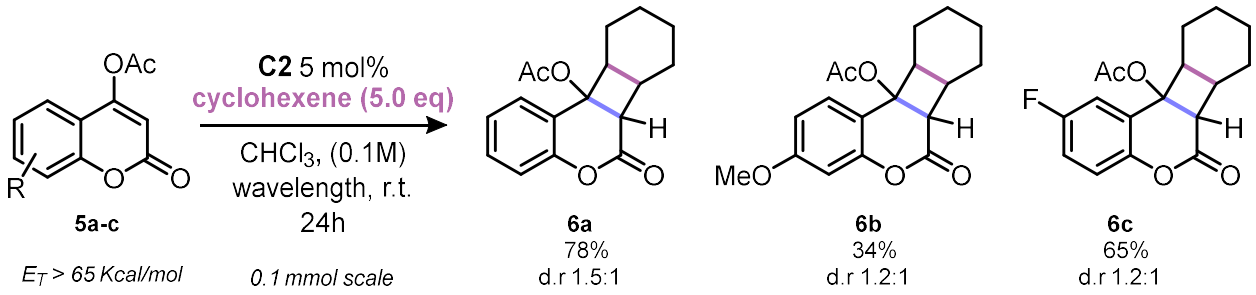


Figure S30: intermolecular cyclization of **5a-c** substrates with cyclohexene.

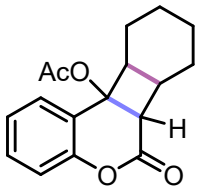
In a Schlenk tube, **coumarins 5a-c** (0.1 mmol), **C2** (5 % mol) and 51 µL (0.5 mmol, 5.0 eq.) of cyclohexene were dissolved in 1 mL of $CHCl_3$. The reaction mixture was degassed by repeated freeze-pump-thaw cycles until gas evolution ceased. Subsequently, the tubes were backfilled with argon and irradiated using a 440 nm Kessil® lamp.

All the results in Table S11 below were determined via ^{1}H-NMR analysis, using dibromomethane as internal standard (0.1 mmol) to observe yield. For the highest yielding entries, the products were isolated by flash chromatography (gradient of *n*-hexane / EtOAc). A background reaction at 390 nm and 440 nm without the addition of photocatalyst was run to confirm the direct excitation of the substrate **5a** was not possible. **C1** and **C2** work the best for the transformation of **5a** to **6a** but **C2** was able to maintain a good activity up to 440 nm.

Table S11 screening for intermolecular [2+2] cycloaddition of substrates **5a-c** with cyclohexene.

Substrate	Catalyst	Wavelength (nm)	Time	Loading	Solvent (conc, temp °C)	yield% (isolated)
5a	**C1**	**390**	**16h**	**5 % mol**	**$CHCl_3$ (0.1M, RT)**	**82**
5a	**C2**	**390**	**16h**	**5 % mol**	**$CHCl_3$ (0.1M, RT)**	**82**
5a	**C3**	390	16h	5 % mol	$CHCl_3$ (0.1M, RT)	68
5a	**C4**	390	16h	5 % mol	$CHCl_3$ (0.1M, RT)	17
5a	**C5**	390	16h	5 % mol	$CHCl_3$ (0.1M, RT)	43
5a	**C1**	427	16h	5 % mol	$CHCl_3$ (0.1M, RT)	18
5a	**C2**	**427**	**16h**	**5 % mol**	**$CHCl_3$ (0.1M, RT)**	**88**
5a	**C5**	427	16h	5 % mol	$CHCl_3$ (0.1M, RT)	20
5a	**C2**	**440**	**16h**	**5 % mol**	**$CHCl_3$ (0.1M, RT)**	**56**
5a	**C2**	456	16h	5 % mol	$CHCl_3$ (0.1M, RT)	12
5a	**no PC**	390	24h	0 % mol	$CHCl_3$ (0.1M, RT)	< 5 %
5a	**no PC**	440	24h	0 % mol	$CHCl_3$ (0.1M, RT)	0 %
5a	**C2**	**440**	**24h**	**5 % mol**	**$CHCl_3$ (0.1M, RT)**	**98 (78)**
5b	**C2**	440	24h	5 % mol	$CHCl_3$ (0.1M, RT)	38 (34)
5c	**C2**	440	24h	5 % mol	$CHCl_3$ (0.1M, RT)	68 (65)

5.2.1 Characterization of products 6a-c



6a

6-oxo-6,6a,6b,7,8,9,10,10a-octahydro-10bH-benzo[3,4]cyclobuta[1,2-c]chromen-10b-yl acetate (**6a**):

White powder; 78 % y*ield (22.3 mg, 0.078 mmol)*.

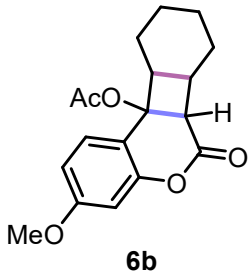
HRMS (MALDI-qTOF) = calculated for $C_{17}H_{18}Na\ O_4^+$([M+Na])$^+$: 309.1097; found: 309.1101

^{1}H NMR *major diasteromer – syn* (600 MHz, $CDCl_3$) δ 7.38 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.32 (ddd, *J* = 8.2, 7.3, 1.7 Hz, 1H), 7.16 (td, *J* = 7.5, 1.2 Hz, 1H), 7.05 (dd, *J* = 8.3, 1.2 Hz, 1H), 3.53 (dd, *J* = 10.6, 1.0 Hz, 1H), 2.70 – 2.57 (m, 1H), 2.38 – 2.31 (m, 1H), 2.09 – 2.01 (m, 1H), 1.96 (s, 3H), 1.81 – 1.66 (m, 4H), 1.47 – 1.36 (m, 2H), 1.09 – 0.99 (m, 1H).

^{13}C NMR *major diasteromer – syn* (151 MHz, $CDCl_3$) δ 170.48, 165.58, 151.65, 130.35, 127.67, 124.91, 123.01, 117.06, 73.29, 45.99, 44.69, 30.58, 24.07, 23.06, 22.10, 21.35, 21.05.

^{1}H NMR *minor diasteromer – anti* (600 MHz, $CDCl_3$) δ 7.27 (td, *J* = 7.4, 2.3 Hz, 1H), 7.09 (m, 3H), 3.82 (d, *J* = 8.8 Hz, 1H), 2.62 – 2.51 (m, 1H), 2.19 (s, 3H), 2.02 – 1.91 (m, 2H), 1.86 – 1.77 (m, 2H), 1.73 – 1.63 (m, 2H), 1.54 – 1.32 (m, 2H), 1.31 – 1.20 (m, 1H).

^{13}C NMR *minor diasteromer– anti* (151 MHz, $CDCl_3$) δ 170.03, 167.20, 149.72, 129.47, 124.81, 124.07, 122.57, 117.67, 82.07, 56.13, 47.39, 44.81, 29.19, 25.87, 25.74, 25.71, 21.56.



6b

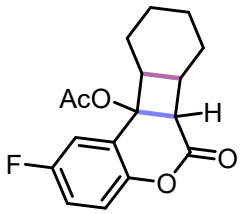
3-methoxy-6-oxo-6,6a,6b,7,8,9,10,10a-octahydro-10bH-benzo[3,4]cyclobuta[1,2-c]chromen-10b-yl acetate (**6b**):

White powder; 34 % y*ield (10.7 mg, 0.034 mmol)*.

HRMS (MALDI-qTOF) = calculated for $C_{18}H_{20}Na\ O_5^+$([M+Na])$^+$: 339.1203; found: 339.1206 (*major diasteromer*).

^{1}H NMR *major diasteromer* (600 MHz, $CDCl_3$) δ 6.98 (d, *J* = 8.4 Hz, 1H), 6.69 – 6.61 (m, 2H), 3.82 (d, *J* = 8.9 Hz, 1H), 3.78 (s, 3H), 2.59 – 2.47 (m, 1H), 2.17 (s, 3H), 1.98 – 1.89 (m, 2H), 1.85 – 1.78 (m, 2H), 1.63 (m, 3H), 1.49 – 1.27 (m, 2H).

^{13}C NMR *major diasteromer* (151 MHz, $CDCl_3$) δ 170.08, 167.38, 160.46, 150.70, 123.43, 116.41, 111.12, 102.89, 82.22, 56.54, 55.67, 47.37, 44.57, 29.85, 29.21, 25.93, 25.83, 21.65.



6c

2-fluoro-6-oxo-6,6a,6b,7,8,9,10,10a-octahydro-10bH-benzo[3,4]cyclobuta[1,2-c]chromen-10b-yl acetate (**6c**):

White powder; 65 % y*ield (19.8 mg, 0.065 mmol)*.

HRMS (MALDI-qTOF) = calculated for $C_{17}H_{17}FNa\ O_4^+$; $[M+Na]^+$: 327.1003; found: 327.1006 (*major diasteromer*)

^{1}H NMR *major diasteromer* (600 MHz, $CDCl_3$) δ 7.10 – 7.05 (m, 1H), 7.05 – 7.03 (m, 2H), 3.52 (dd, *J* = 10.6, 1.0 Hz, 1H), 2.64 (dt, *J* = 10.7, 7.9 Hz, 1H), 2.41 – 2.31 (m, 1H), 2.08 – 2.02 (m, 1H), 1.99 (s, 3H), 1.81 – 1.66 (m, 4H), 1.47 – 1.38 (m, 2H), 1.05 (qt, *J* = 12.9, 3.1 Hz, 1H).

^{13}C NMR *major diasteromer* (151 MHz, $CDCl_3$) δ 170.49, 165.21, 160.15, 158.54, 147.81 (d, *J* = 2.7 Hz), 124.34 (d, *J* = 7.2 Hz), 118.67 (d, *J* = 8.2 Hz), 117.59 (d, *J* = 23.6 Hz), 113.76 (d, *J* = 23.8 Hz), 73.25, 45.54, 44.66, 30.60, 24.03, 23.02, 21.33, 21.05.

5.4 Intermolecular cyclization of 5a using different alkenes

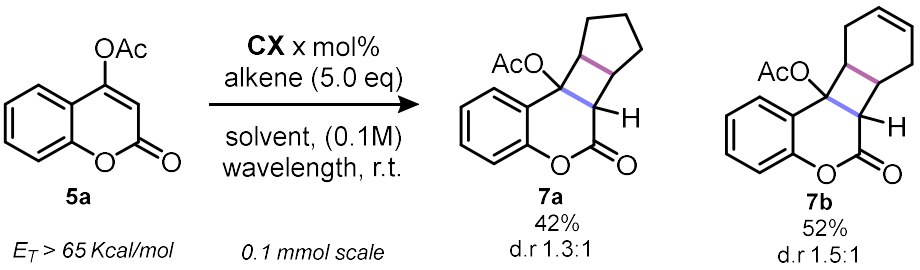


Figure S31: intermolecular cyclization of **5a** with different alkenes.

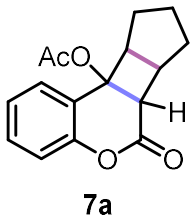
In a Schlenk tube, **coumarin 5a** (0.1 mmol), **C2** (5 % mol) and the alkene (0.5 mmol, 5.0 eq.) were dissolved in 1 mL of $CHCl_3$. The reaction mixture was degassed by repeated freeze-pump-thaw cycles until gas evolution ceased. Subsequently, the tubes were backfilled with argon and irradiated using a 440 nm Kessil® lamp.

All the results in the tables below were determined via ^{1}H-NMR analysis, using dibromomethane as internal standard (0.1 mmol) to observe yield. For the highest yielding entries, the products were isolated by flash chromatography (gradient of *n*-hexane / EtOAc).

Table S12 screening for intermolecular [2+2] cycloaddition of **5a** with different alkenes.

Alkene	Catalyst	Wavelength (nm)	Time	Loading	Solvent (conc, temp °C)	yield% (isolated)
cyclopentene	**C2**	440	24h	5 % mol	$CHCl_3$ (0.1M, RT)	45 (42)
cyclohexadiene	**C2**	440	24h	5 % mol	$CHCl_3$ (0.1M, RT)	56 (52)

5.3.1 Characterization of products 7a-b



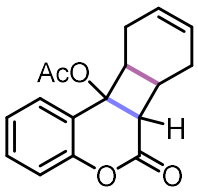
6-oxo-6a,6b,7,8,9,9a-hexahydrocyclopenta[3,4]cyclobuta[1,2-c]chromen-9b(6H)-yl acetate (**7a**):

White powder; 42 % y*ield (11.4 mg, 0.04 mmol)*.

HRMS (MALDI-qTOF) = calculated for $C_{16}H_{16}Na\ O_4^+$([M+Na]$^+$): 295.0941; found: 295.0943.

^{1}H NMR *major diasteromer* (600 MHz, $CDCl_3$) δ 7.35 – 7.29 (m, 1H), 7.17 (td, *J* = 7.3, 1.2 Hz, 1H), 7.07 (dd, *J* = 8.7, 1.2 Hz, 1H), 3.10 (dd, *J* = 7.1, 1.2 Hz, 1H), 2.93 (ddt, *J* = 9.5, 6.8, 1.5 Hz, 1H), 2.77 (q, *J* = 6.6 Hz, 1H), 2.36 – 2.29 (m, 1H), 1.99 (s, 3H), 1.98-1.82 (m, 3H), 1.72 (dddd, *J* = 14.2, 10.7, 9.5, 8.2 Hz, 1H), 1.65 – 1.58 (m, 1H).

^{13}C NMR *major diasteromer* (151 MHz, $CDCl_3$) δ 170.21, 166.04, 150.88, 130.23, 126.97, 125.26, 123.84, 117.39, 72.07, 51.37, 47.39, 39.59, 31.86, 25.99, 25.62, 21.14.



7b

6-oxo-6,6a,6b,7,10,10a-hexahydro-10bH-benzo[3,4]cyclobuta[1,2-c]chromen-10b-yl acetate (**7b**):

White powder; 52 % y*ield (14.8 mg, 0.052 mmol)*.

HRMS (MALDI-qTOF) = calculated for $C_{17}H_{16}NaO_4^+$([M+Na]$^+$): 307.0941; found: 307.0944 (*major diasteromer*).

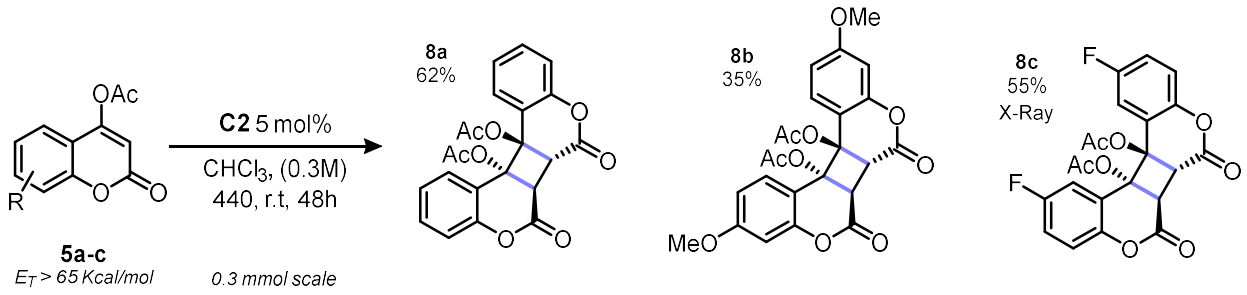
^{1}H NMR *major diasteromer* (400 MHz, cdcl$_3$) δ 7.37 – 7.30 (m, 2H), 7.23 – 7.13 (m, 1H), 7.12 – 7.05 (m, 1H), 6.03 (m, 1H), 5.85 (m, 1H), 3.40 (d, *J* = 9.4 Hz, 1H), 2.83 (dd, *J* = 9.1, 2.9 Hz, 1H), 2.74 – 2.55 (m, 2H), 2.33 – 2.20 (m, 2H), 2.14 (s,1H), 1.98 (s, 3H).

The major diastereomer resulted to co-elute with the minor. For this reason, only ^{1}H NMR is here presented.

^{1}H NMR *minor diasteromer* (600 MHz, CDCl$_3$) δ 7.35 – 7.27 (m, 1H), 7.14 – 7.07 (m, 3H), 5.75 – 5.59 (m, 2H), 3.92 (d, *J* = 9.0 Hz, 1H), 2.82 (dddd, *J* = 13.2, 10.4, 9.0, 6.3 Hz, 1H), 2.57 – 2.43 (m, 1H), 2.30 – 2.23 (m, 3H), 2.19 (s, 3H), 2.02 – 1.96 (m, 1H).

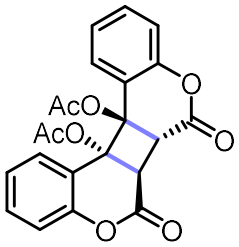
^{13}C NMR *minor diasteromer* (151 MHz, CDCl$_3$) δ 169.91, 166.88, 149.73, 129.63, 127.42, 126.38, 124.93, 124.01, 122.56, 117.74, 81.39, 51.28, 47.16, 40.02, 28.95, 25.48, 21.55.

5.5 [2+2] dimerization of 5a-c



In a Schlenk tube, **coumarins 5a-c** (0.3 mmol) and **C2** (5 % mol) were dissolved in 1 mL chloroform (0.3 M). The reaction mixture was degassed by repeated freeze-pump-thaw cycles until gas evolution ceased. Subsequently, the tubes were backfilled with argon and irradiated using a 440 nm Kessil® lamp. The products were isolated by flash chromatography (gradient of *n*-hexane / EtOAc).

5.4.1 Characterization of products 8a-c



8a

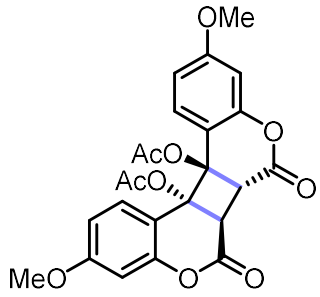
(6aR,6bR,12bR,12cR)-6,7-dioxo-6,6a,6b,7-tetrahydrocyclobuta[1,2-c:4,3-c']dichromene-12b,12c-diyl diacetate (**8a**):

White powder; 62 % y*ield (40.0 mg, 0.093 mmol)*.

HRMS (MALDI-qTOF) = calculated for $C_{22}H_{16}Na\ O_8^+$([M+Na]$^+$): 431.0737; found: 431.0745.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 7.8, 1.6 Hz, 2H), 7.49 (ddd, *J* = 8.3, 7.3, 1.6 Hz, 2H), 7.29 (ddd, *J* = 7.8, 7.3, 1.2 Hz, 2H), 7.20 (dd, *J* = 8.3, 1.2 Hz, 2H), 3.43 (s, 2H), 1.88 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 169.25, 160.29, 151.65, 131.85, 130.49, 124.33, 117.80, 114.78, 77.84, 43.51, 20.74.



8b

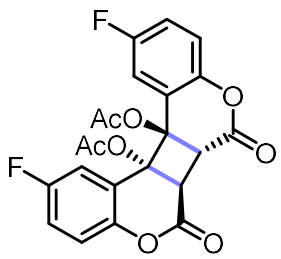
(6aR,6bR,12bR,12cR)-3,10-dimethoxy-6,7-dioxo-6,6a,6b,7-tetrahydrocyclobuta[1,2-c:4,3-c']dichromene-12b,12c-diyl diacetate (**8b**):

white powder; 35 % y*ield (25.8 mg, 0.053 mmol)*.

HRMS (MALDI-qTOF) = calculated for $C_{24}H_{20}Na\ O_{10}^+$([M+Na]$^+$): 491.0948; found: 491.0952.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.8 Hz, 2H), 6.84 (dd, *J* = 8.8, 2.6 Hz, 2H), 6.67 (d, *J* = 2.6 Hz, 2H), 3.86 (s, 6 H), 3.38 (s, 2H), 1.88 (s, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 169.37, 162.07, 160.58, 152.86, 131.30, 112.26, 106.77, 101.43, 77.87, 55.66, 43.49, 20.83.



8c

(6aR,6bR,12bR,12cR)-2,11-difluoro-6,7-dioxo-6,6a,6b,7-tetrahydro cyclobuta[1,2-c:4,3-c']dichromene-12b,12c-diyl diacetate (**8c**):

White powder; 55 % y*ield (38.5 mg, 0.083 mmol)*.

HRMS (MALDI-qTOF) = calculated for $C_{22}H_{14}F_2Na\ O_8^+$([M+Na]$^+$): 467.0549; found: 467.0552.

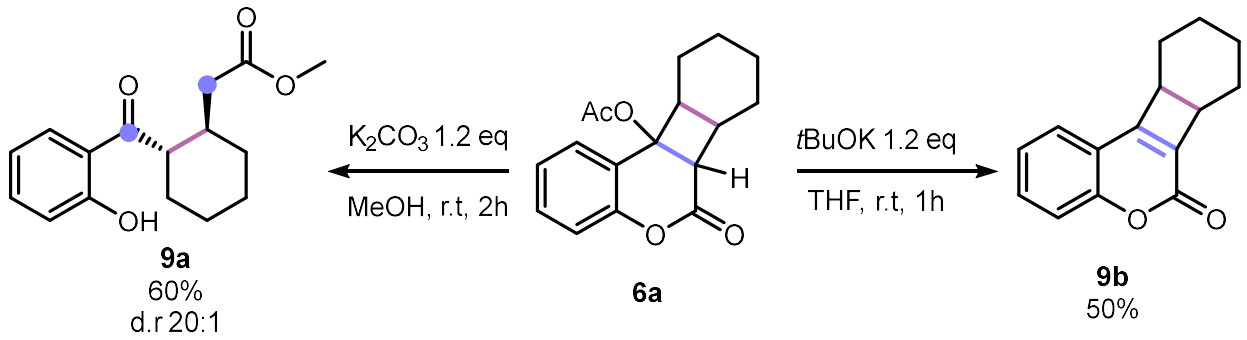
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.32 (dd, *J* = 8.4, 2.9 Hz, 2H), 7.25 – 7.18 (m, 4H), 3.41 (s, 2H), 1.95 (s, 6H).

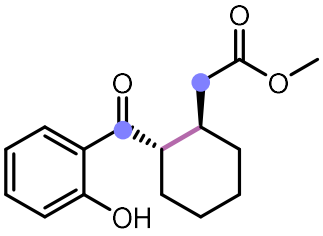
^{19}F NMR (565 MHz, CDCl3) δ -116.90 (td, *J* = 7.9, 4.5 Hz).

^{13}C NMR (151 MHz, $CDCl_3$) δ 169.16, 159.69, 158.71 (d, *J* = 245 Hz, 1C), 147.77 (d, *J* = 2.77 Hz, 1C), 119.43 (d, *J* = 8.22 Hz, 1C), 119.42 (d, *J* = 23.5 Hz, 1C), 116.39 (d, *J* = 24.7 Hz, 1C), 115.80 (d, *J* = 7.88 Hz, 1C), 77.53, 43.02, 20.71.

Single crystals suitable for X-ray diffraction analysis (see 9.2.2 X-Ray Crystallography of product 8c) were obtained within the NMR sample. The sample was dissolved in deuterated chloroform ($CDCl_3$) and left to stand in the original NMR tube for more than two weeks. To facilitate slow evaporation of the solvent and promote gradual crystallization, the tube was loosely capped with a pierced cap.

5.6 Synthetic elaborations of 6a





9a

Methyl 2-((1R,2S)-2-(2-hydroxybenzoyl)cyclohexyl)acetate chromen-6-one (9a): 141 mg (0.49 mmol, 1.0 eq.) of **6a** and 74.6 mg (0.54 mmol, 1.1 eq.) of potassium carbonate were dissolved in 5 mL of MeOH (100 mM) and stirred at room temperature for 2 hours. The solvent was removed under reduced pressure. The product was isolated by flash chromatography (gradient of *n*-hexane / EtOAc) as white powder; 60 % y*ield (81.8 mg, 0.29 mmol)*. The NMR spectrum agrees with the reported data:[54]

^{1}H NMR (600 MHz, $CDCl_3$) δ 12.58 (s, 1H), 7.79 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.48 (ddd, *J* = 8.5, 7.1, 1.7 Hz, 1H), 6.99 (dd, *J* = 8.4, 1.1 Hz, 1H), 6.91 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 3.59 (s, 3H), 3.30 (td, *J* = 11.0, 3.4 Hz, 1H), 2.37 (dddd, *J* = 14.4, 12.0, 7.6, 3.5 Hz, 1H), 2.31 (dd, *J* = 14.7, 4.0 Hz, 1H), 2.12 (dd, *J* = 14.7, 8.3 Hz, 1H), 1.97 (ddd, *J* = 12.9, 3.5, 2.1 Hz, 1H), 1.92 (ddd, *J* = 13.1, 3.4, 1.5 Hz, 1H), 1.86 – 1.77 (m, 2H), 1.47 – 1.34 (m, 2H), 1.24 – 1.17 (m, 1H).

***Determination of relative configuration of* 9a:**

The determination of the relative configuration of **9a** was assessed via 1D NOE experiments. The Figure S32 below shows relevant correlations that were investigated:

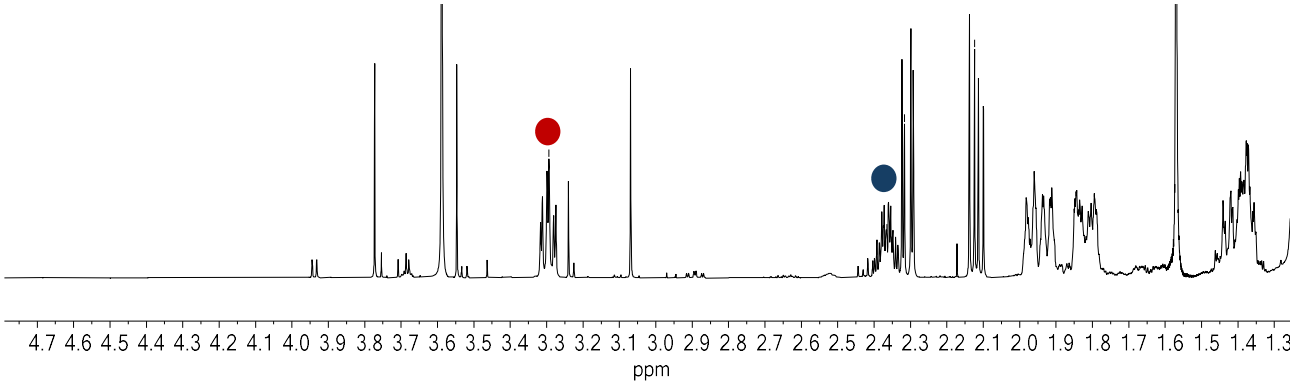


Figure S32 Zoom on aliphatic region for **9a**. The signal at 3.29 ppm (red dot) was chosen for 1D NOE irradiation.

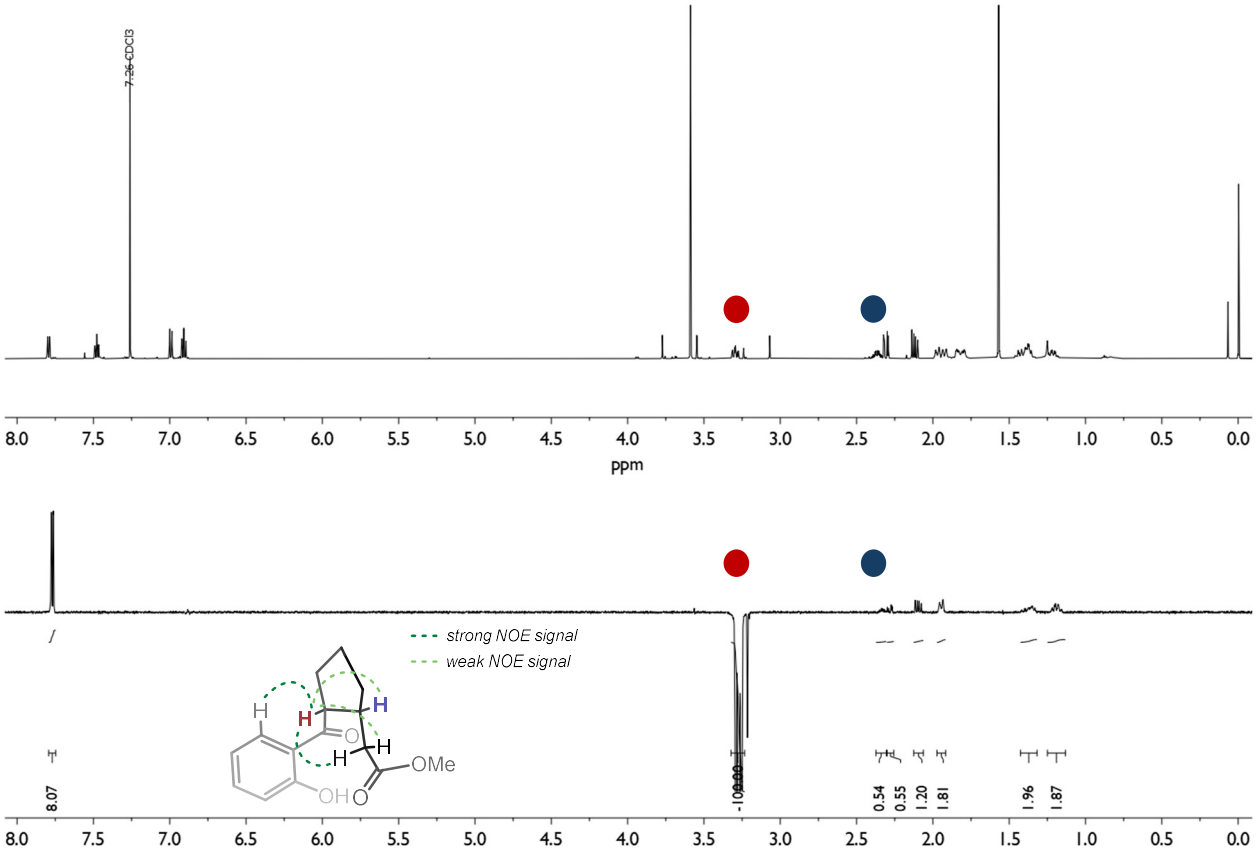
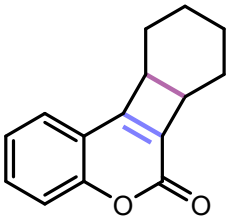


Figure S33 Top: ^{1}H NMR of **9a**; bottom: 1D NOE observed when irradiating signal at 3.29 ppm. The stronger relationships were found with the *ortho* aromatic signal (7.79 ppm), the cyclohexane protons and one of the two methylene protons α to the ester moiety suggesting the relationship between the ester and the ketone moiety to be *anti*.



9b

6b,7,8,9,10,10a-Hexahydro-6H-benzo[3,4]cyclobuta[1,2-c]chromen-6-one (9b):

28.6 mg (0.1 mmol, 1.0 eq.) of **6a** and 13.5 mg (0.12 mmol, 1.2 eq.) of potassium *tert*-butoxide were dissolved in 1 mL of dry THF under argon atmosphere and stirred at room temperature for 1 hour. The solvent was removed under reduced pressure. The product was isolated by flash chromatography (gradient of *n*-hexane / EtOAc) as white powder; 50 % y*ield (11.3 mg, 0.05 mmol)*.

HRMS (MALDI-qTOF) = calculated for $C_{15}H_{14}Na\ O_2^+$([M+Na]$^+$): 249.0886; found: 249.0888.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48 (ddd, *J* = 8.7, 7.3, 1.6 Hz, 1H), 7.41 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.36 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.24 (td, *J* = 7.5, 1.1 Hz, 1H), 3.11 (ddt, *J* = 11.5, 7.6, 3.7 Hz, 2H), 2.17 (ddd, *J* = 11.8, 4.9, 2.4 Hz, 2H), 1.98 (m, 3H), 1.87 (qd, *J* = 12.0, 3.9 Hz, 1H), 1.69 – 1.58 (m, 2H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 166.86, 156.92, 156.84, 132.51, 131.21, 124.10, 123.68, 118.30, 117.78, 52.76, 51.95, 28.65, 27.82, 26.88, 26.40.

6. Mechanistic experiments

6.1 Stern Volmer Plot with 1a-E in chloroform

A saturated solution (1 M – 114.13 mg/mL) of the quencher substrate (dimethyl fumarate **1a-*E***) in degassed $CHCl_3$ (HPLC grade) was prepared and incremental aliquots (20-40-50 µL) of this stock solution were added to a solution ($5 \cdot 10^{-5}$ M in $CHCl_3$ HPLC grade) of the photocatalyst **C2**. After each addition, the solution was mixed, and the emission spectra of the excited catalyst was acquired from 350 nm to 750 nm (the excitation wavelength was fixed at 338 nm). A solvent blank was subtracted from all the measurements. The results shown in Figure S34 indicate that substrate **1a-*E*** quenched the excited-state emission of **C2**. The Stern-Volmer plot in Figure S35 shows a linear correlation between the amounts of substrates and the ratio I_0/I, following the relationship: $\mathbf{I_0/I = 1 + K_{SV}[Q]}$ **(Q = Quencher)**.

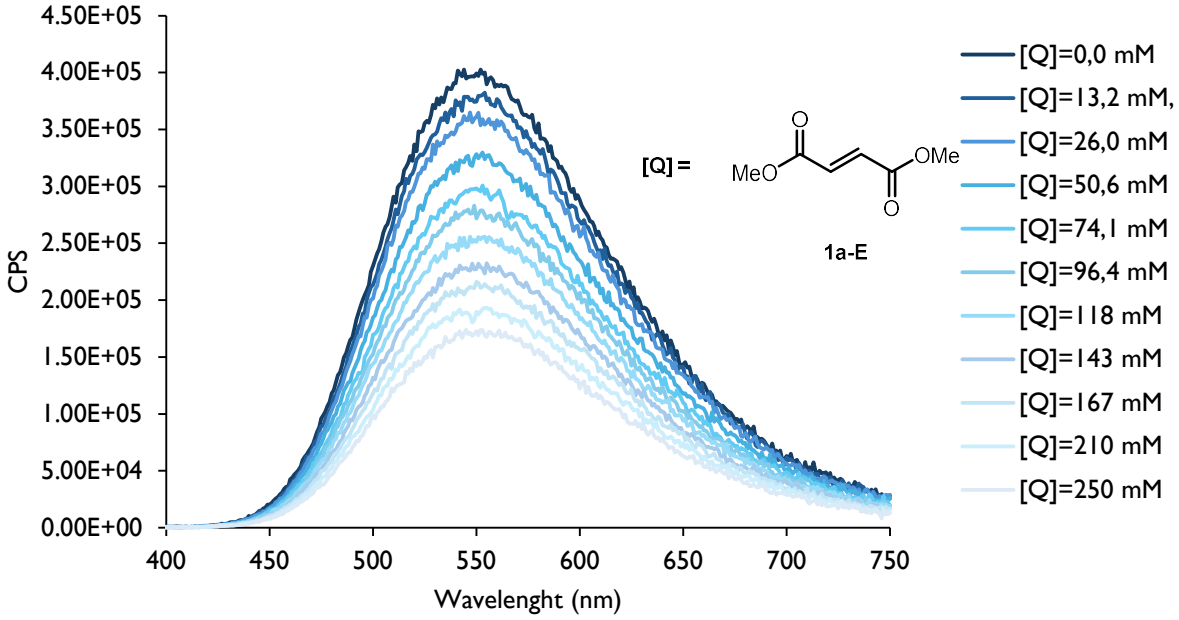


Figure S34 Emission quenching of **C2** in the presence of increasing amounts of quencher **1a-*E*.** The solvent ($CHCl_3$) was chosen because of the better solubility of substrate **1a-*E*** and a small screening conducted for the photosensitization rate of **1a-*E*** (Table S5)

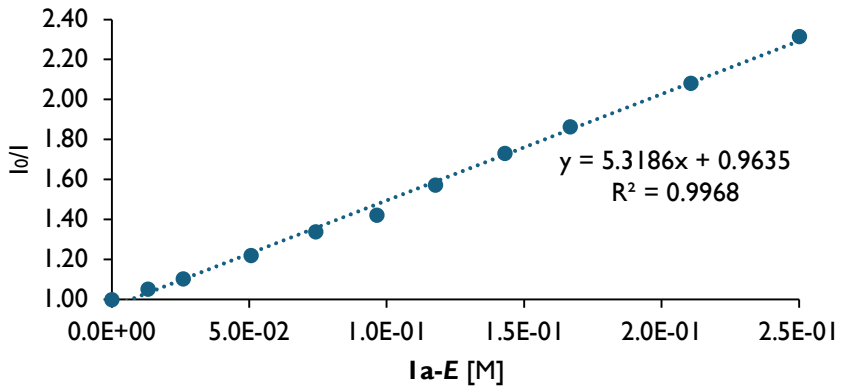


Figure S35: Stern-Volmer plot of **C2** in the presence of increasing amounts of quencher **1a-*E*** in $CDCl_3$.

We obtained a Stern-Volmer constant ($\mathbf{K_{SV}}$) of 5.32 L/mol. The Stern-Volmer constant provides information about the sensitivity of the quenching system and, for dynamic quenching, $\mathbf{K_{SV}}$ follows the relationship: $\mathbf{K_{SV} = k_q \cdot \tau_0}$. Where $\boldsymbol{\tau_0}$ in the case of triplet-triplet energy transfer (EnT) is the phosphorescence lifetime of the emitter in the absence of a quencher, and $\mathbf{k_q}$ is the bimolecular quenching constant. The constant $\mathbf{k_q}$ describes how efficiently the quencher suppresses the emission intensity of the system. In our system, **C2** T_1 lifetime in $CHCl_3$ at room temperature ($\boldsymbol{\tau_{T1}}$) is 8.71 μs (Table S1) which implies a bimolecular quenching constant ($\mathbf{k_q}$) of 6.2 x 10^5 $M^{-1}s^{-1}$.

6.2 Stern-Volmer Plot with 1a-E in n-hexane

We also conducted a similar Stern-Volmer quenching experiment changing the solvent to *n*-hexane, to better understand if the improved isomerization ratio (*E:Z*) in the more apolar solvent seen during the reaction optimization (Table S5) was also attributable to a higher quenching rate of the catalyst emission.

A saturated solution (0.02 M – 2.3 mg/mL) of the quencher substrate (dimethyl fumarate **1a-*E***) in degassed *n*-hexane (HPLC grade) was prepared and incremental aliquots (0-40-80 μL) of this stock solution were added to a solution ($5 \cdot 10^{-6}$ M in *n*-hexane HPLC grade) of the photocatalyst **C2**. After each addition, the solution was mixed, and the emission spectra of the excited catalyst was acquired from 350 nm to 750 nm (the excitation wavelength was fixed at 338 nm). A solvent blank was subtracted from all the measurements. The results shown in Figure S36 indicate that substrate **1a-*E*** quenched the excited-state emission of **C2**. The Stern-Volmer plot in Figure S37 shows a linear correlation between the amounts of substrates and the ratio I_0/I, following the relationship: $\mathbf{I_0/I = 1 + K_{SV}[Q]}$ **(Q = Quencher)**.

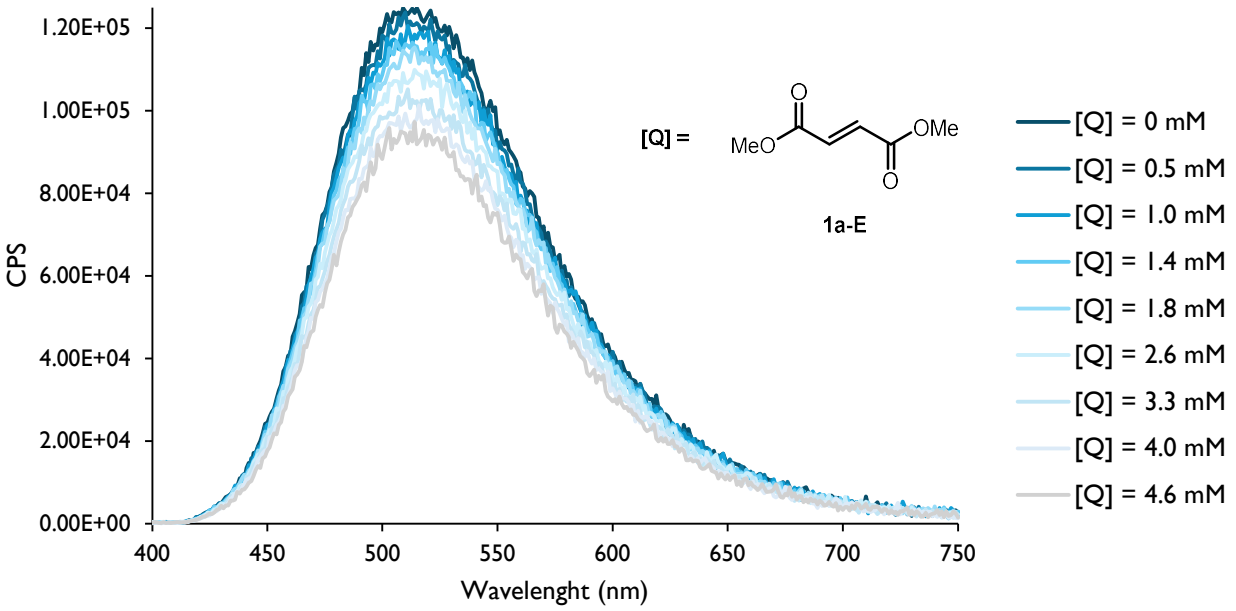


Figure S36 Emission quenching of **C2** in the presence of increasing amounts of quencher **1a-*E*** *in n*-hexane.

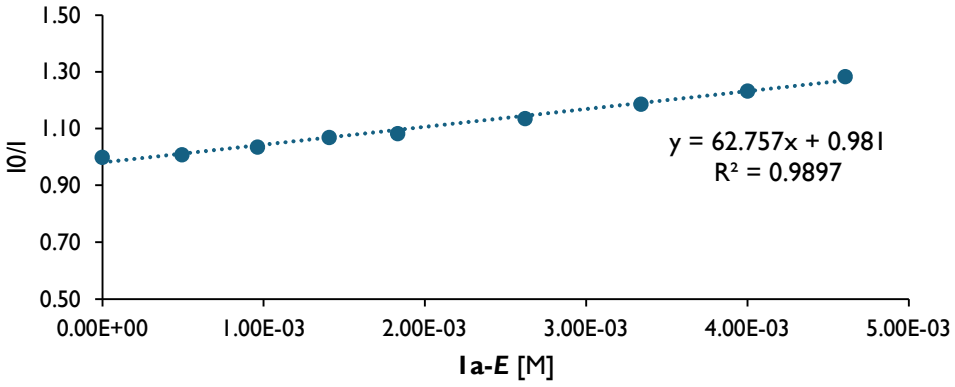


Figure S37 Stern-Volmer plot of **C2** in the presence of increasing amounts of quencher **1a-*E*** in *n*-hexane.

Even with a much higher dilution we obtained a Stern-Volmer constant ($\mathbf{K_{SV}}$) of 62.8 L/mol and a good linearity in the resulting plot in Figure S37. In our system, **C2** T_1 lifetime in *n*-hexane at room temperature ($\boldsymbol{\tau_{T1}}$) is 8.61 µs (Table S1) which implies a bimolecular quenching constant ($\mathbf{k_q}$) of 7.3 x 10^6 $M^{-1}s^{-1}$ which is more than a 10-fold increase compared to the one in chloroform. This aspect corroborates our hypothesis of a better efficiency of this catalytic system in apolar solvents, which was observed for several of our catalytic transformations.

6.3 Photostability of C2 in optimized conditions at 440 nm

The photostability of **C2** was evaluated by irradiating a degassed 5 mM $CDCl_3$ solution of **C2**, with and without 100 mM 4-acetyloxycoumarin (**5a**) and 500 mM cyclohexene, at room temperature under 440 nm Kessil® lamp irradiation. ^{1}H-NMR spectra were recorded at various time points using dibromomethane (CH_2Br_2, 100 mM) as an internal standard. These conditions were designed to mimic the intermolecular [2+2] cyclization of **5a** with cyclohexene, as described in 5.3 Intermolecular cyclization of 5a-c with cyclohexene.

The results, presented in Figure S38, shows that **C2** exhibits significant photostability. In the absence of substrate **5a**, 80% of **C2** remained intact after 60 hours of irradiation. When acting as a sensitizer in the presence of **5a**, **C2** showed even greater stability, with 100% of the photocatalyst detectable after 60 hours. Degradation of **C2** was observed only after complete consumption of **5a**, highlighting its robustness under reaction conditions.[53]

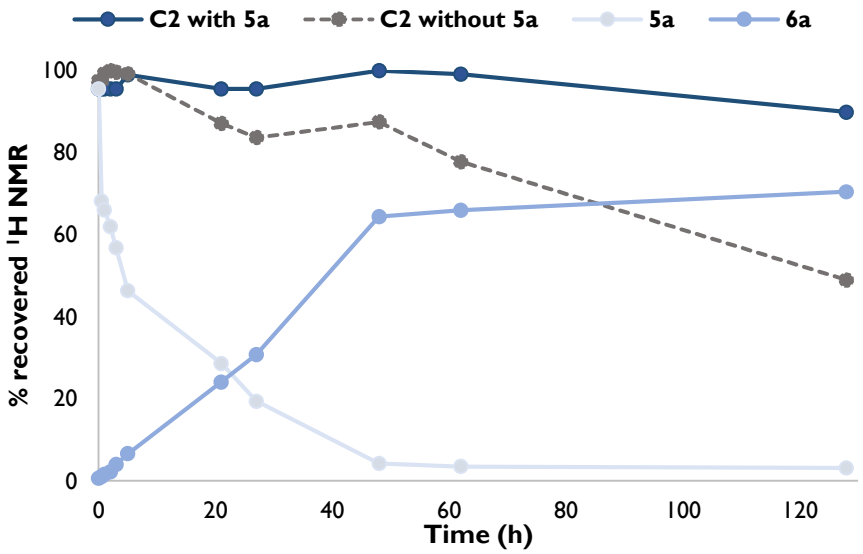


Figure S38 Photostability measurement of PC **C2;** Dotted grey line: **C2** 5 mM solution in $CDCl_3$; Dark blue line: **C2** 5 mM solution in $CDCl_3$ along with 100 mM of **5a** and 500 mM of cyclohexene.

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8. NMR Spectra

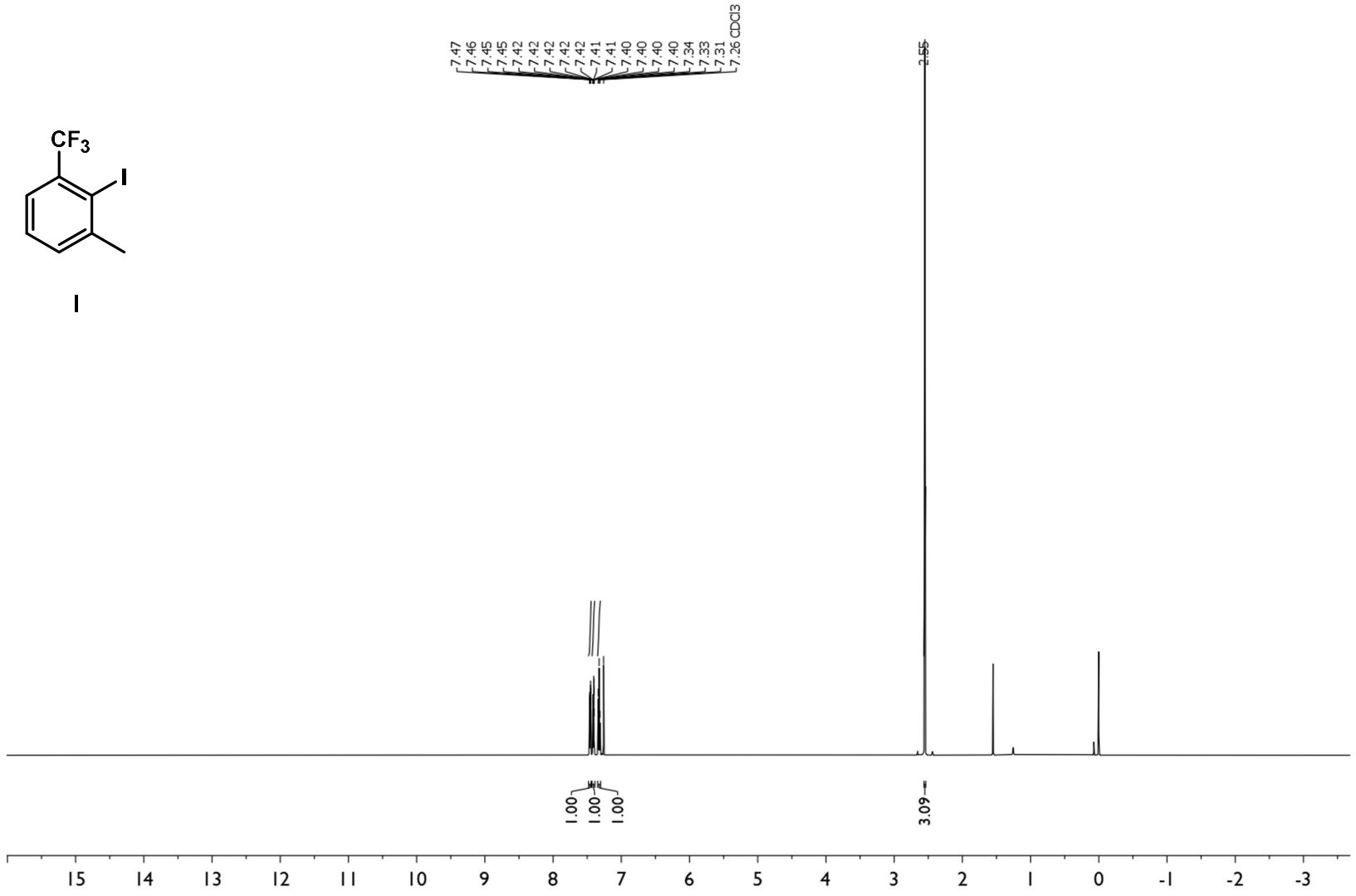


Figure S39 ^{1}H NMR of **I**. Recorded at 600 MHz NMR.

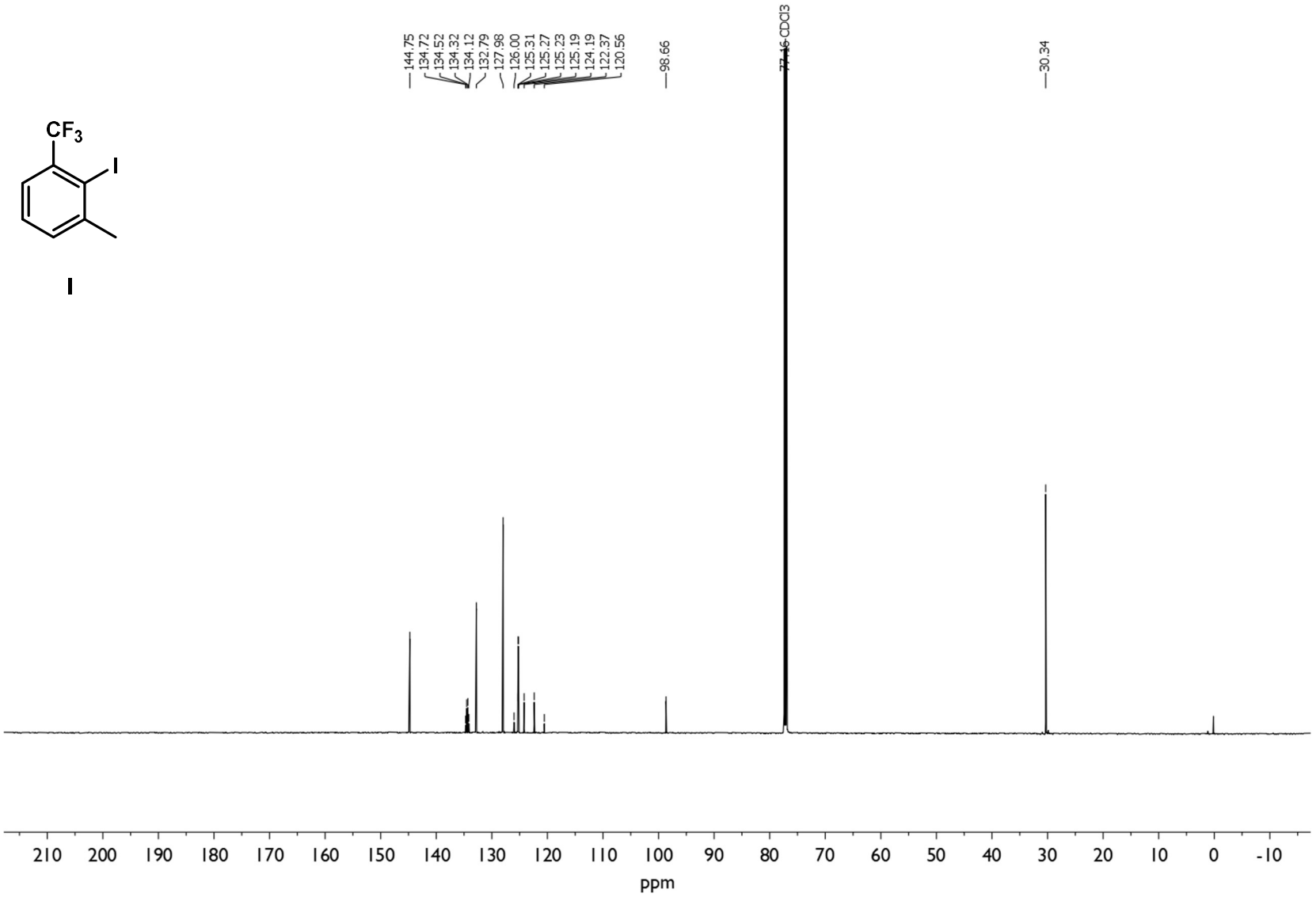


Figure S40 ^{13}C NMR of **I**. Recorded at 151 MHz NMR.

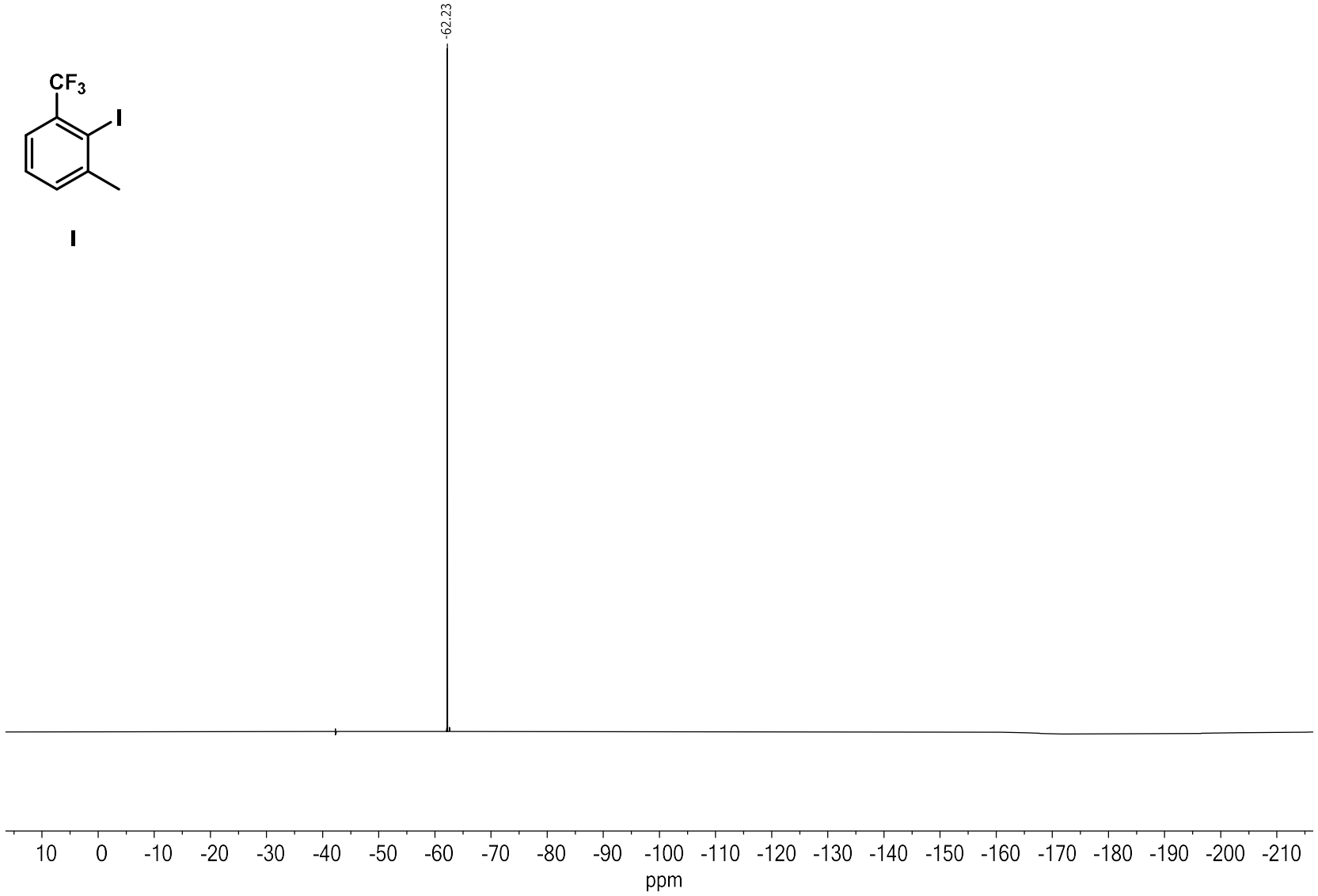


Figure S41 ^{19}F NMR of **I**. Recorded at 565 MHz NMR.

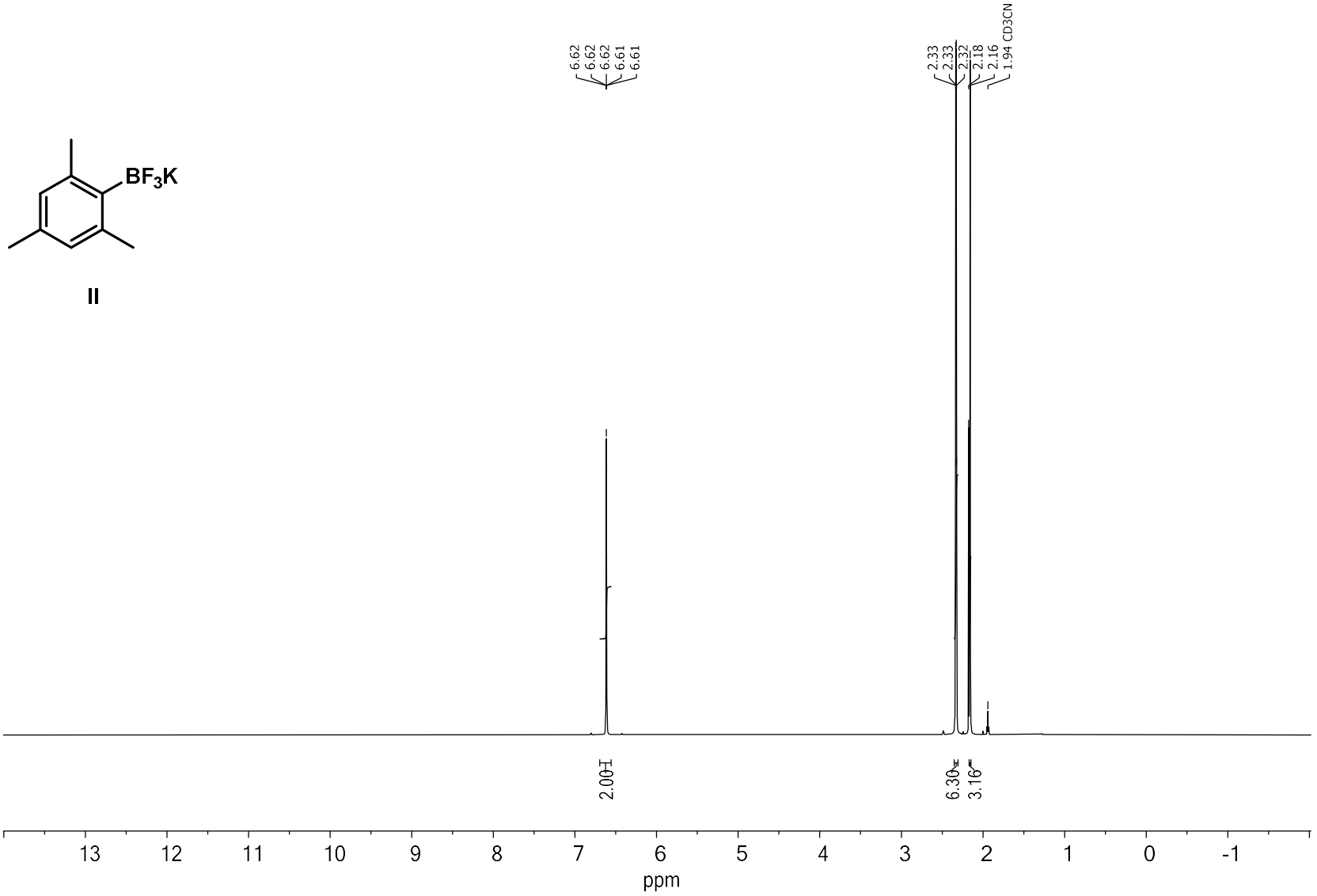


Figure S42 ^{1}H NMR of **II**. Recorded at 600 MHz NMR.

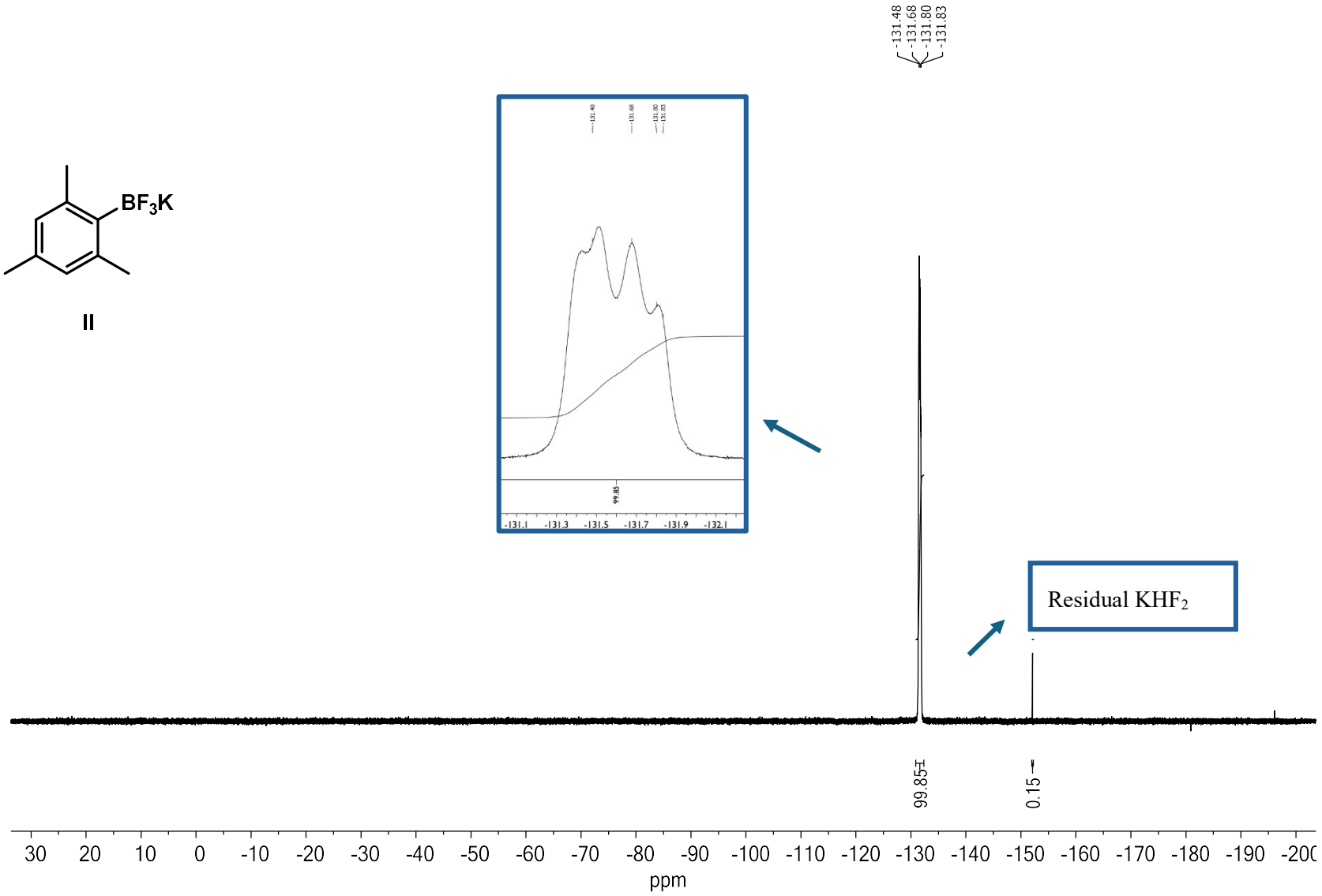


Figure S43 ^{19}F NMR of **II**. Recorded at 565 MHz NMR.

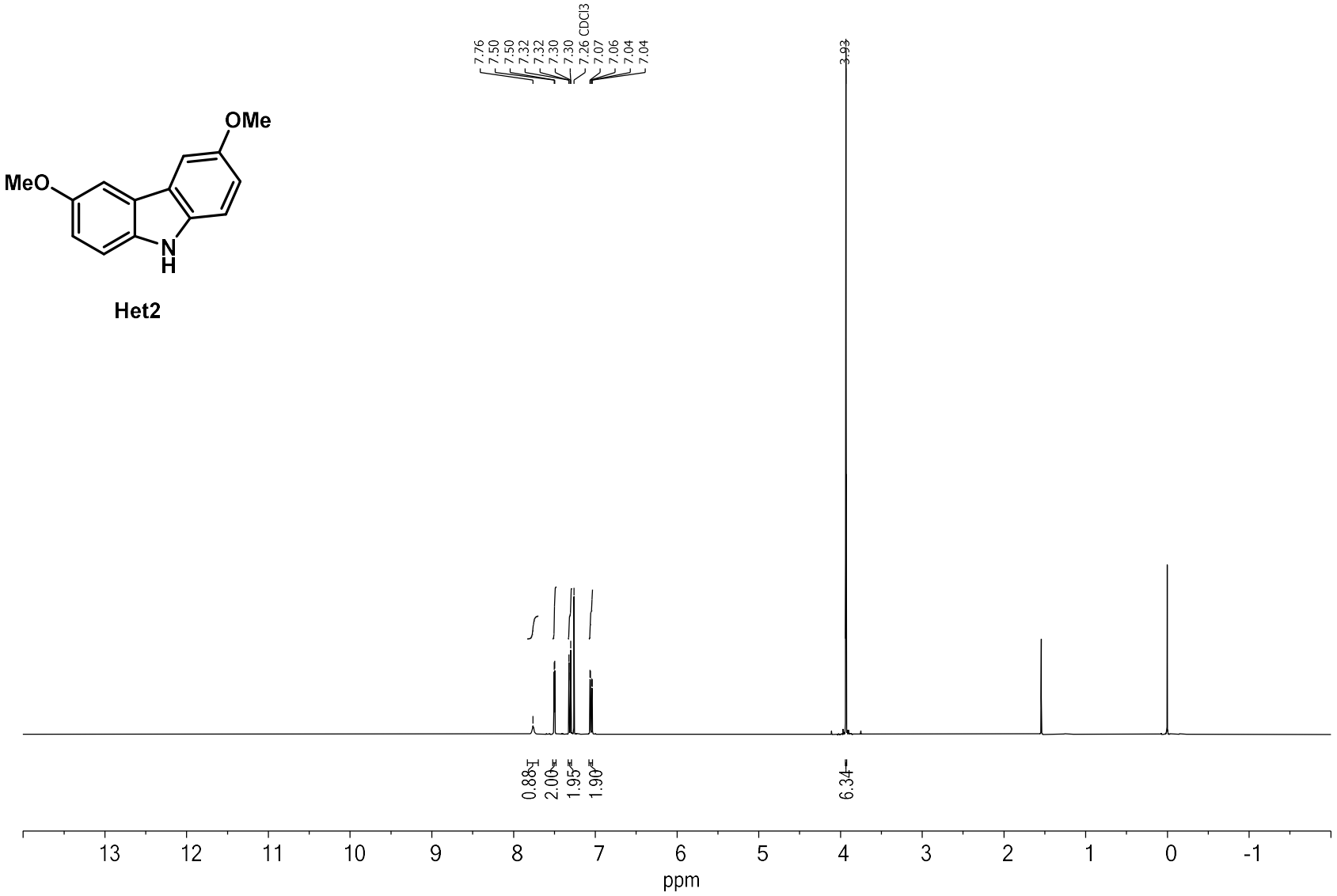


Figure S44 ^{1}H NMR of **Het2**. Recorded at 600 MHz NMR.

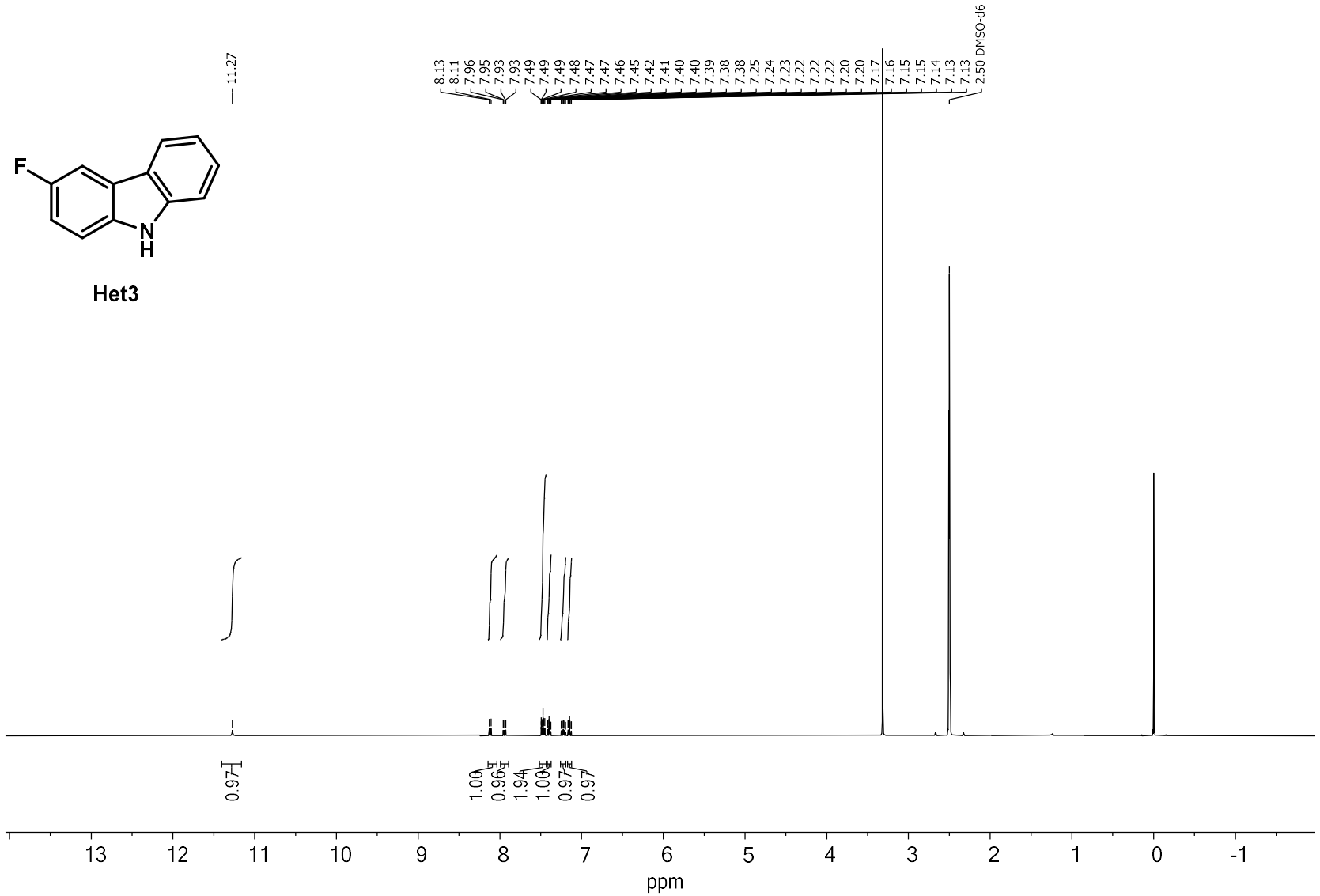


Figure S45 ^{1}H NMR of **Het3**. Recorded at 600 MHz NMR.

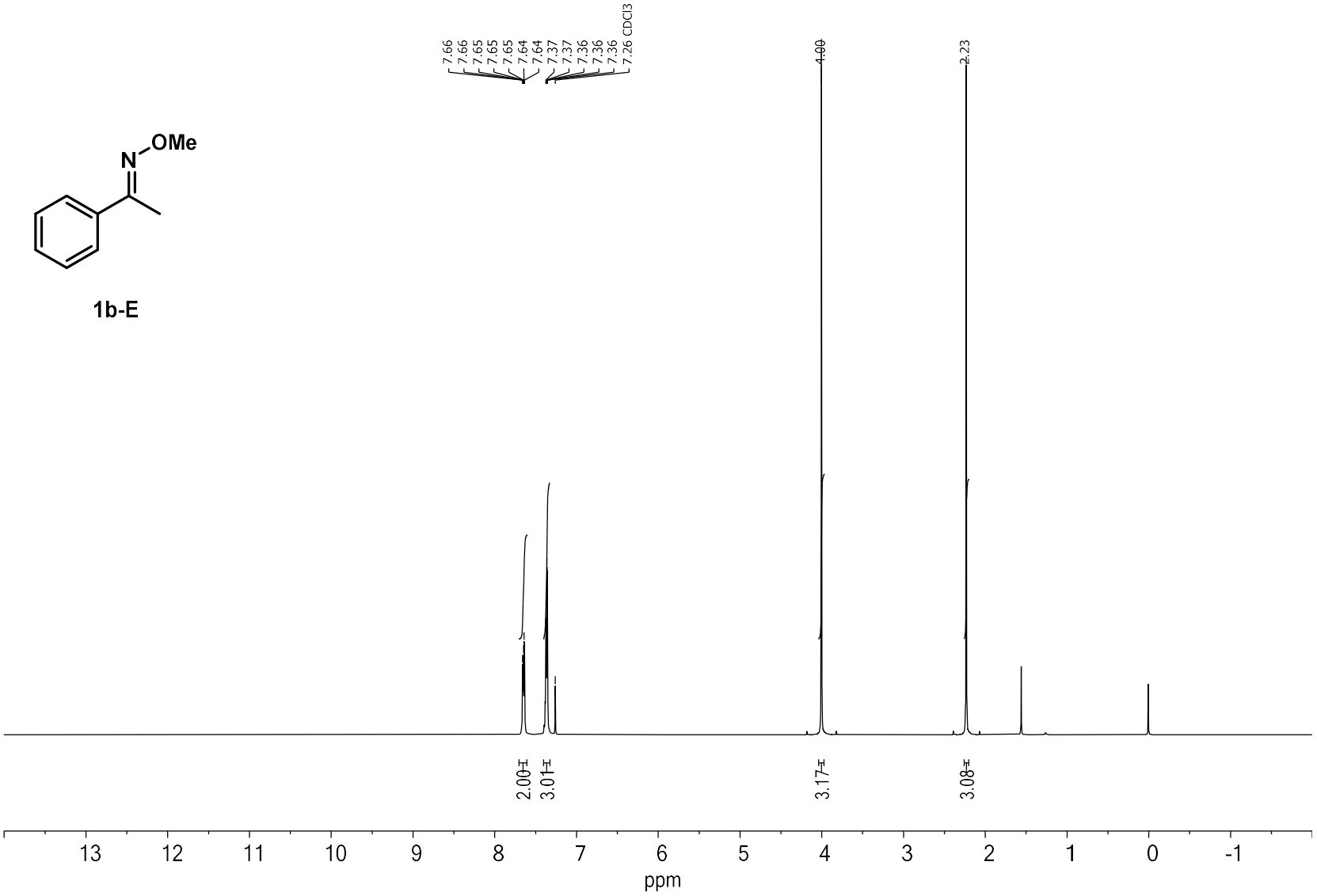


Figure S46 ^{1}H NMR of **1b-*E***. Recorded at 600 MHz NMR.

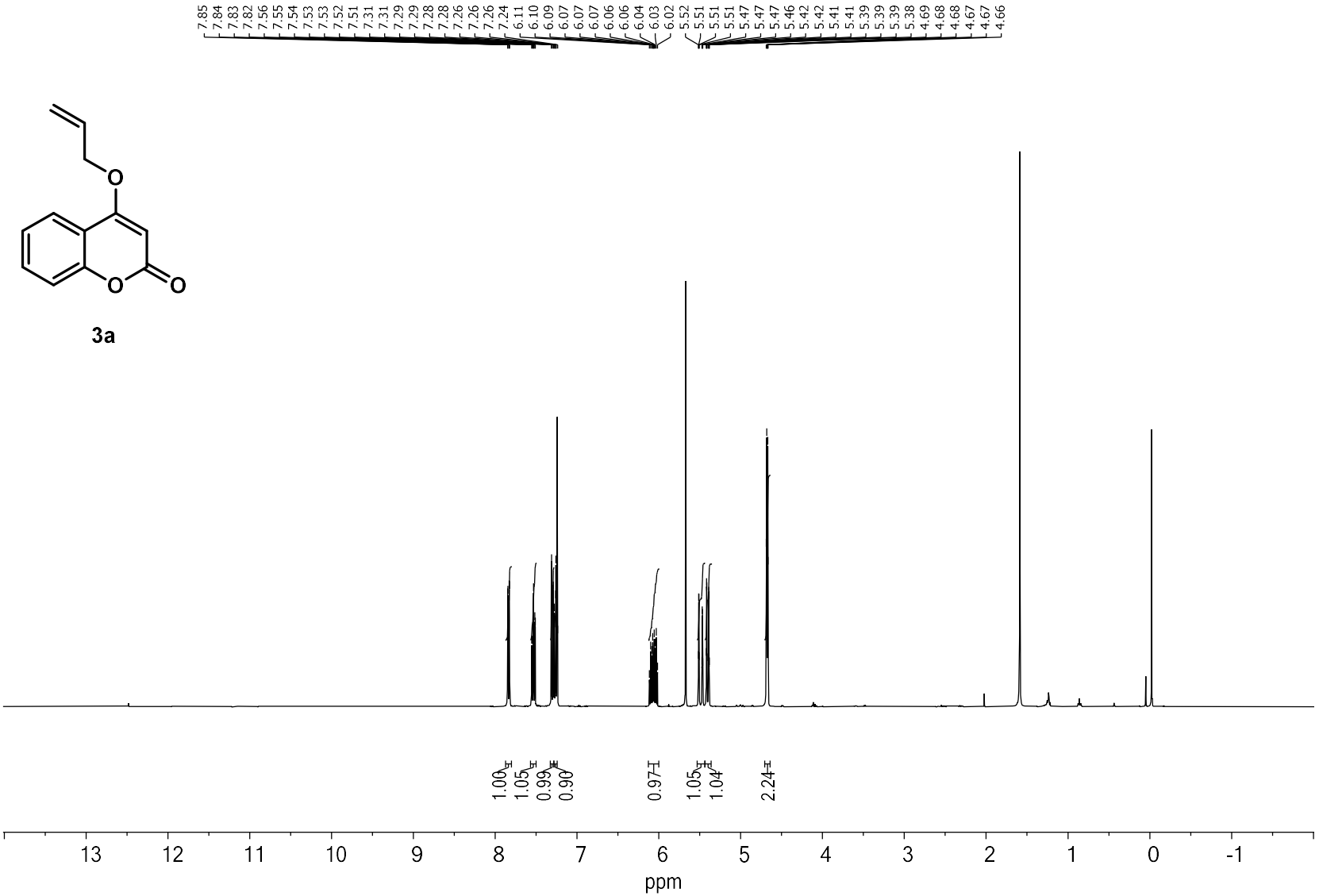


Figure S47 ^{1}H NMR of **3a**. Recorded at 600 MHz NMR.

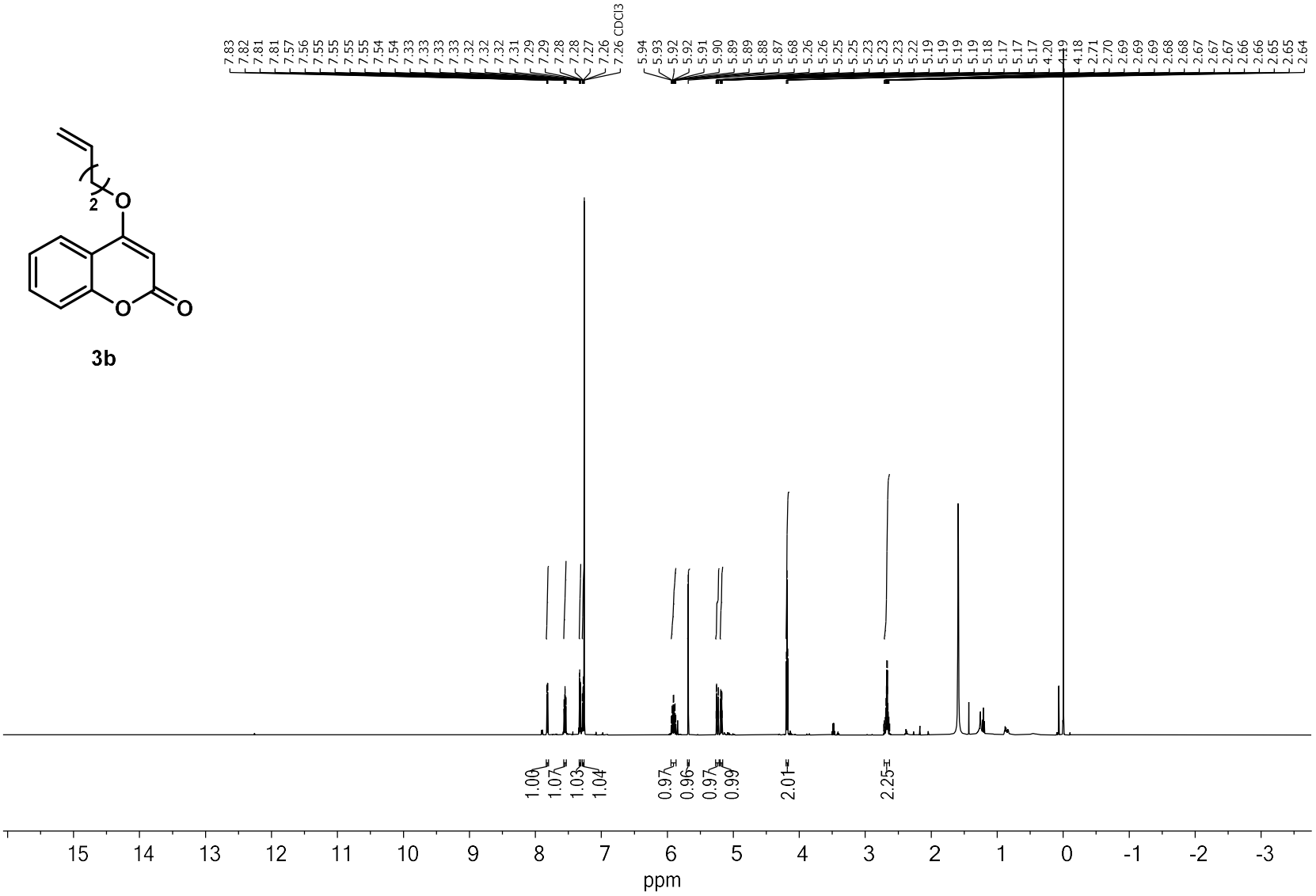


Figure S48 ^{1}H NMR of **3b**. Recorded at 600 MHz NMR.

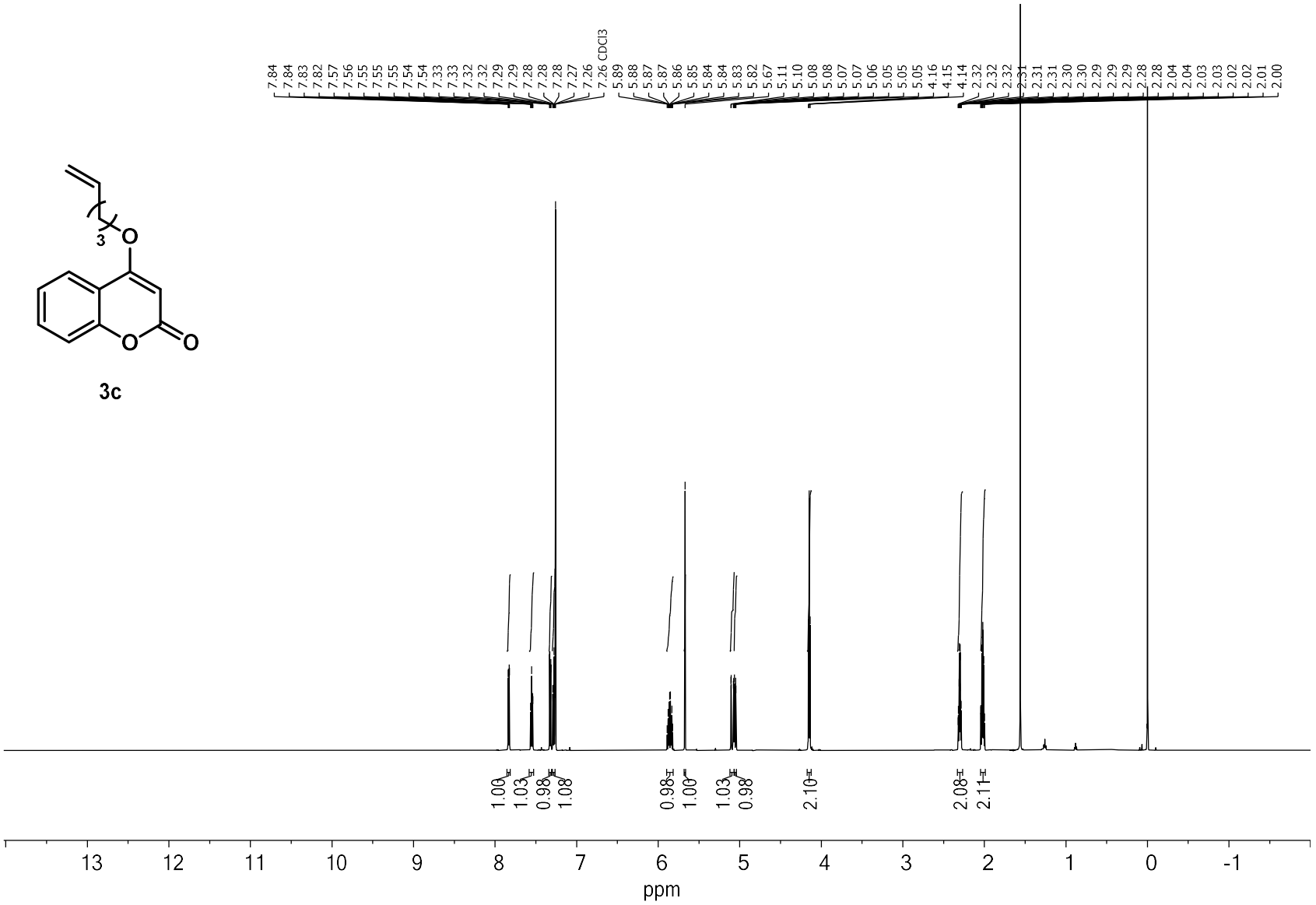


Figure S49 ^{1}H NMR of **3c**. Recorded at 600 MHz NMR.

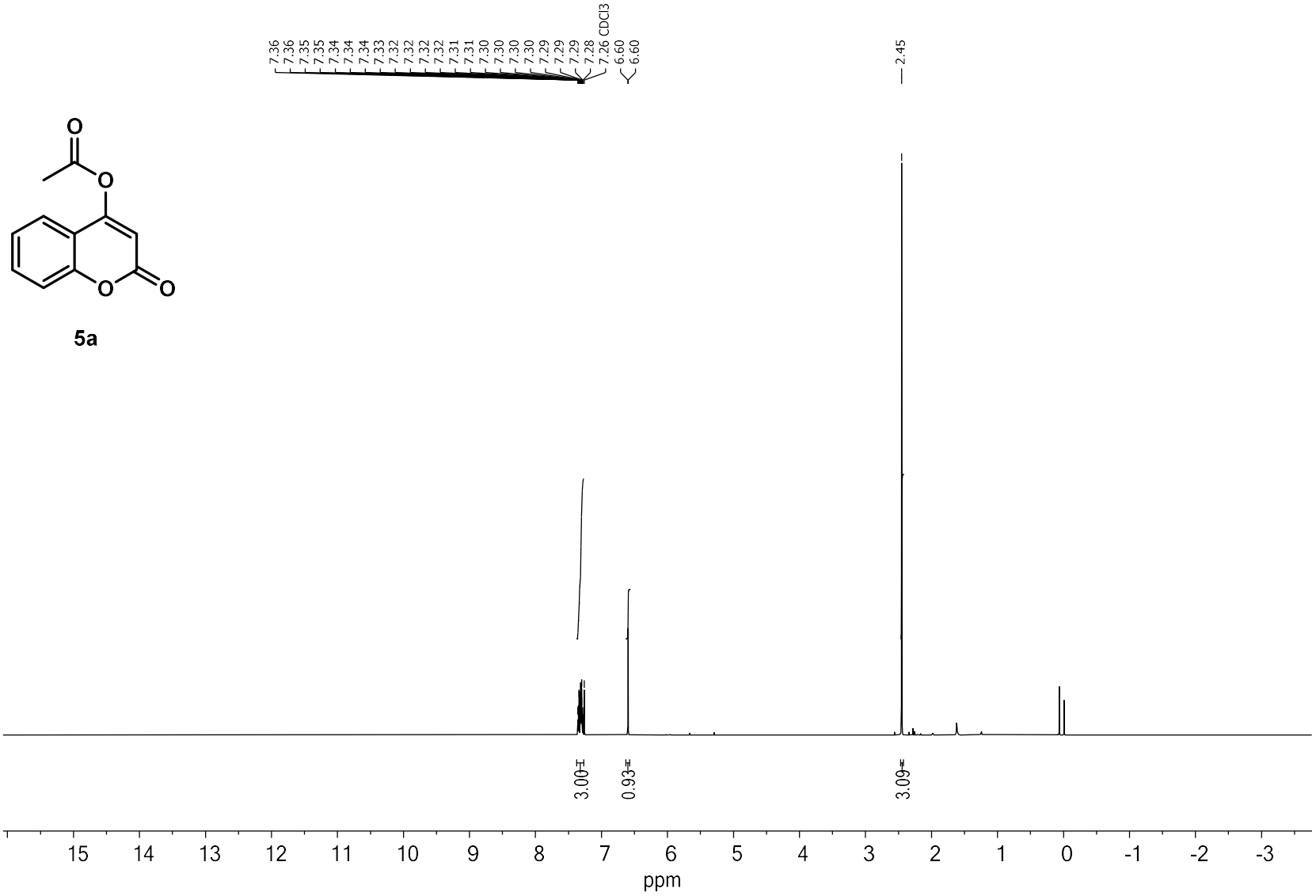


Figure S50 ^{1}H NMR of **5a**. Recorded at 600 MHz NMR.

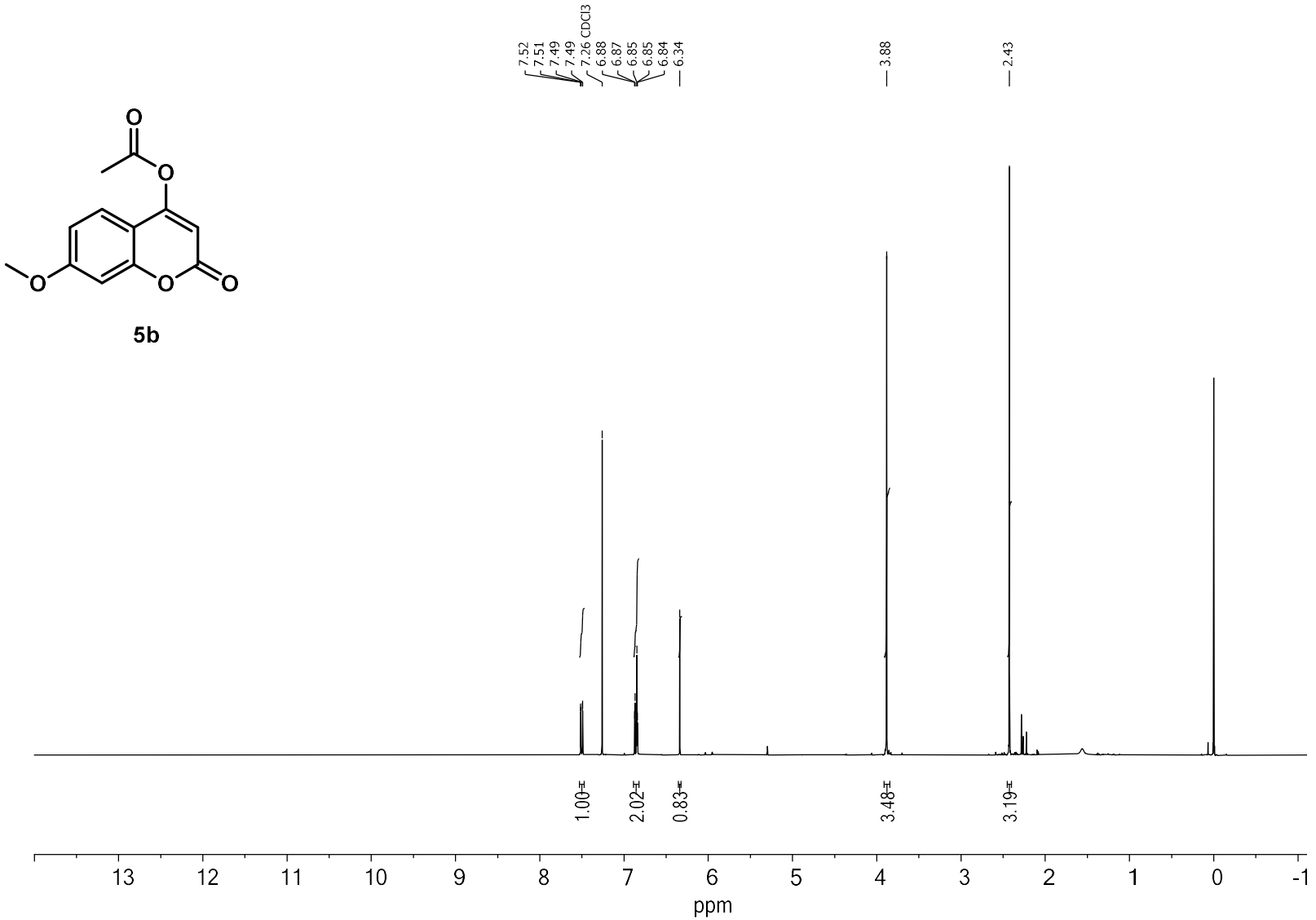


Figure S51 ^{1}H NMR of **5b**. Recorded at 600 MHz NMR.

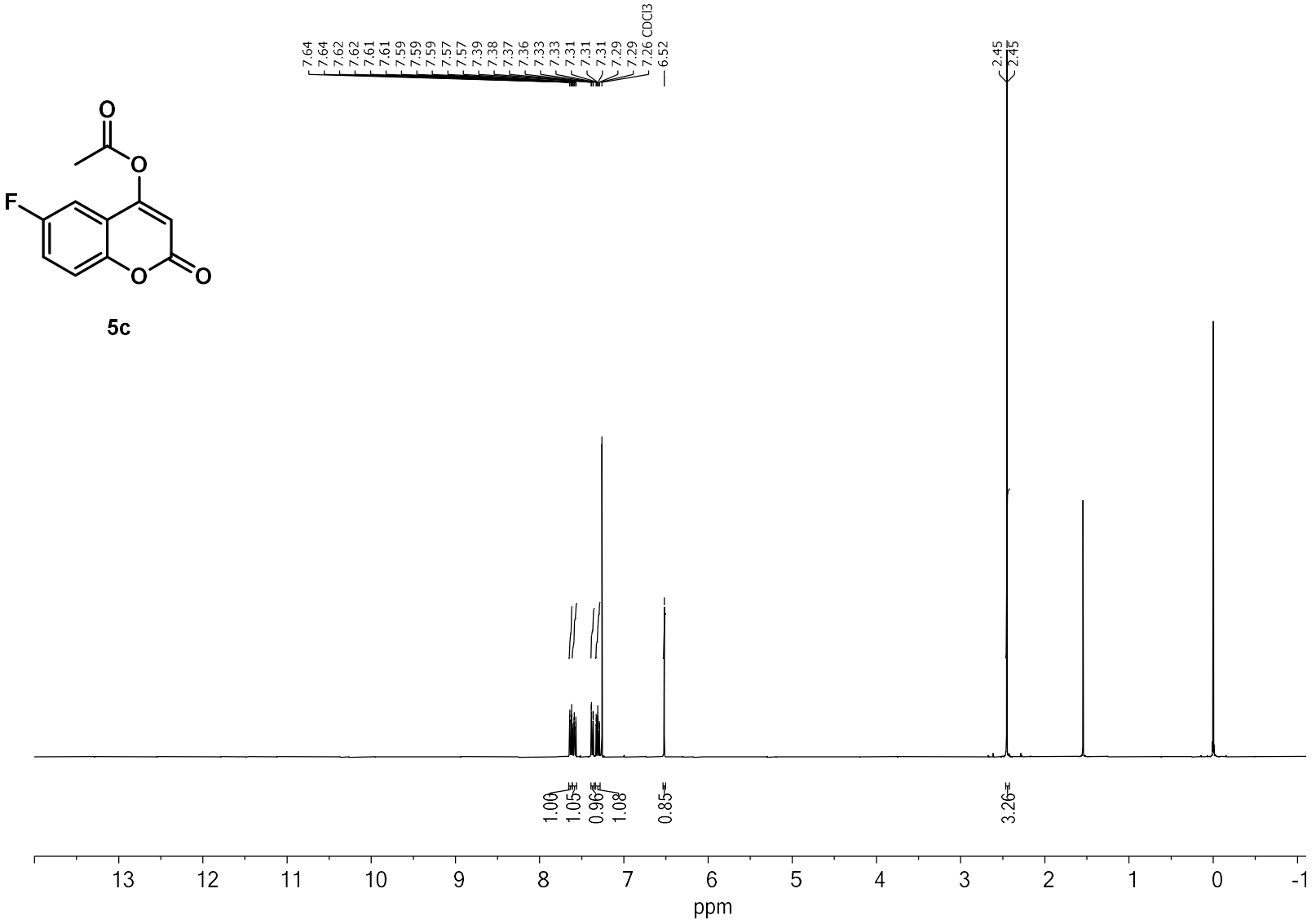


Figure S52 ^{1}H NMR of **5c**. Recorded at 600 MHz NMR.

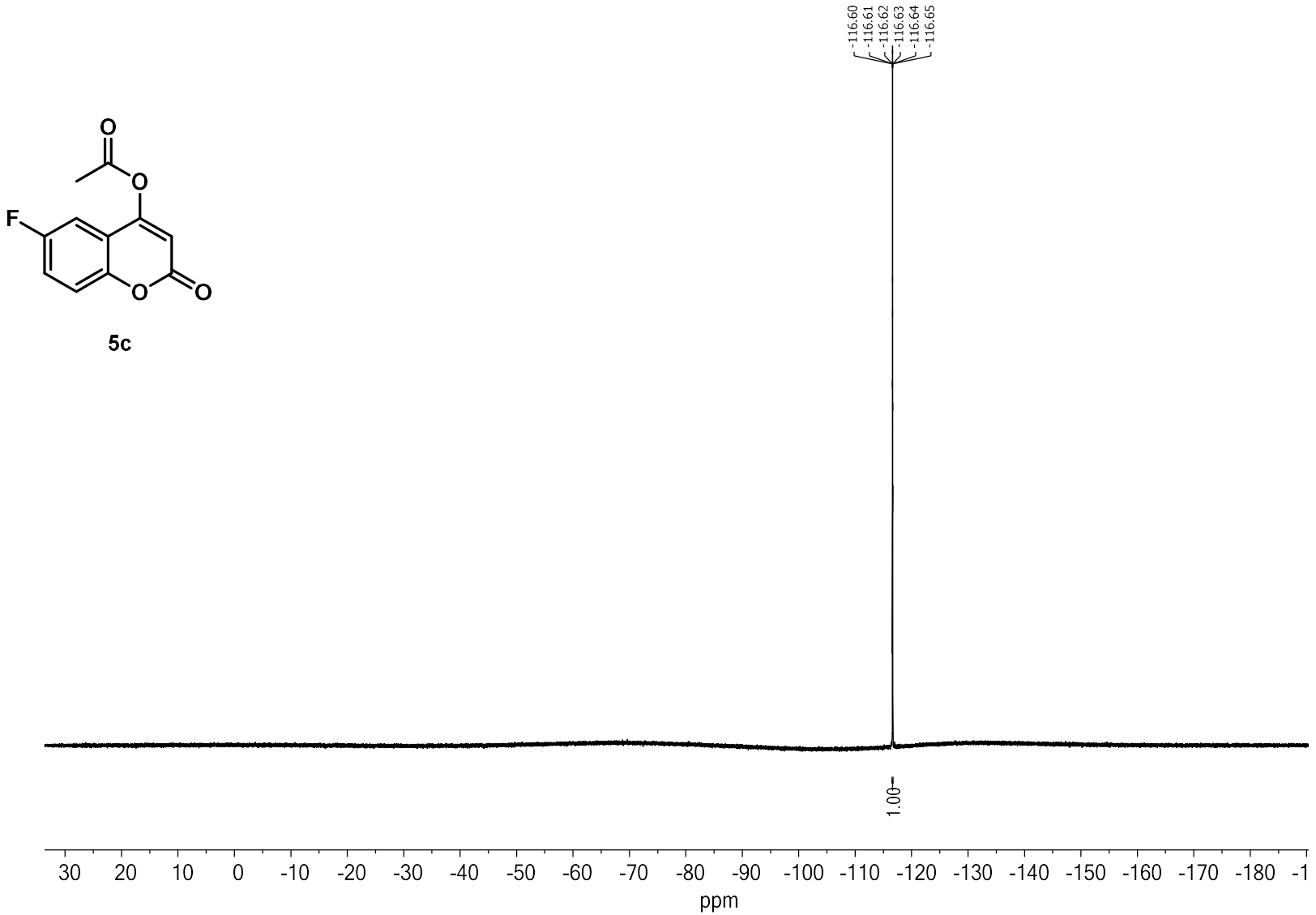


Figure S53 ^{19}F NMR of **5c** recorded at 565 MHz NMR.

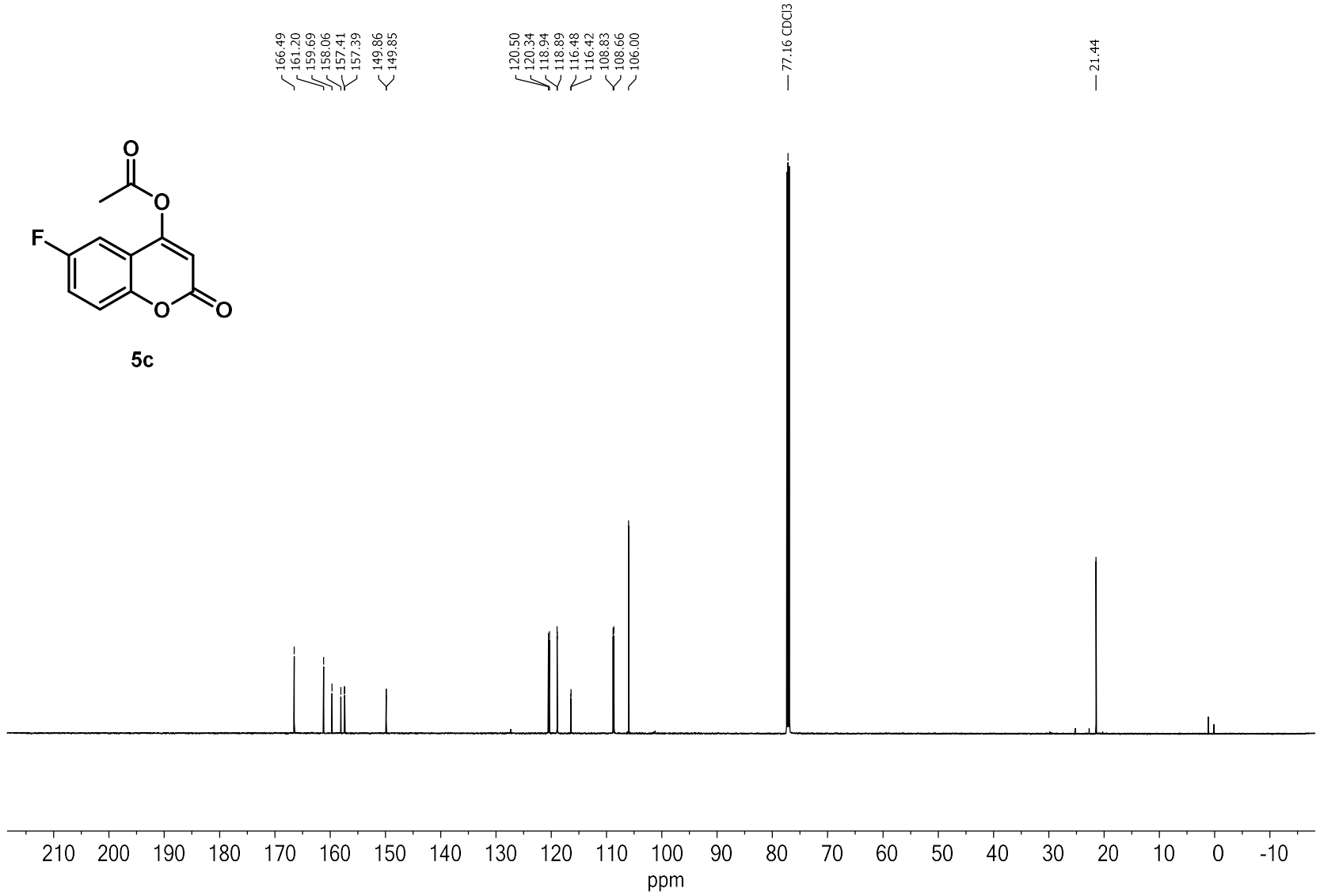


Figure S54 ^{13}C NMR of **5c**. Recorded at 151 MHz NMR.

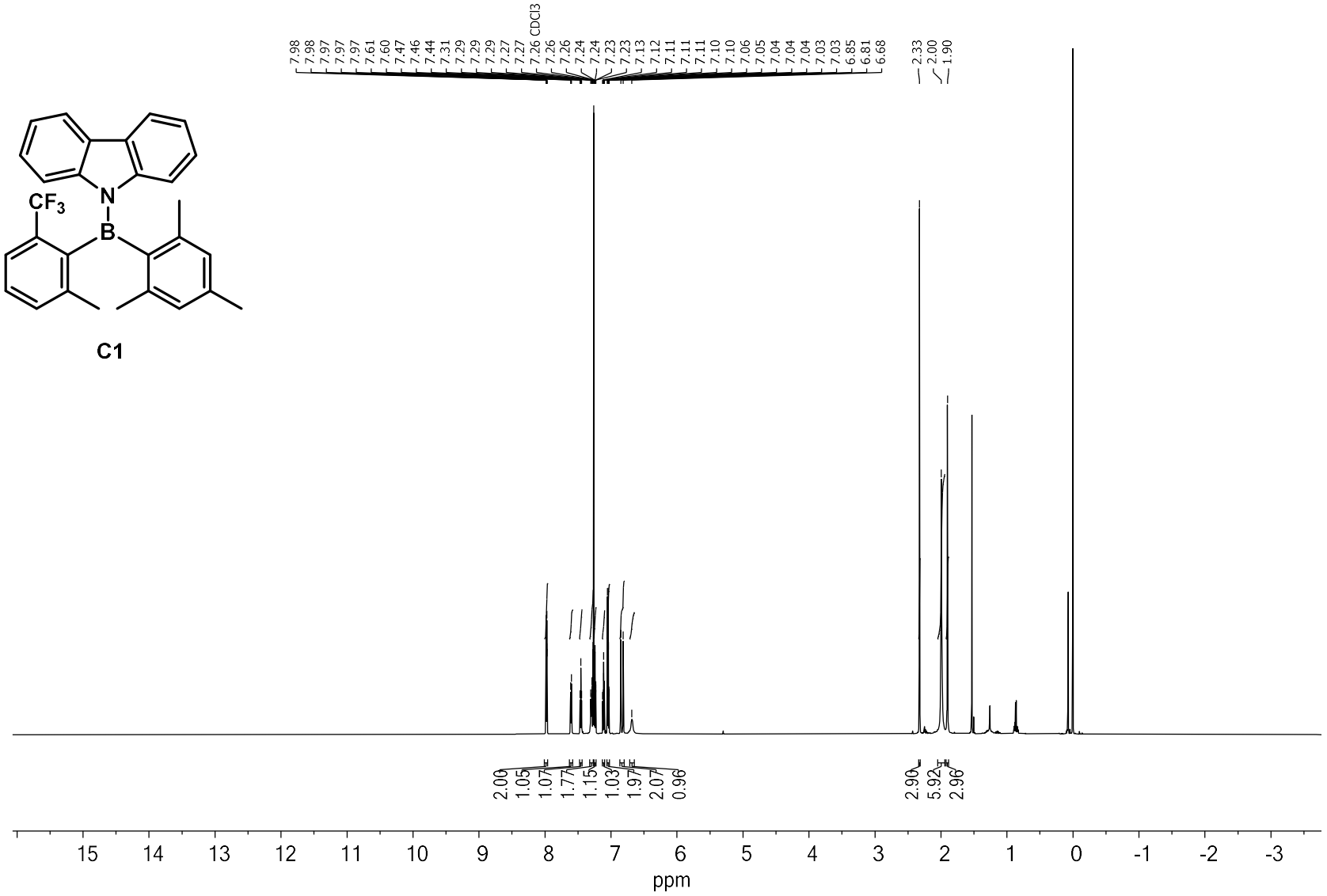


Figure S55 ^{1}H NMR of **C1**. Recorded at 600 MHz NMR.

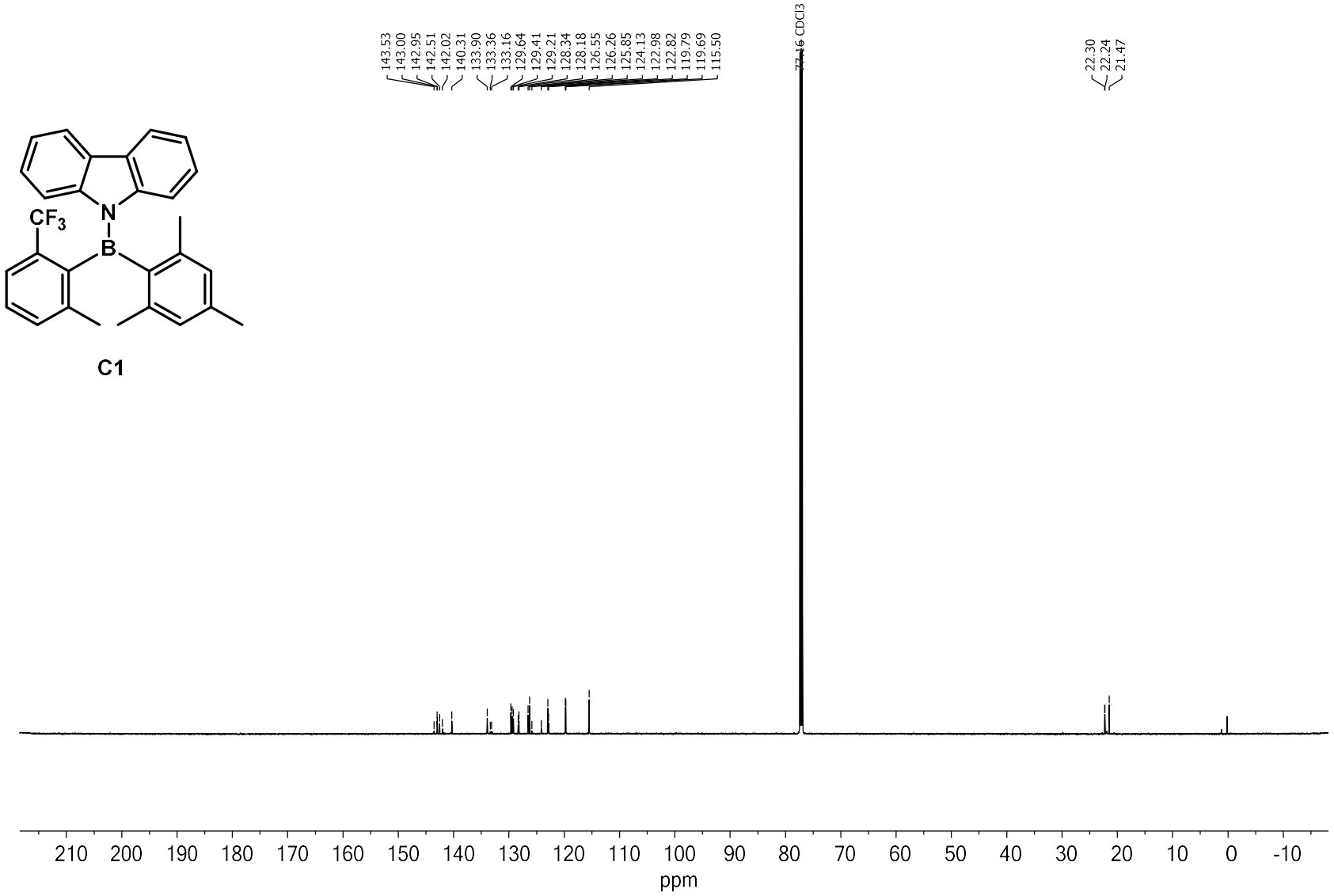


Figure S56 ^{13}C NMR of **C1**. Recorded at 151 MHz NMR.

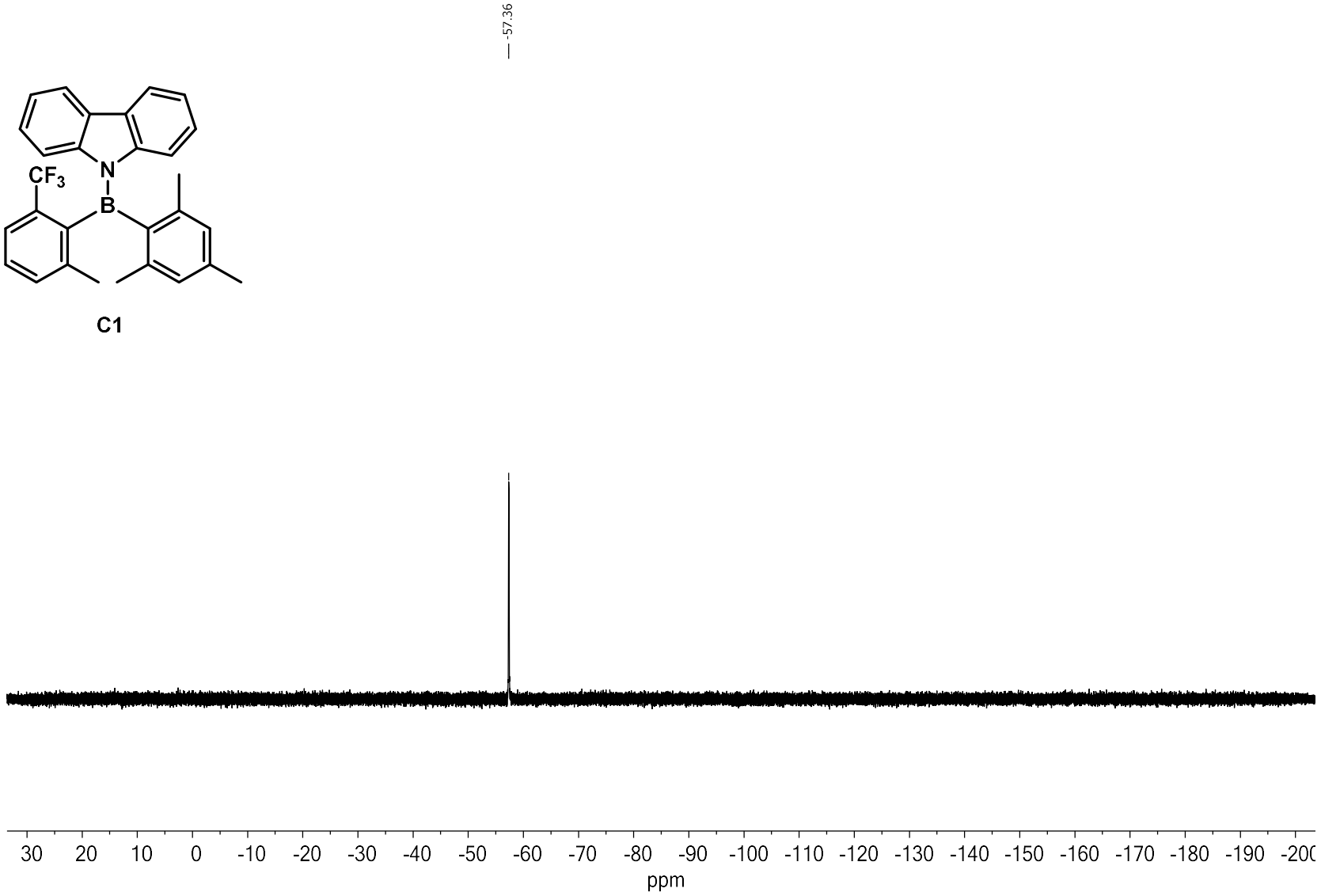


Figure S57 ^{19}F NMR of **C1**. Recorded at 565 MHz NMR.

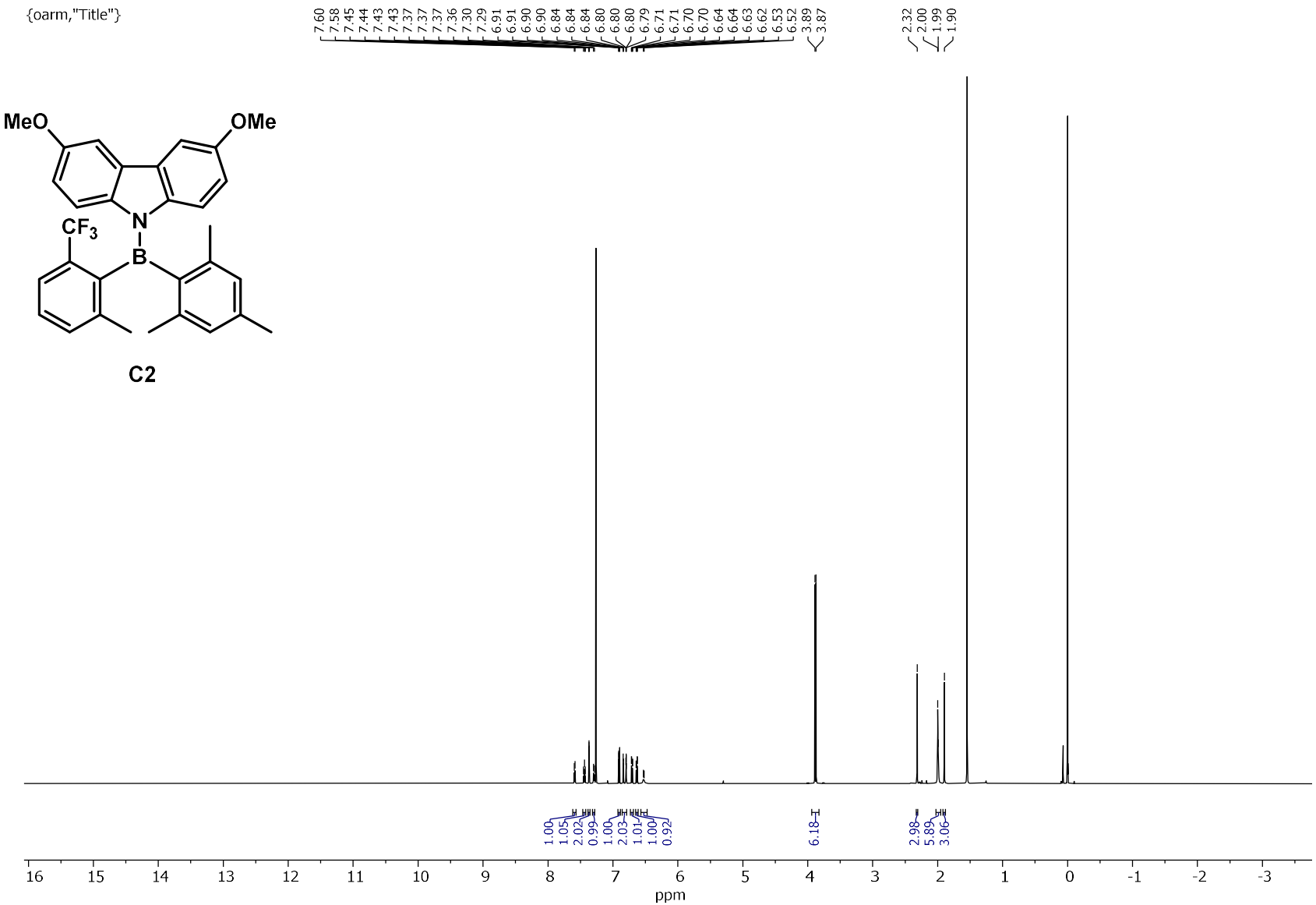


Figure S58 ^{1}H NMR of **C2**. Recorded at 600 MHz NMR.

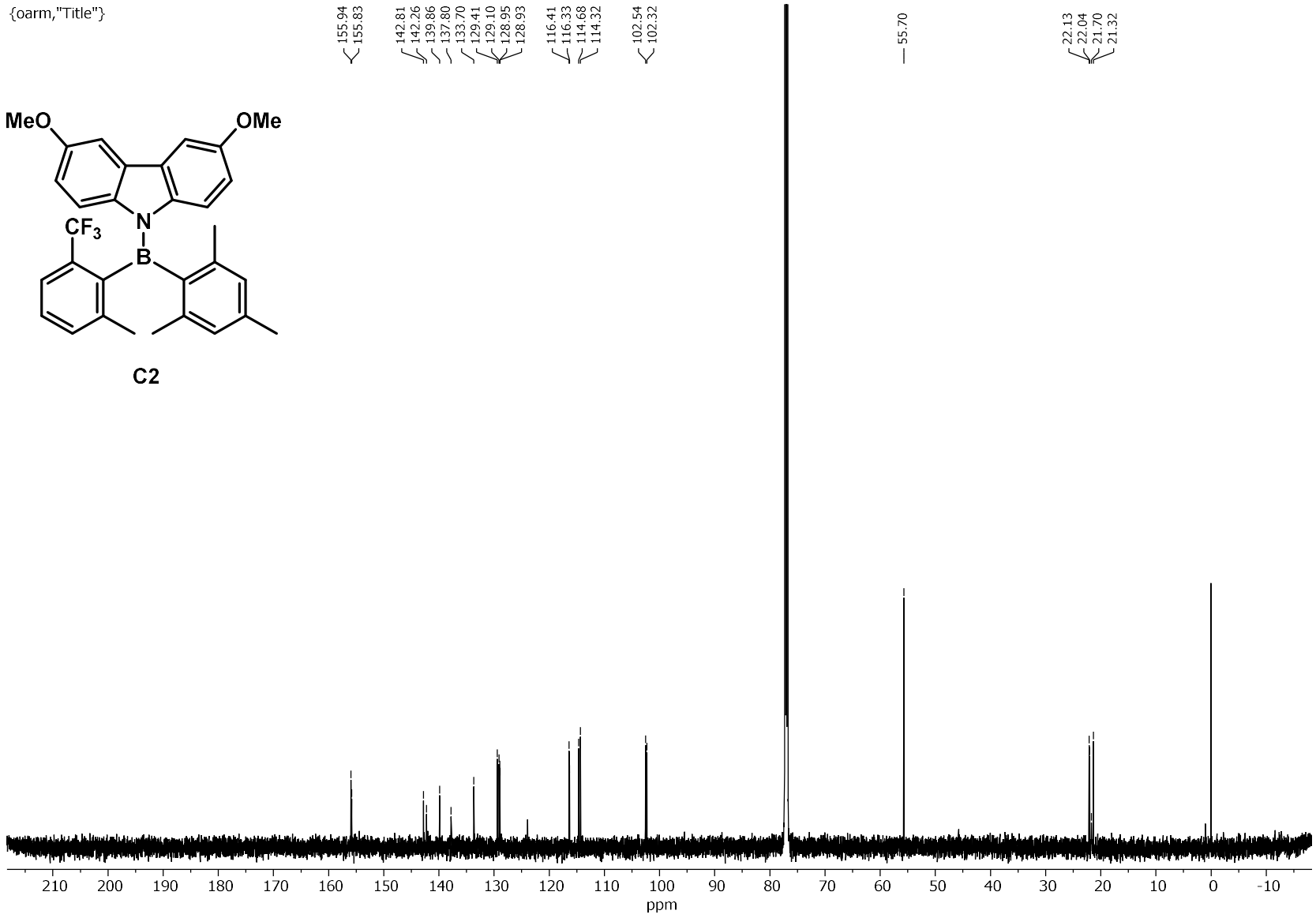


Figure S59 ^{13}C NMR of **C2**. Recorded at 151 MHz NMR.

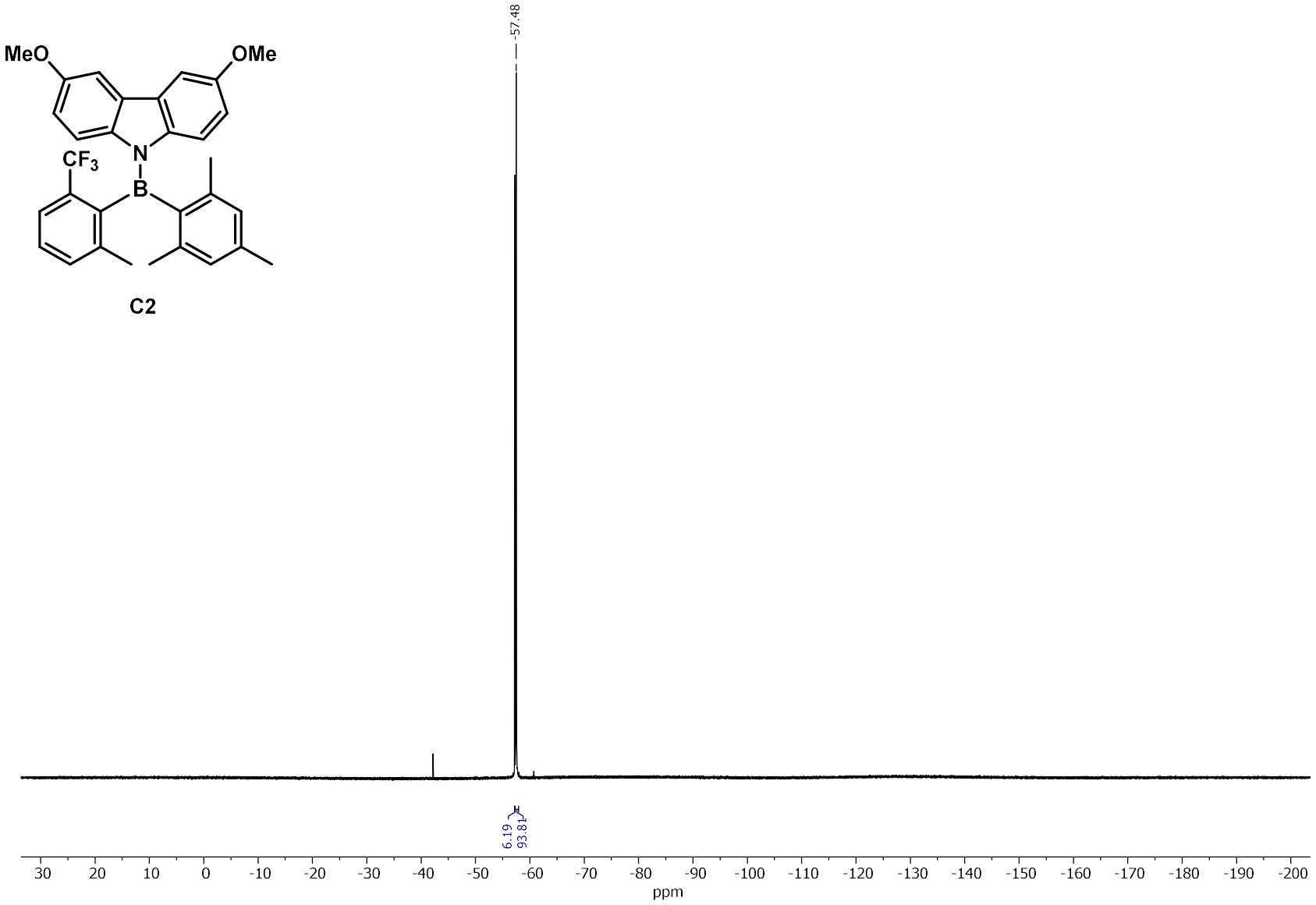


Figure S60 ^{19}F NMR of **C2**. Recorded at 565 MHz NMR.

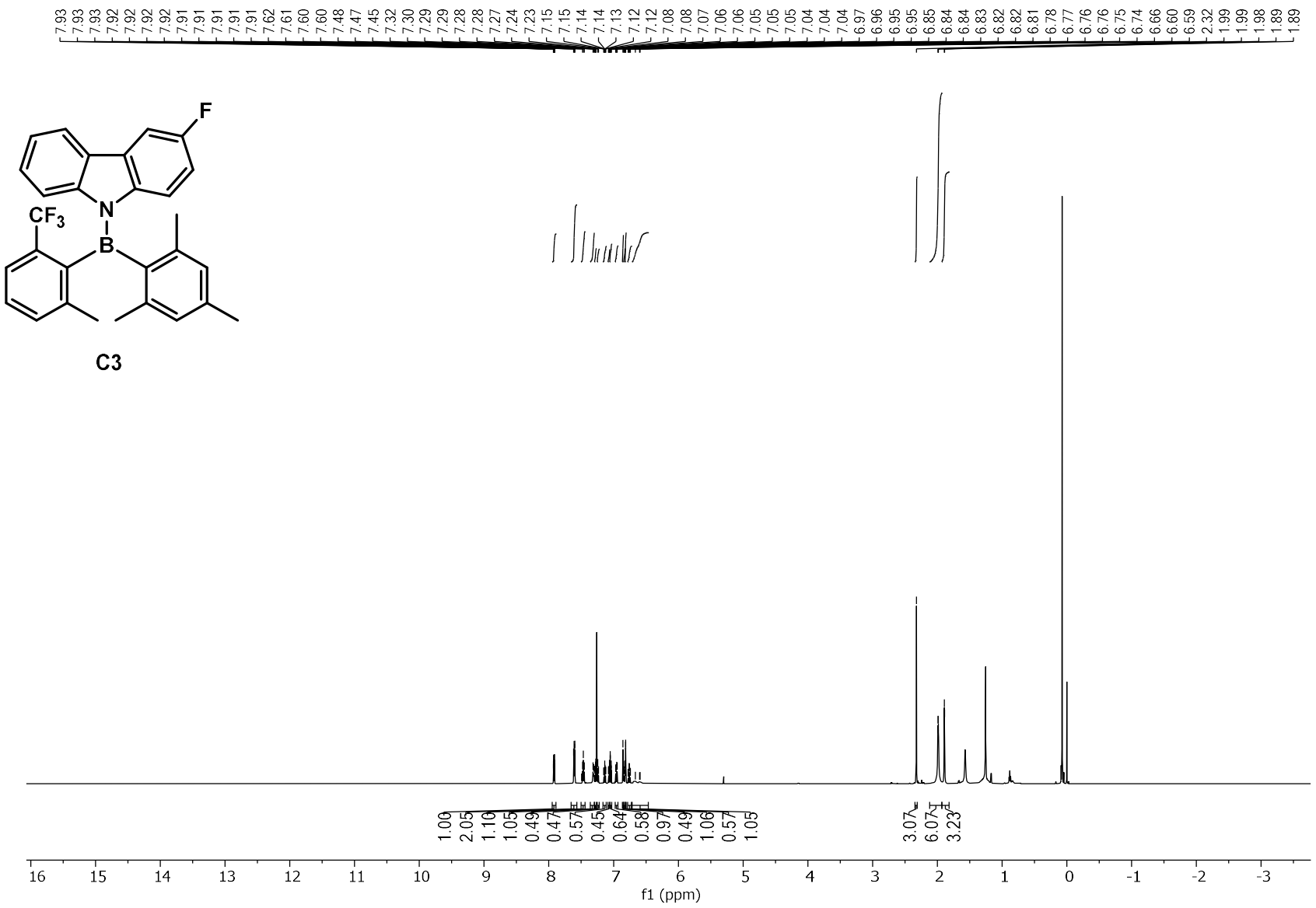


Figure S61 ^{1}H NMR of **C3**. Recorded at 600 MHz NMR.

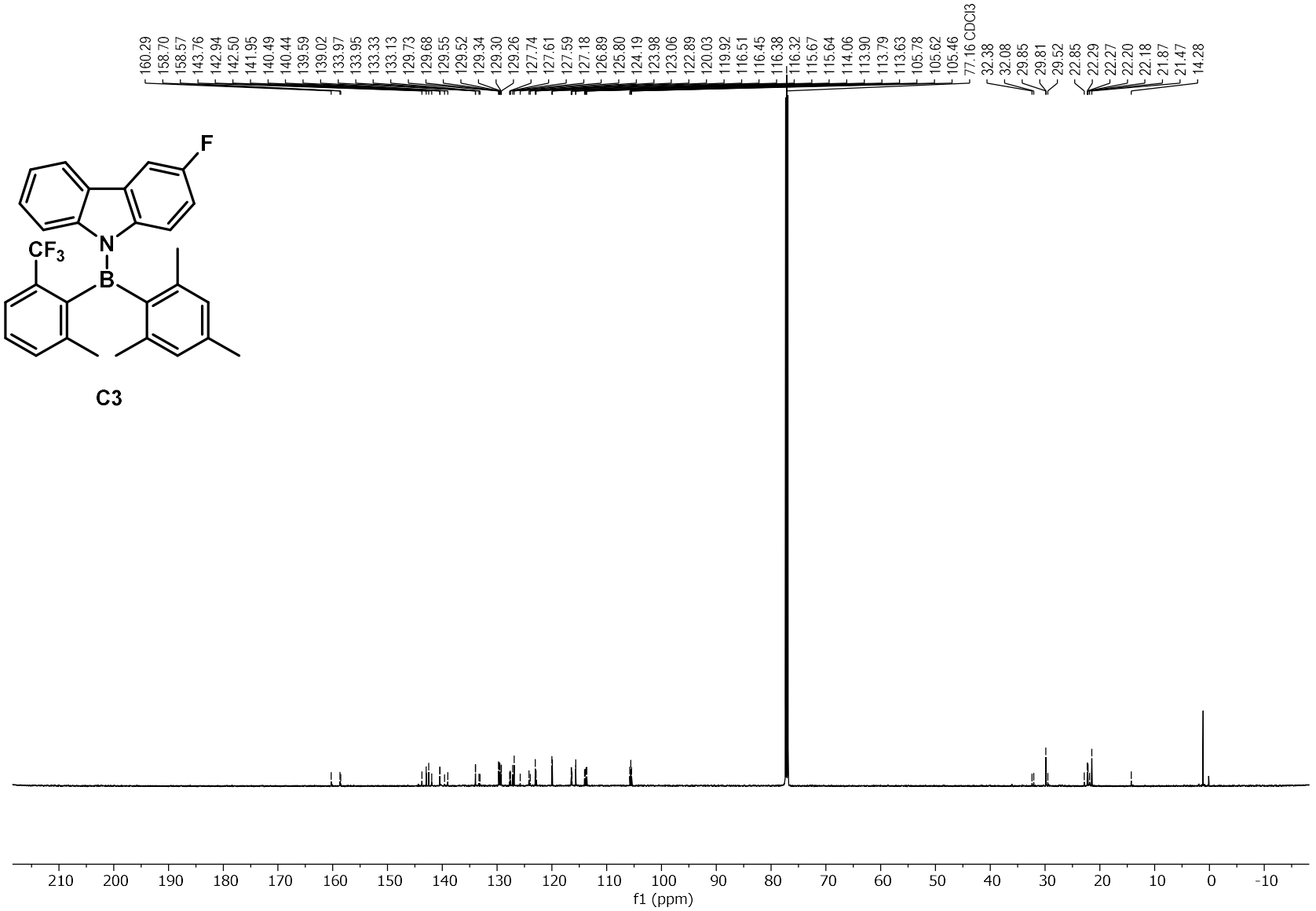


Figure S62 ^{13}C NMR of **C3**. Recorded at 151 MHz NMR.

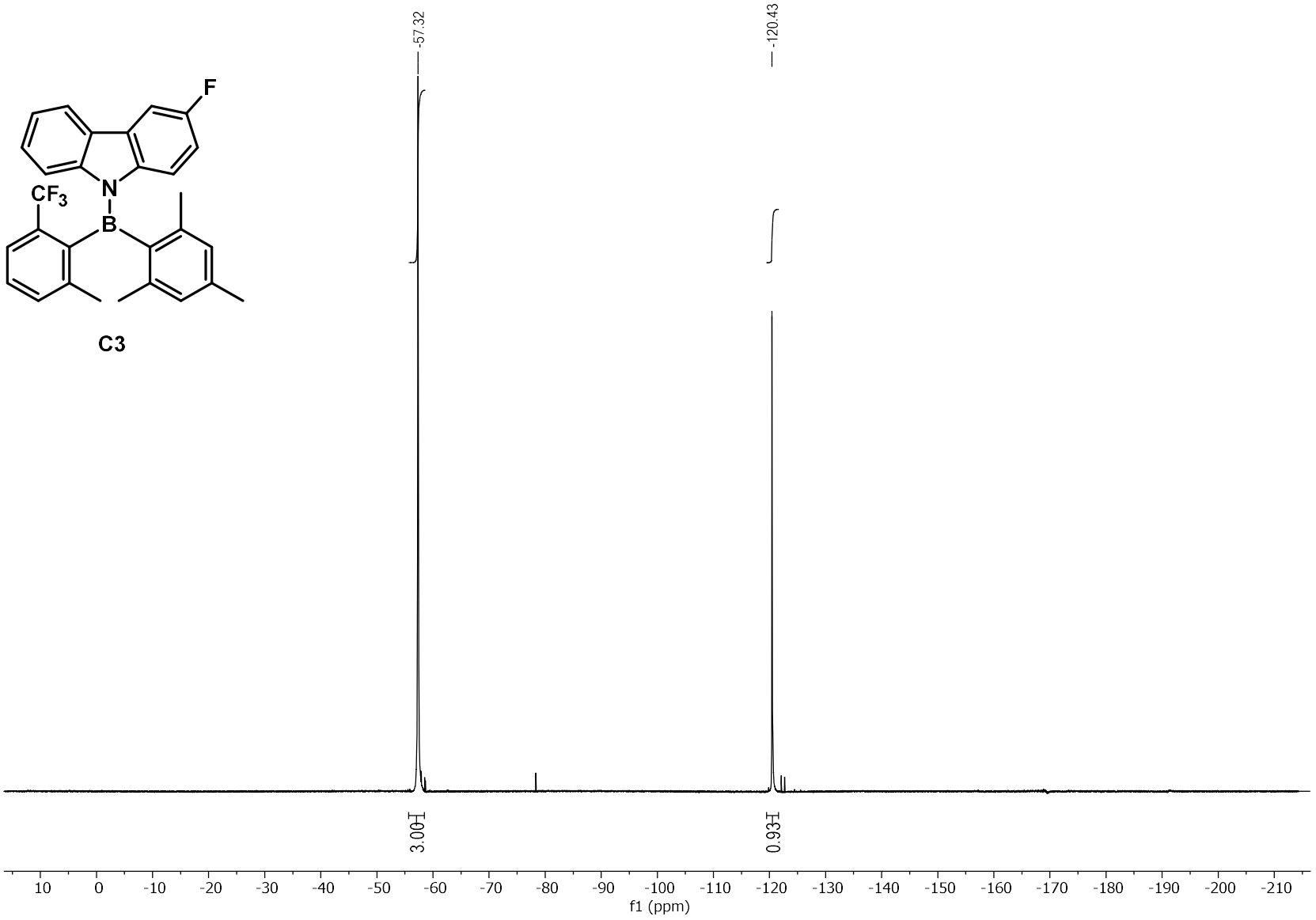


Figure S63 ^{19}F NMR of **C3**. Recorded at 565 MHz NMR.

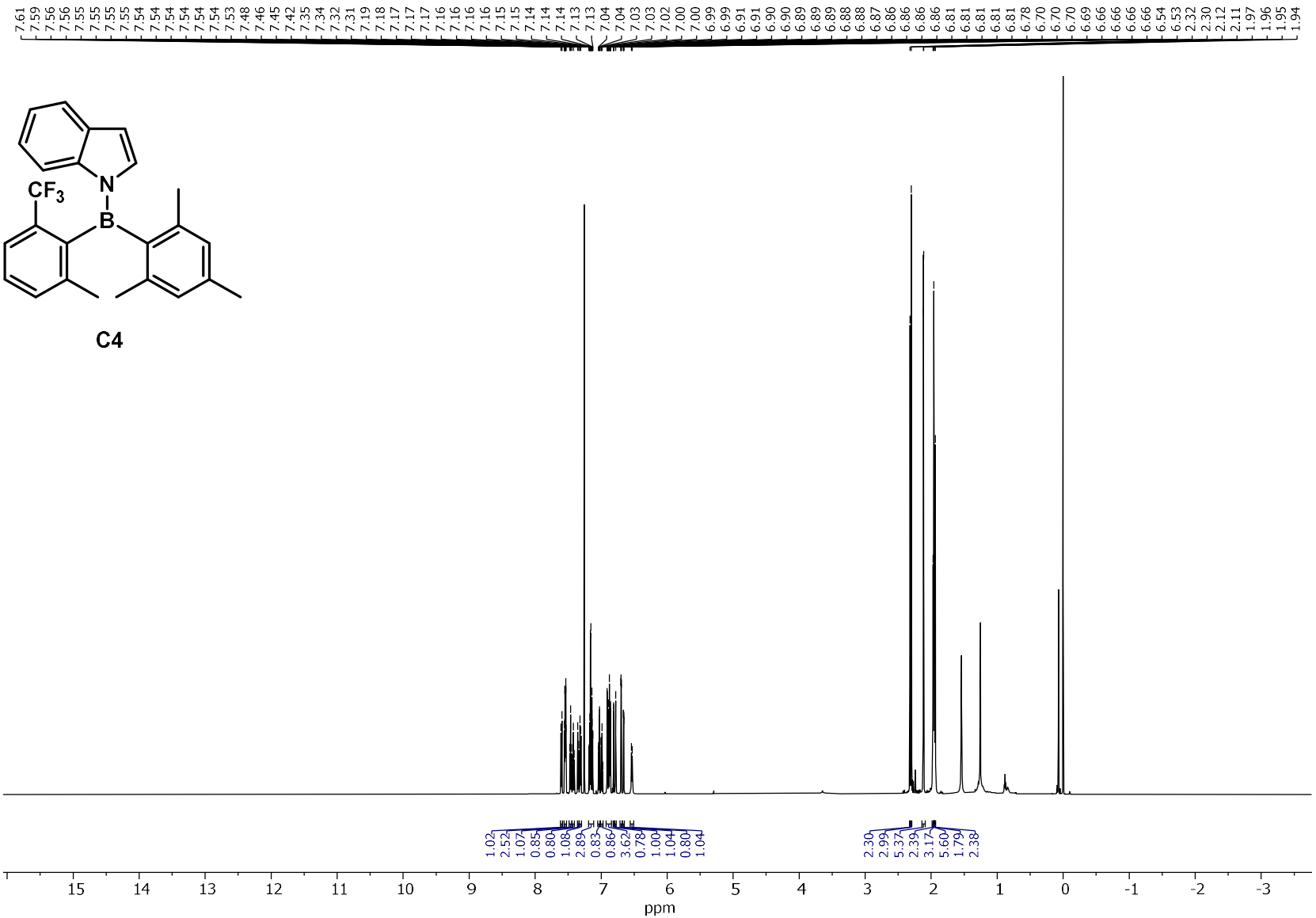


Figure S64 ^{1}H NMR of **C4**. Recorded at 600 MHz NMR.

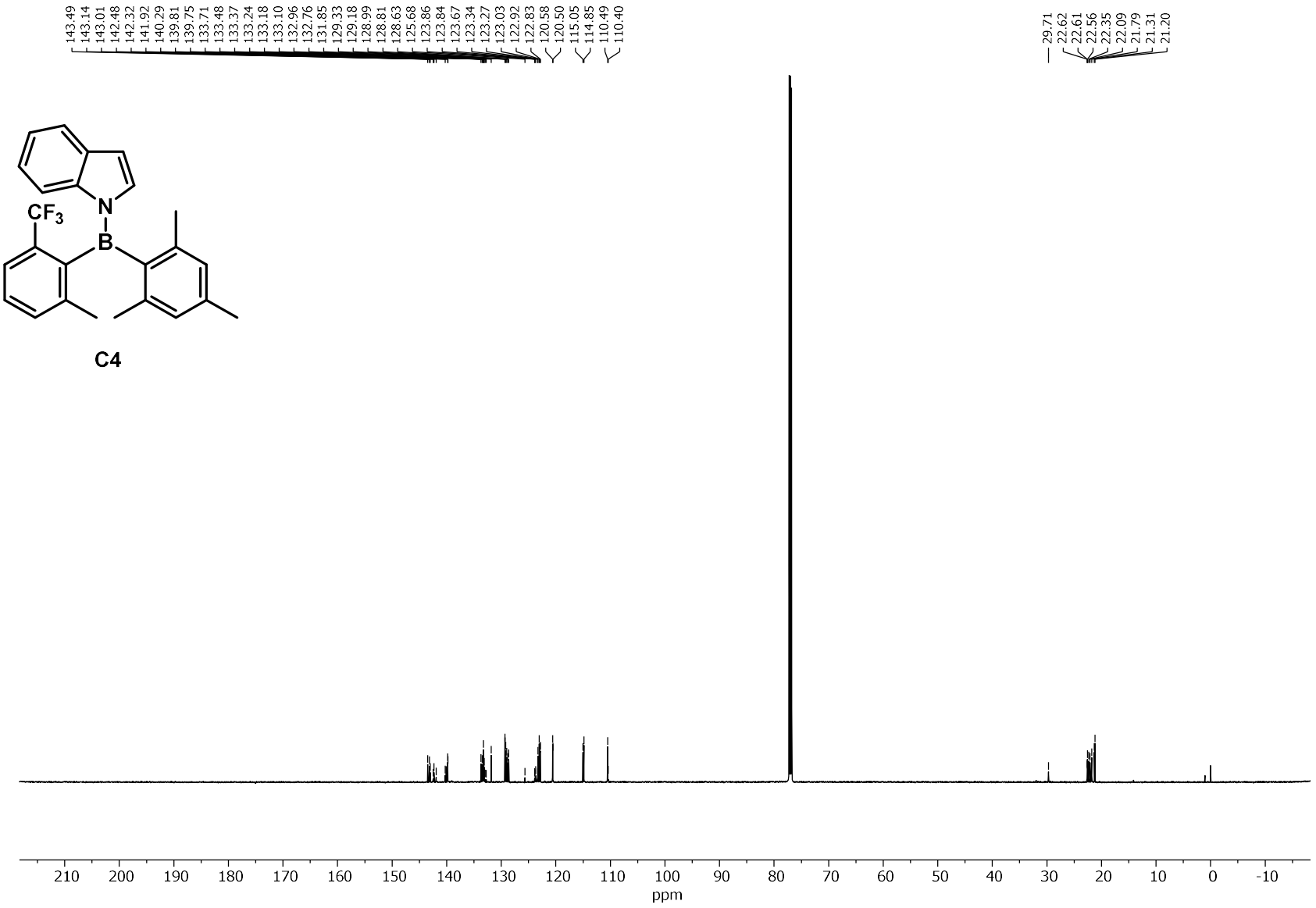


Figure S65 ^{13}C NMR of **C4**. Recorded at 151 MHz NMR.

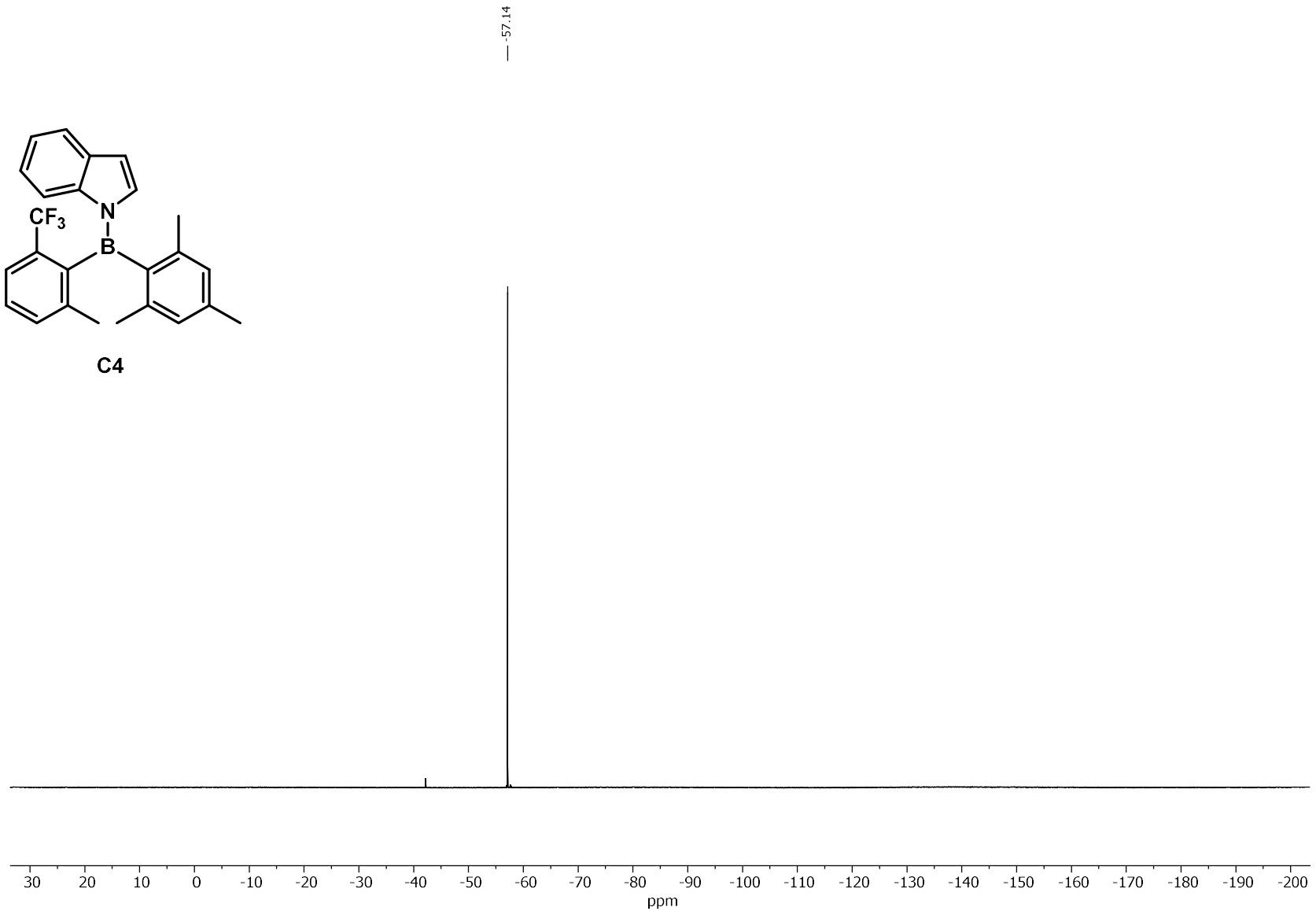


Figure S66 ^{19}F NMR of **C4**. Recorded at 565 MHz NMR.

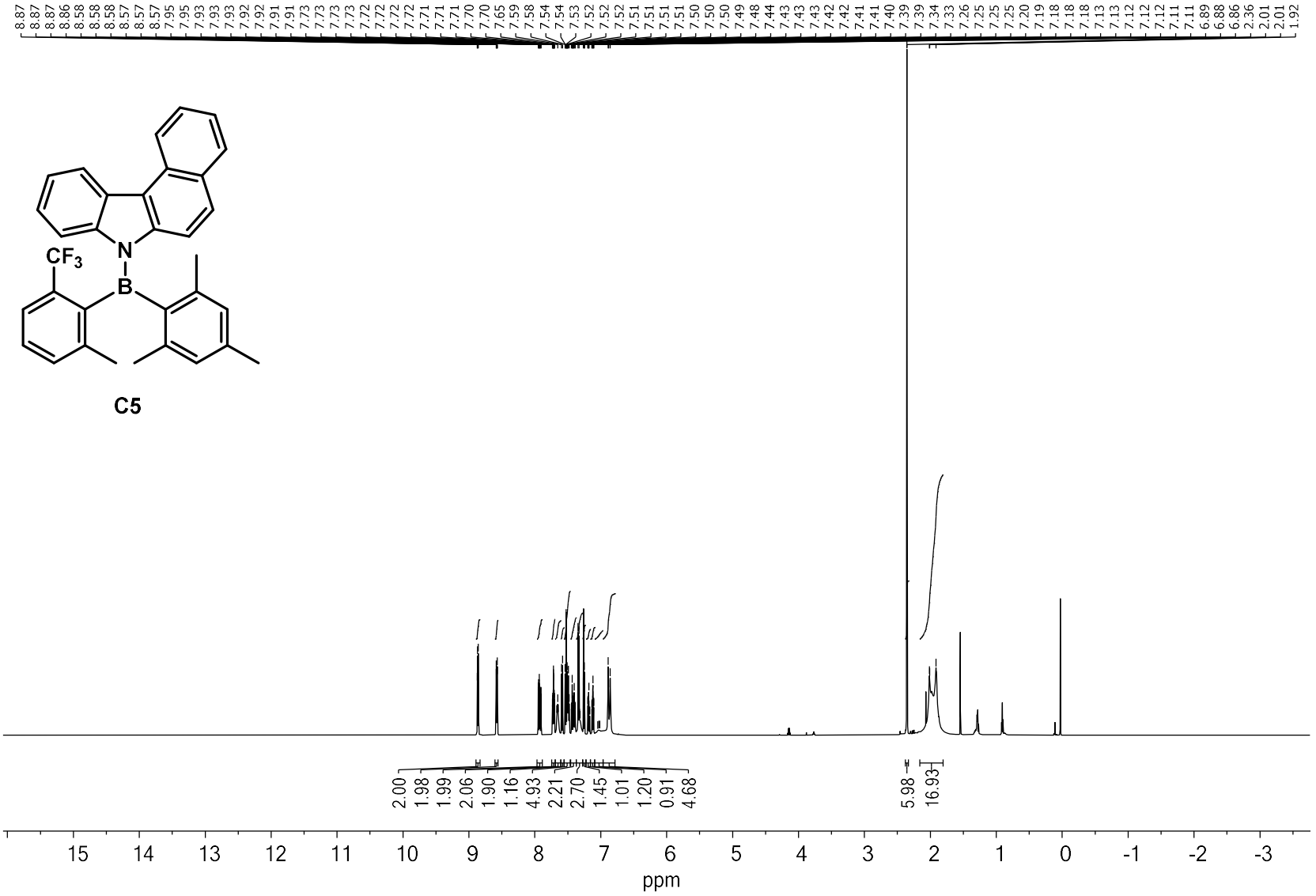


Figure S67 ^{1}H NMR of **C5**. Recorded at 600 MHz NMR.

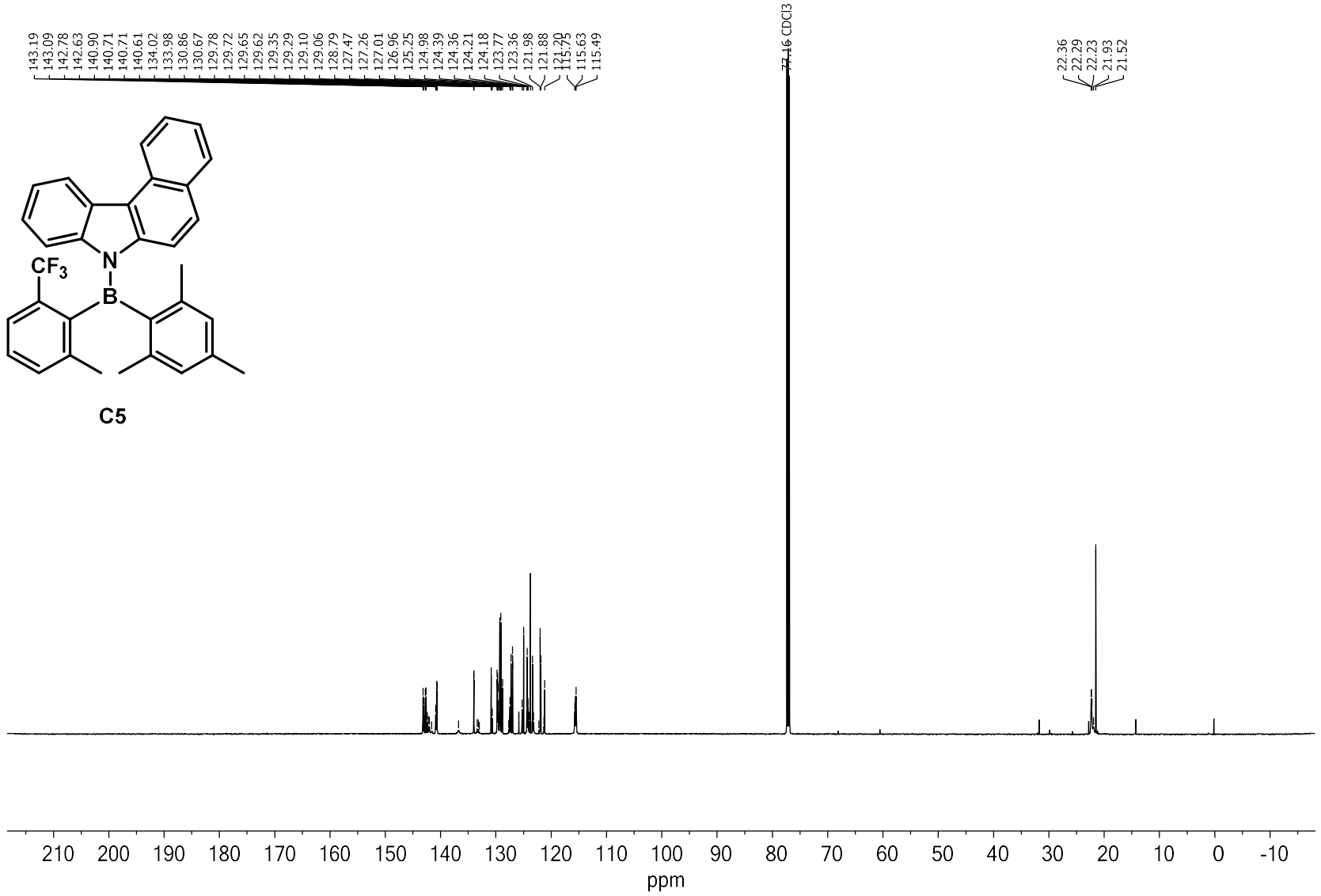


Figure S68 ^{13}C NMR of **C5**. Recorded at 151 MHz NMR.

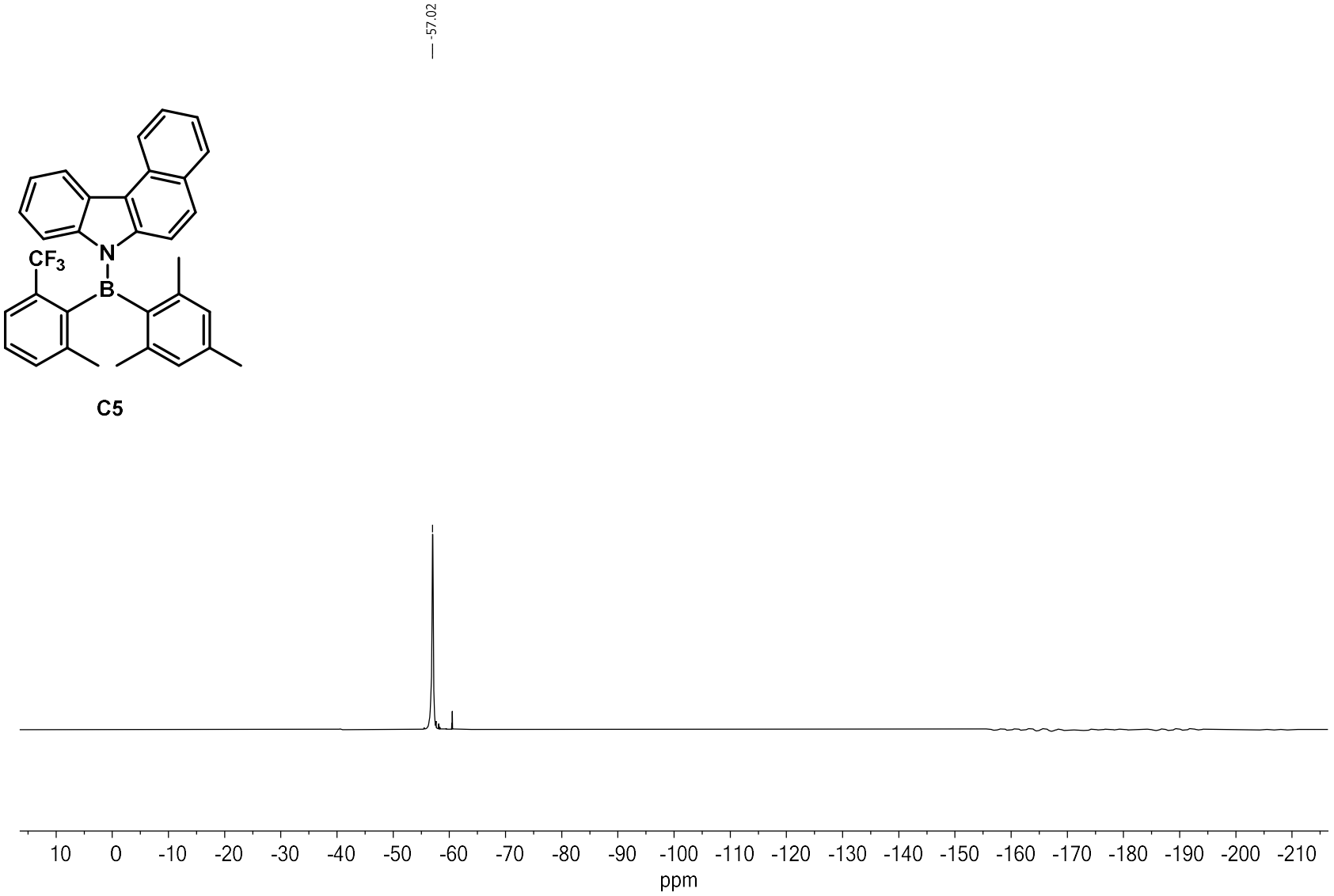


Figure S69 ^{19}F NMR of **C5**. Recorded at 565 MHz NMR.

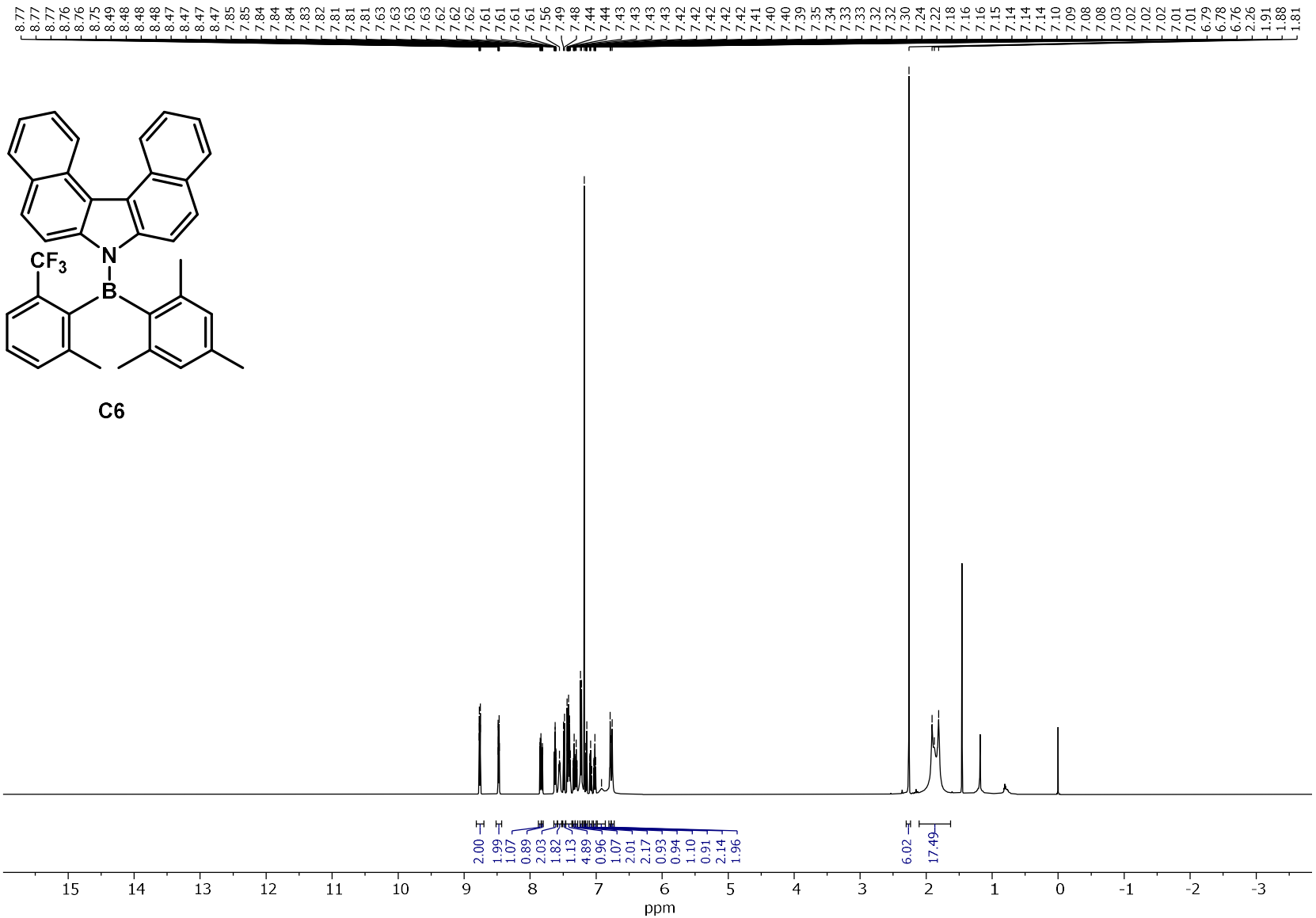


Figure S70 ^{1}H NMR of **C6**. Recorded at 600 MHz NMR.

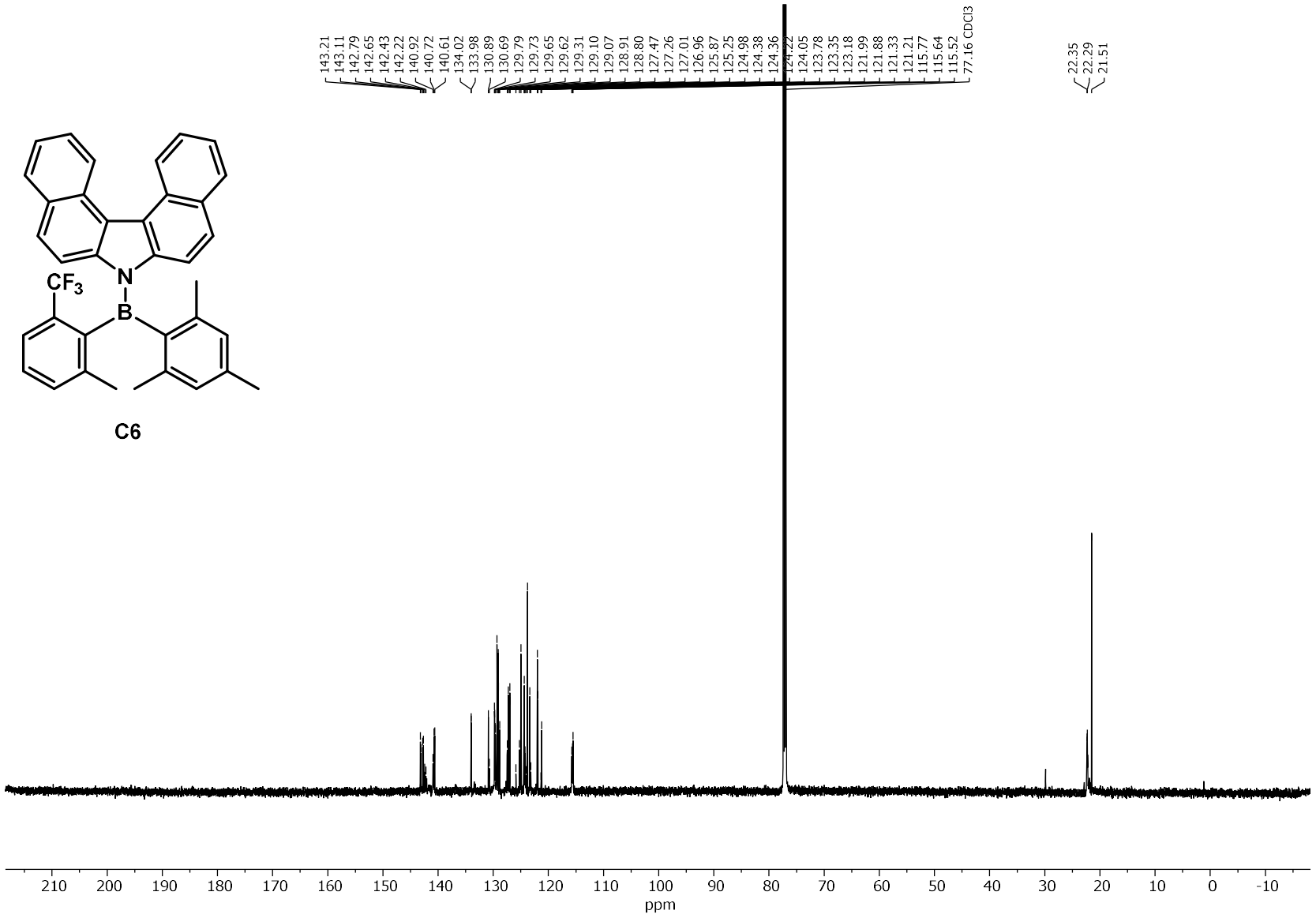
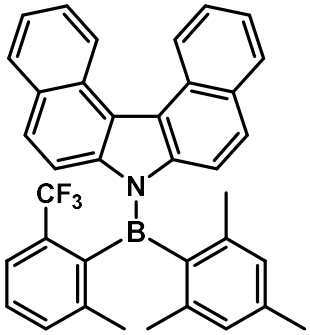


Figure S71 ^{13}C NMR of **C6**. Recorded at 151 MHz NMR.



C6

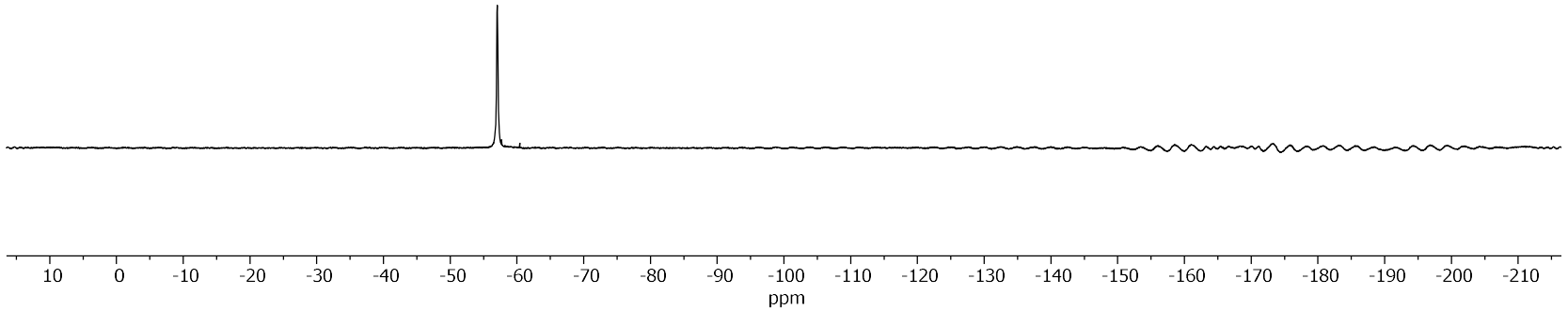


Figure S72 ^{19}F NMR of **C6**. Recorded at 565 MHz NMR.

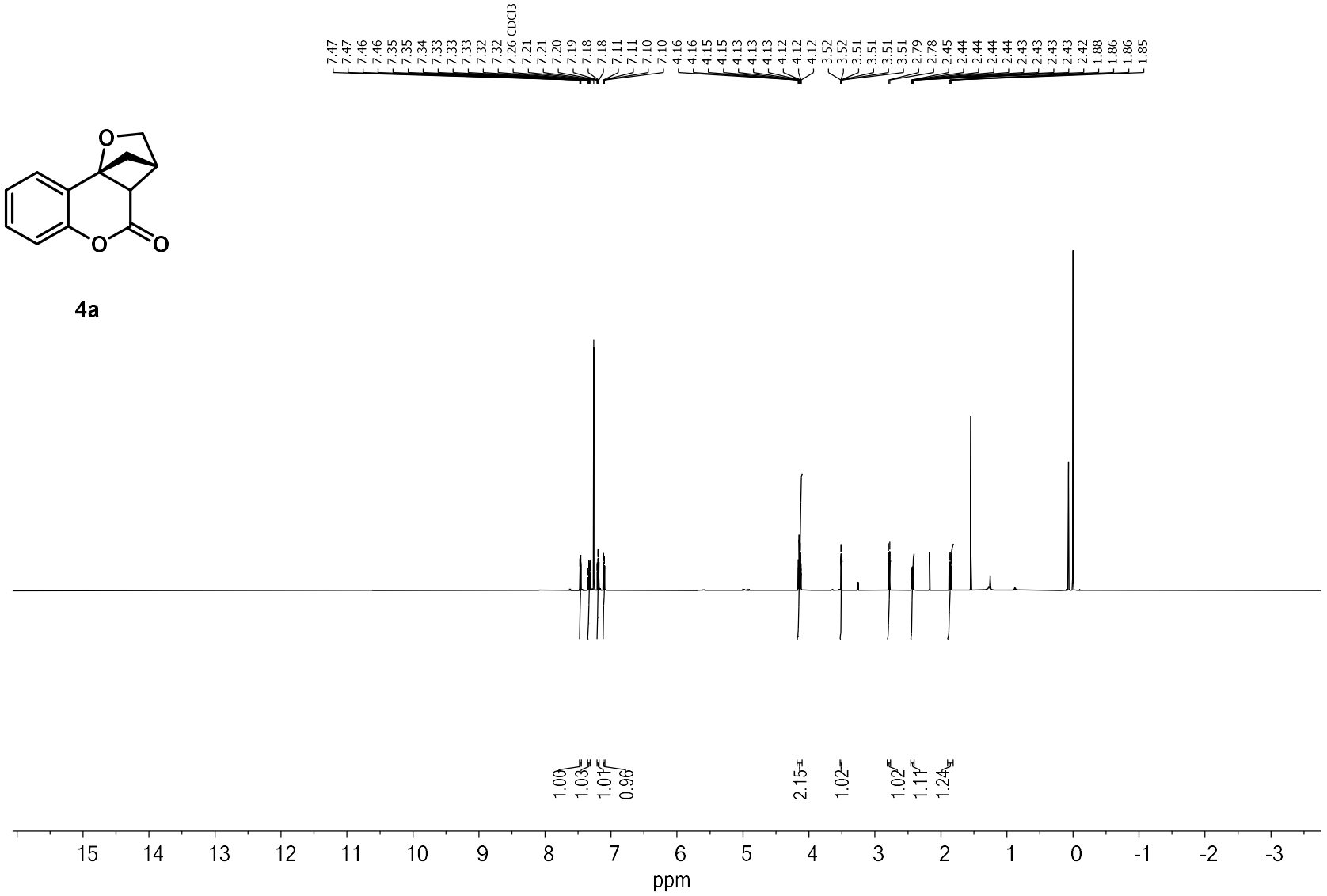


Figure S73 ^{1}H NMR of **4a**. Recorded at 600 MHz NMR.

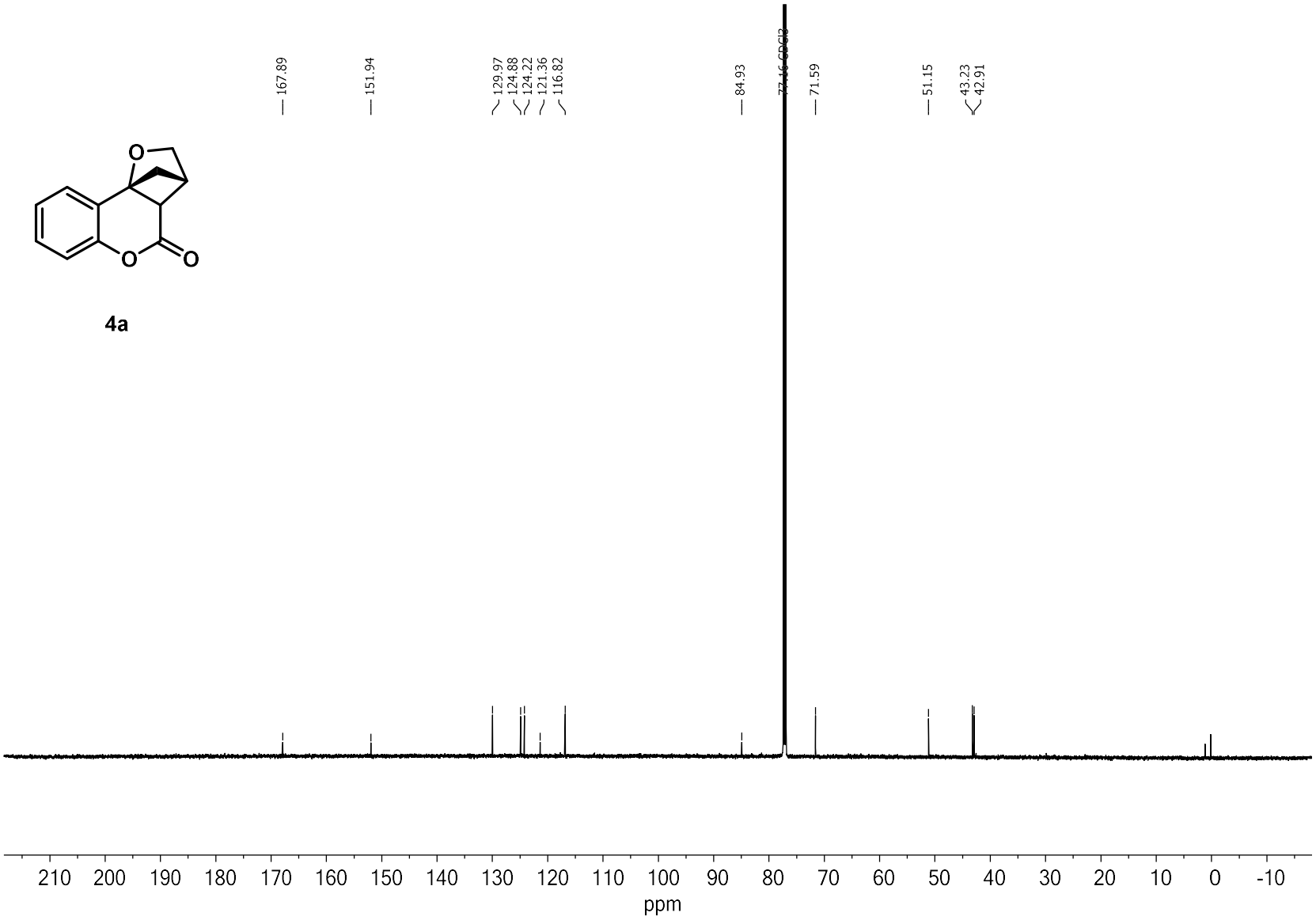


Figure S74 ^{13}C NMR of **4a**. Recorded at 151 MHz NMR.

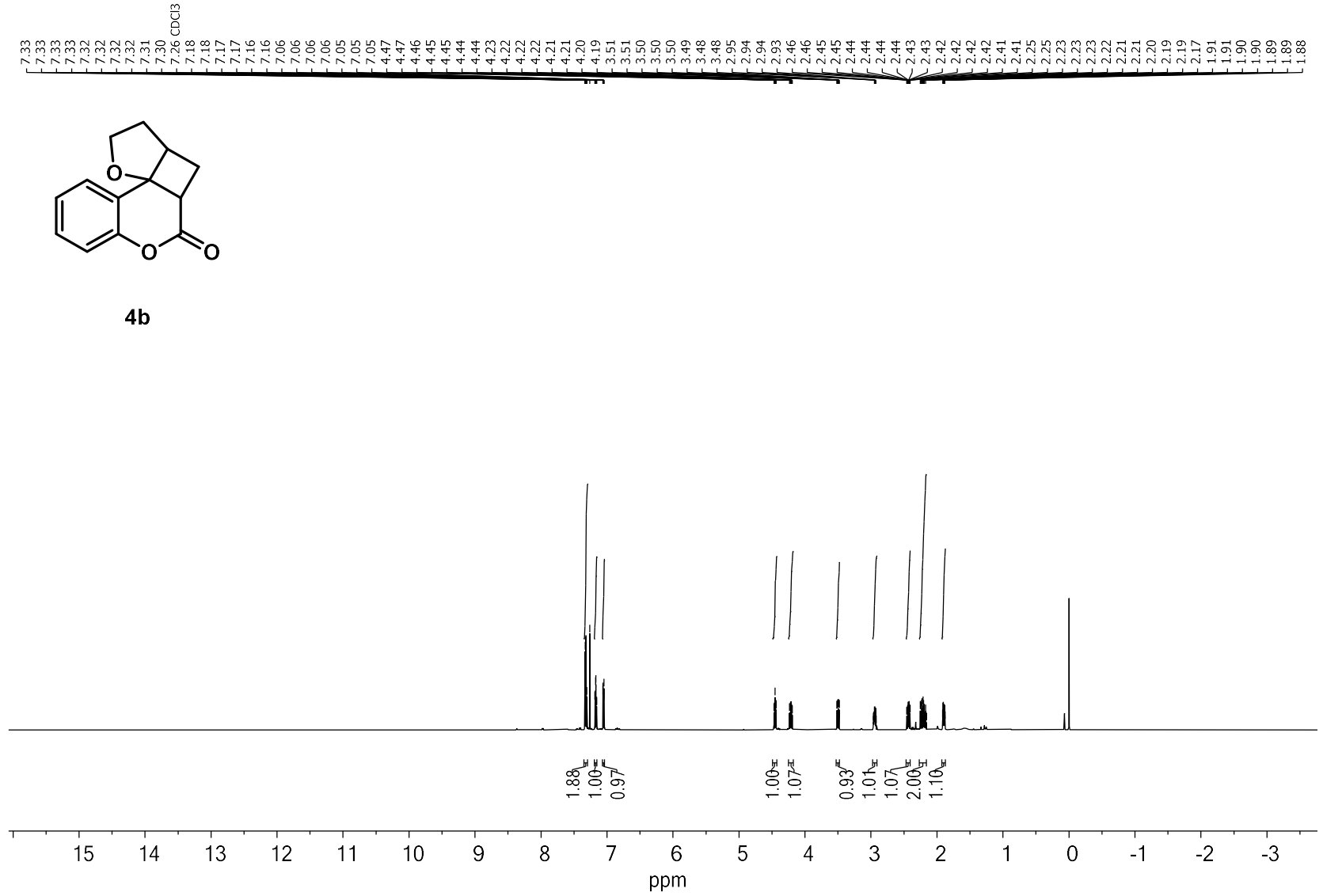


Figure S75 ^{1}H NMR of **4b**. Recorded at 600 MHz NMR.

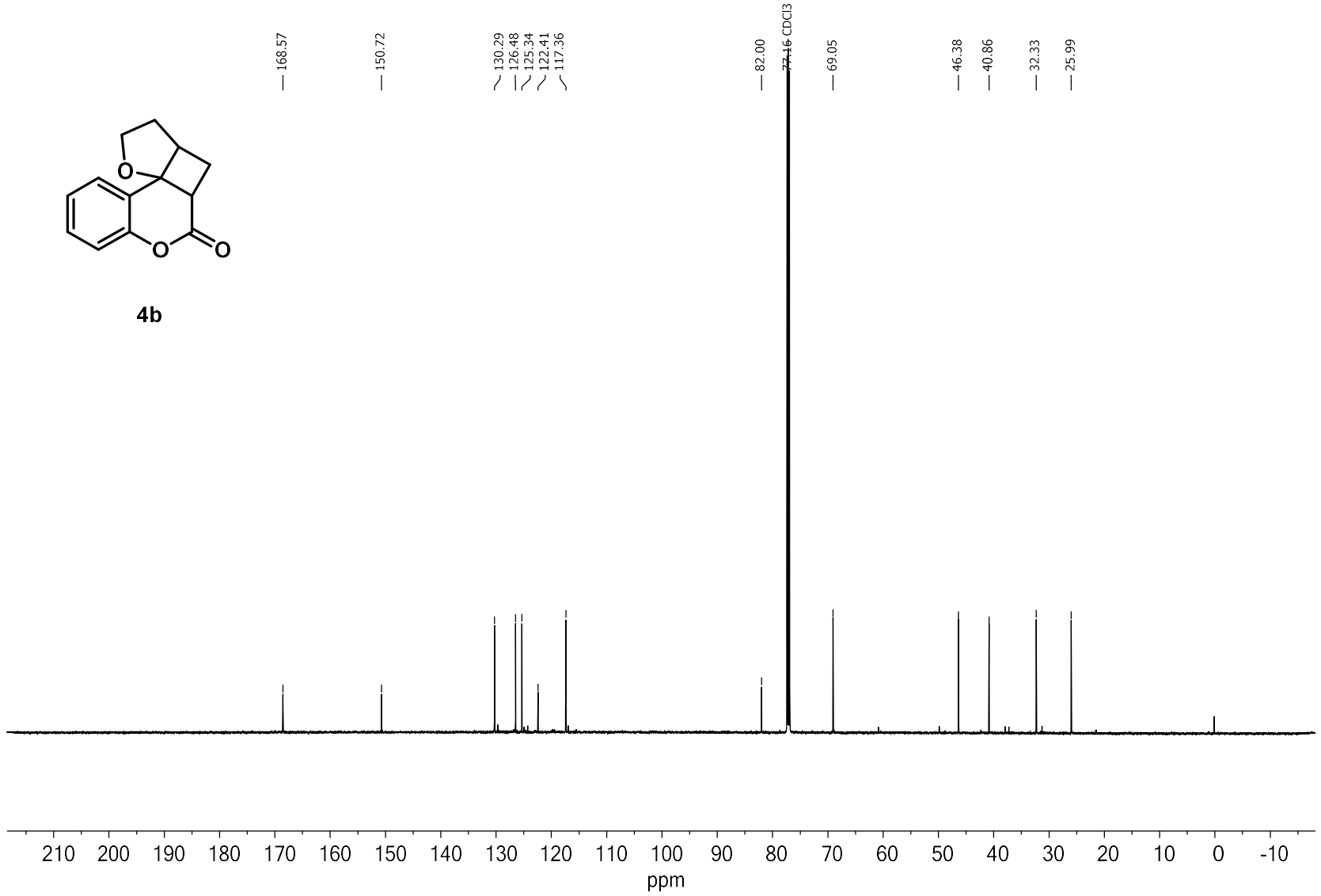


Figure S76 ^{13}C NMR of **4b**. Recorded at 151 MHz NMR.

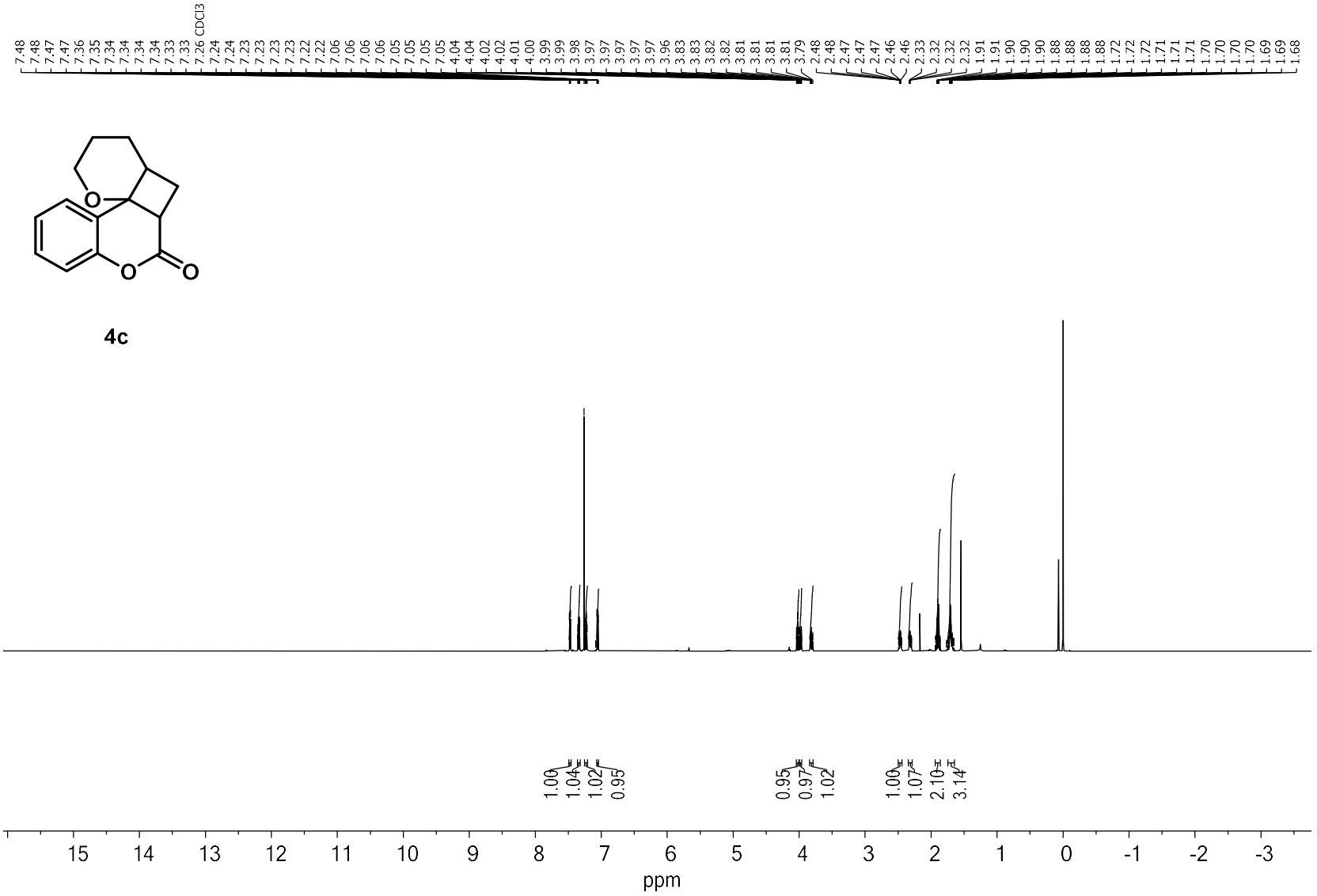


Figure S77 ^{1}H NMR of **4c**. Recorded at 600 MHz NMR.

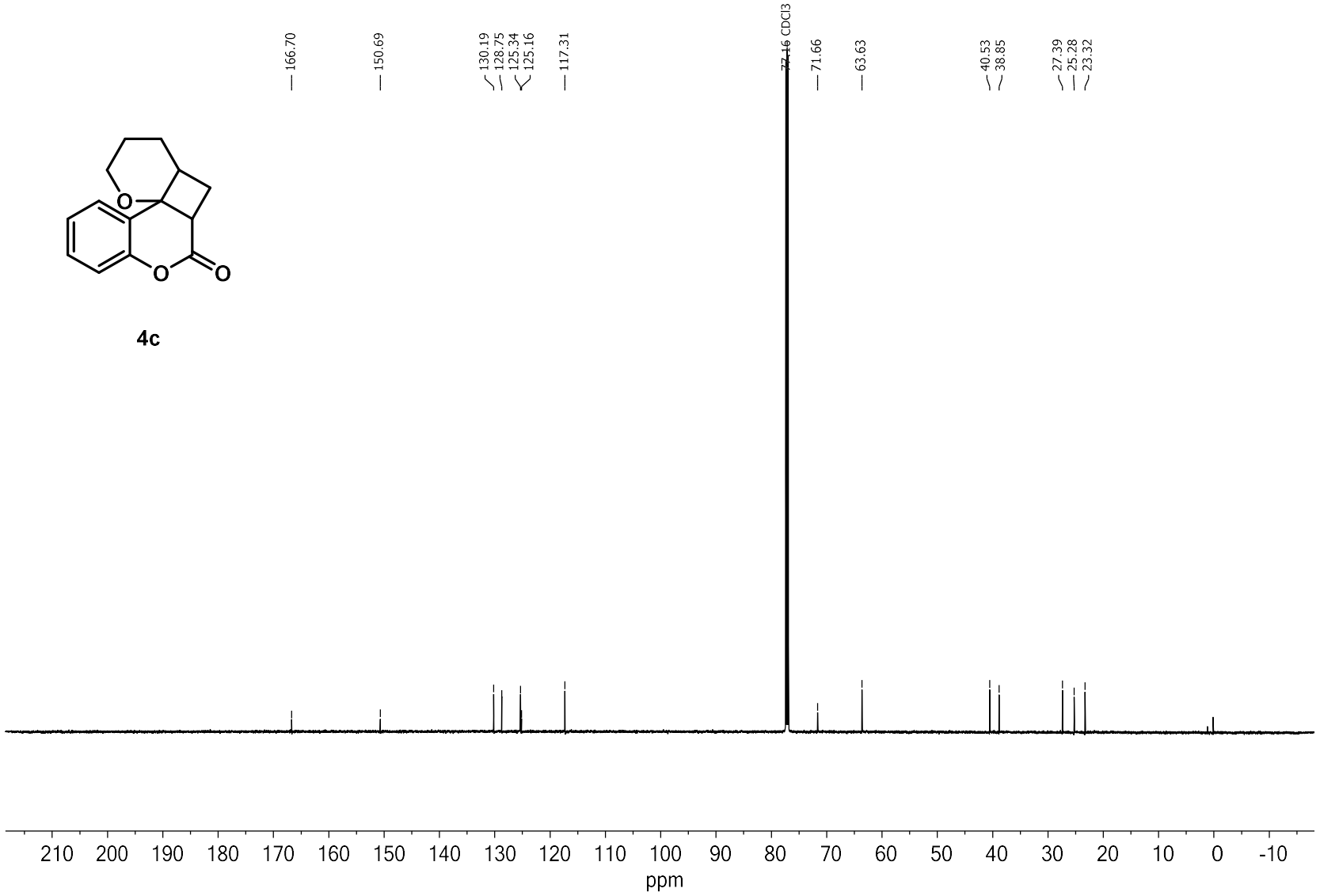


Figure S78 ^{13}C NMR of **4c**. Recorded at 151 MHz NMR.

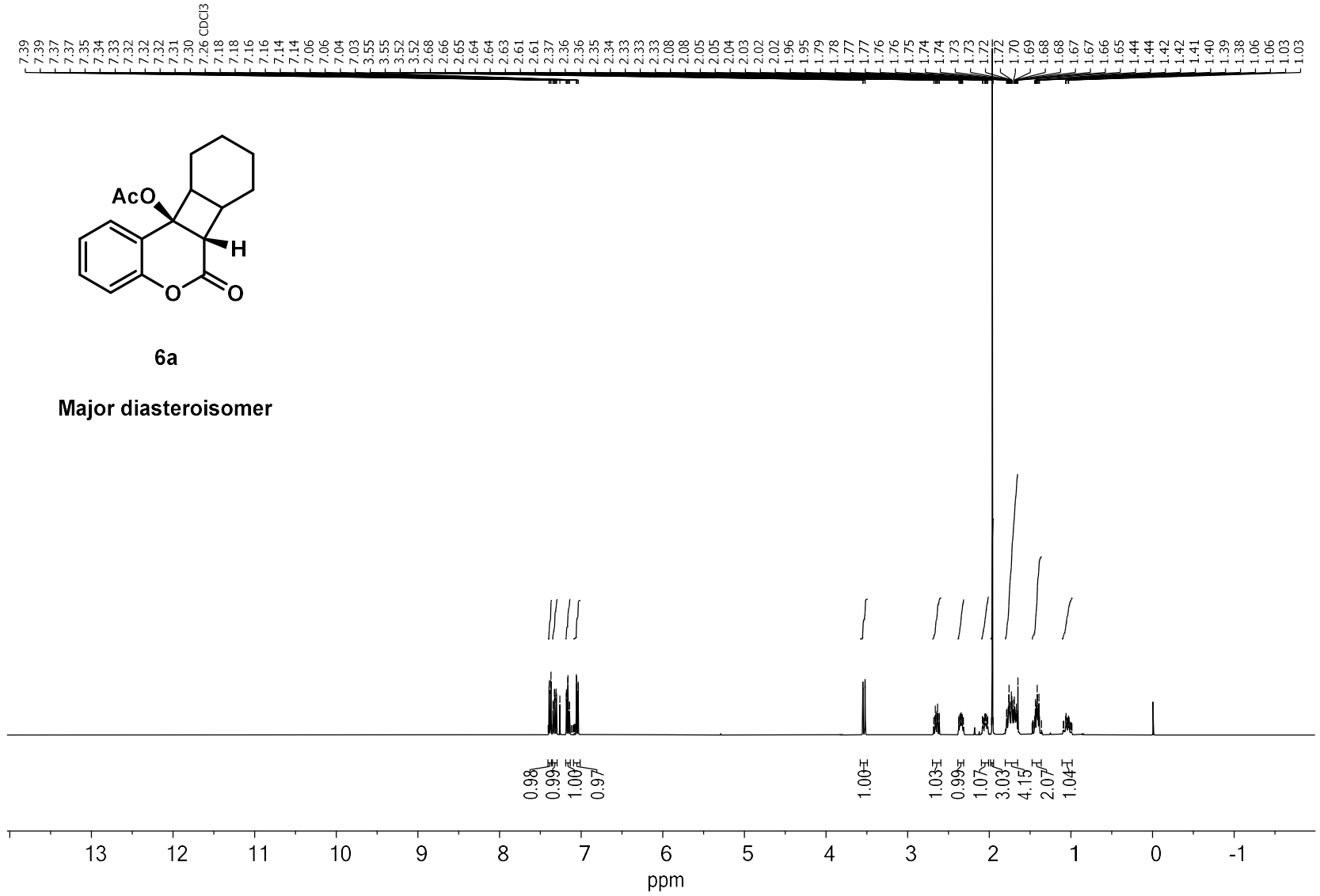


Figure S79 ^{1}H NMR of **6a**. Recorded at 600 MHz NMR.

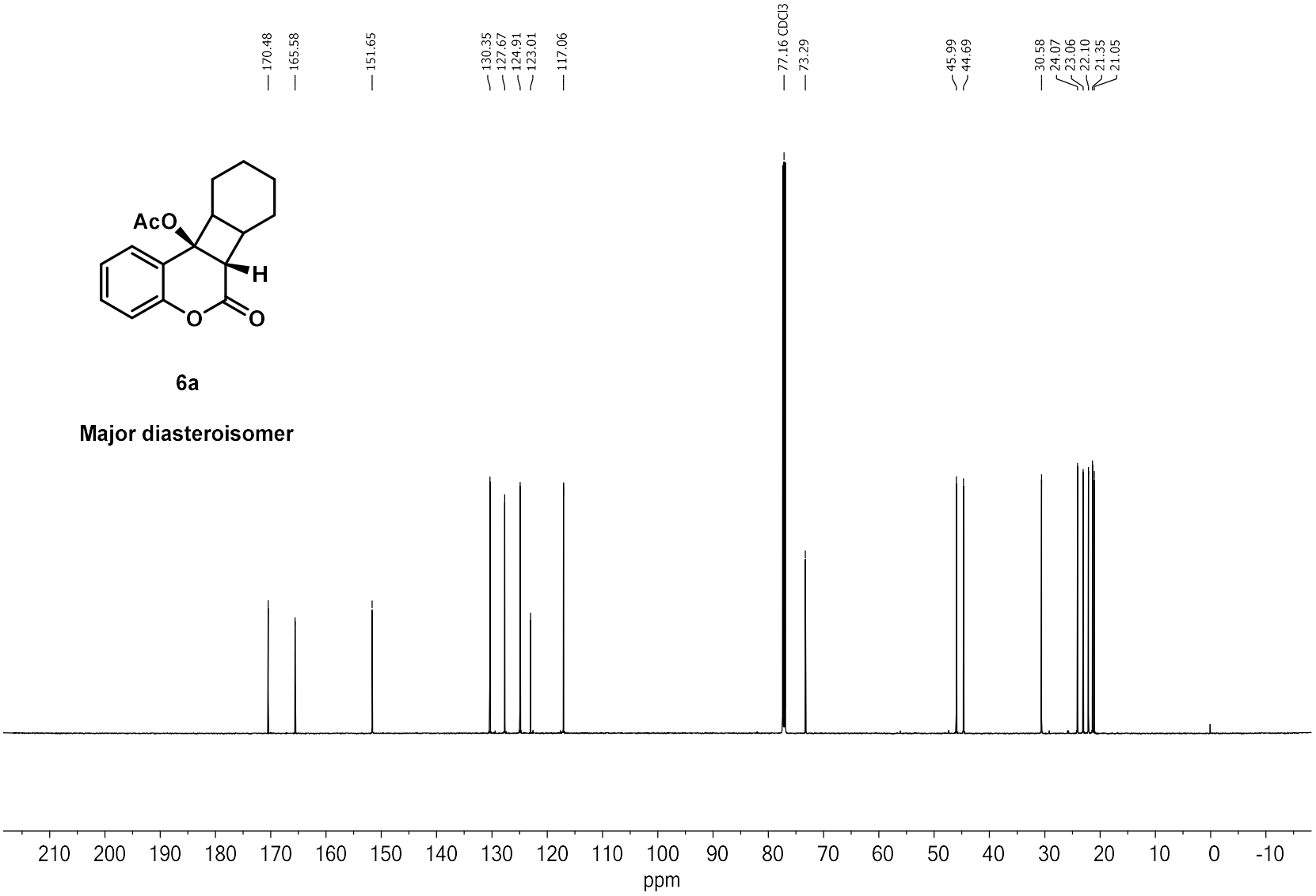


Figure S80 ^{13}C NMR of **6a**. Recorded at 151 MHz NMR.

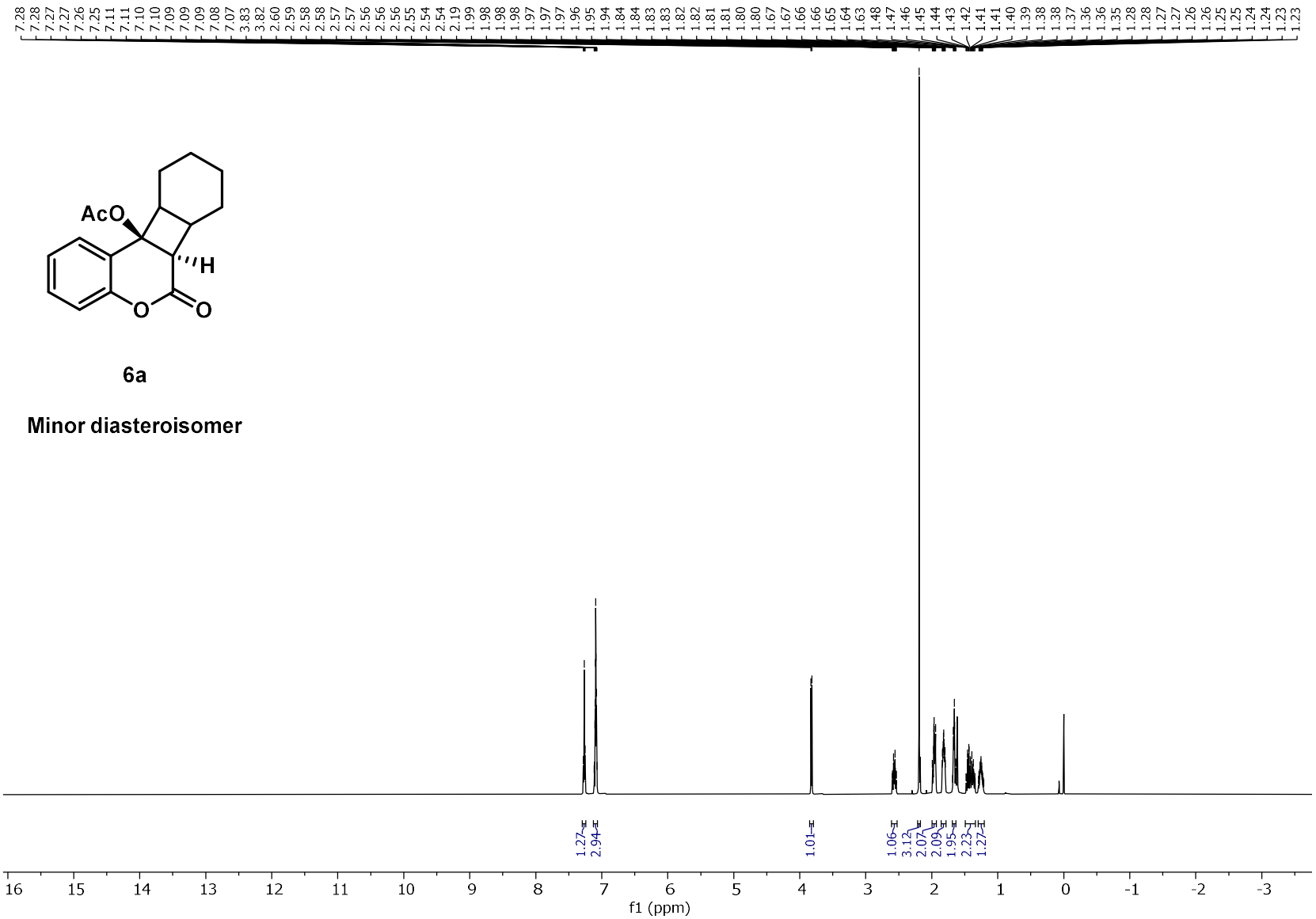


Figure S81 ^{1}H NMR of **6a**. Recorded at 600 MHz NMR.

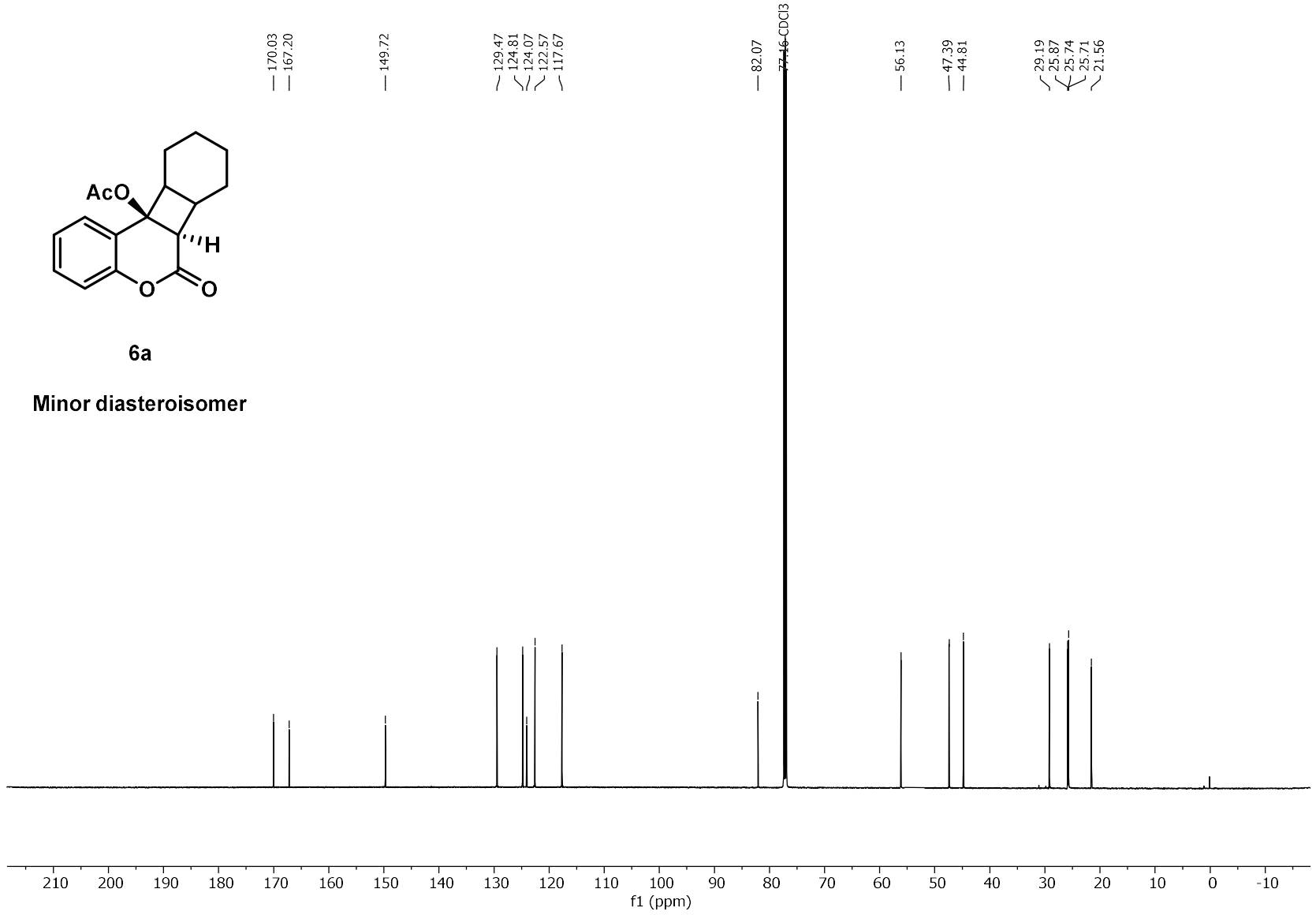


Figure S82 ^{13}C NMR of **6a**. Recorded at 151 MHz NMR.

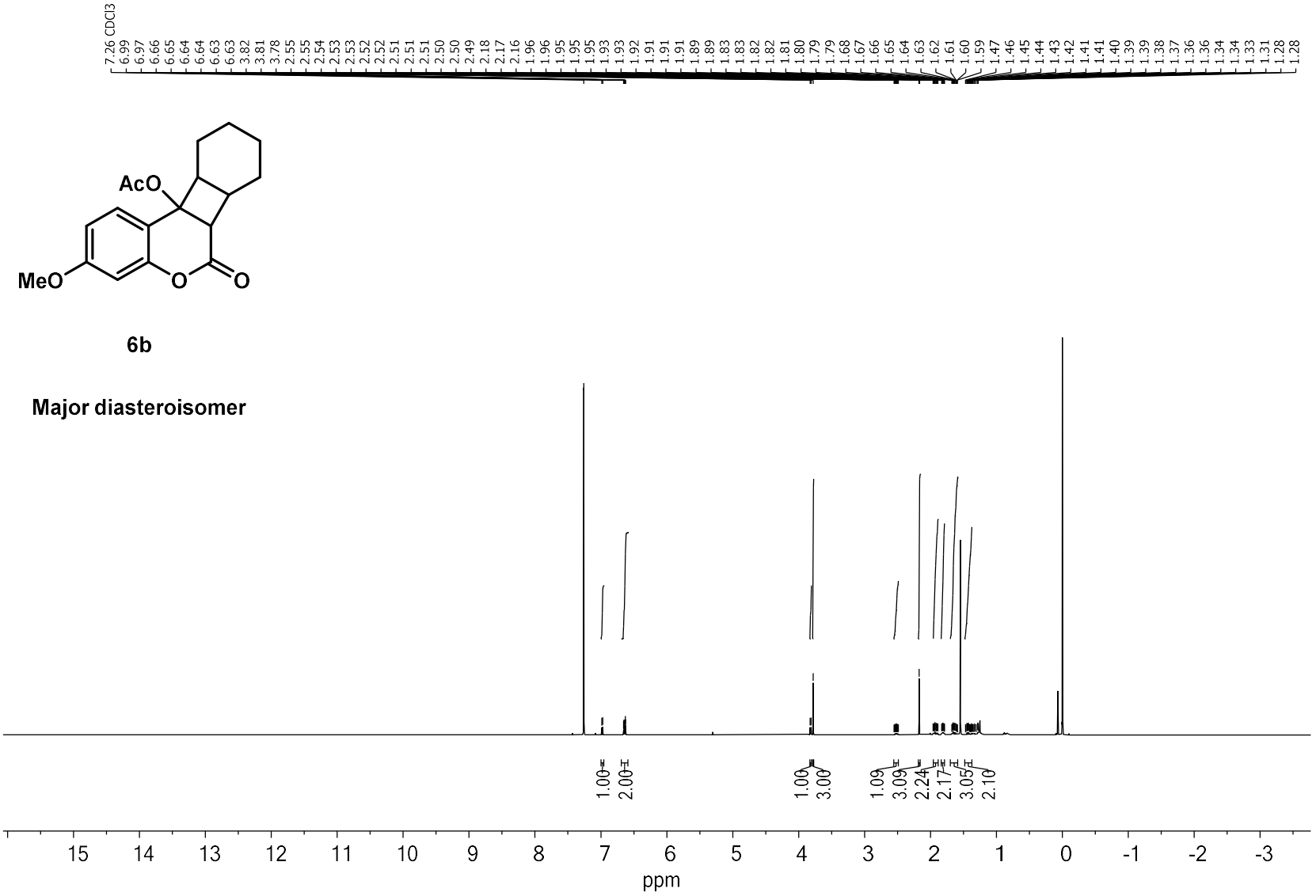


Figure S83 ^{1}H NMR of **6b**. Recorded at 600 MHz NMR.

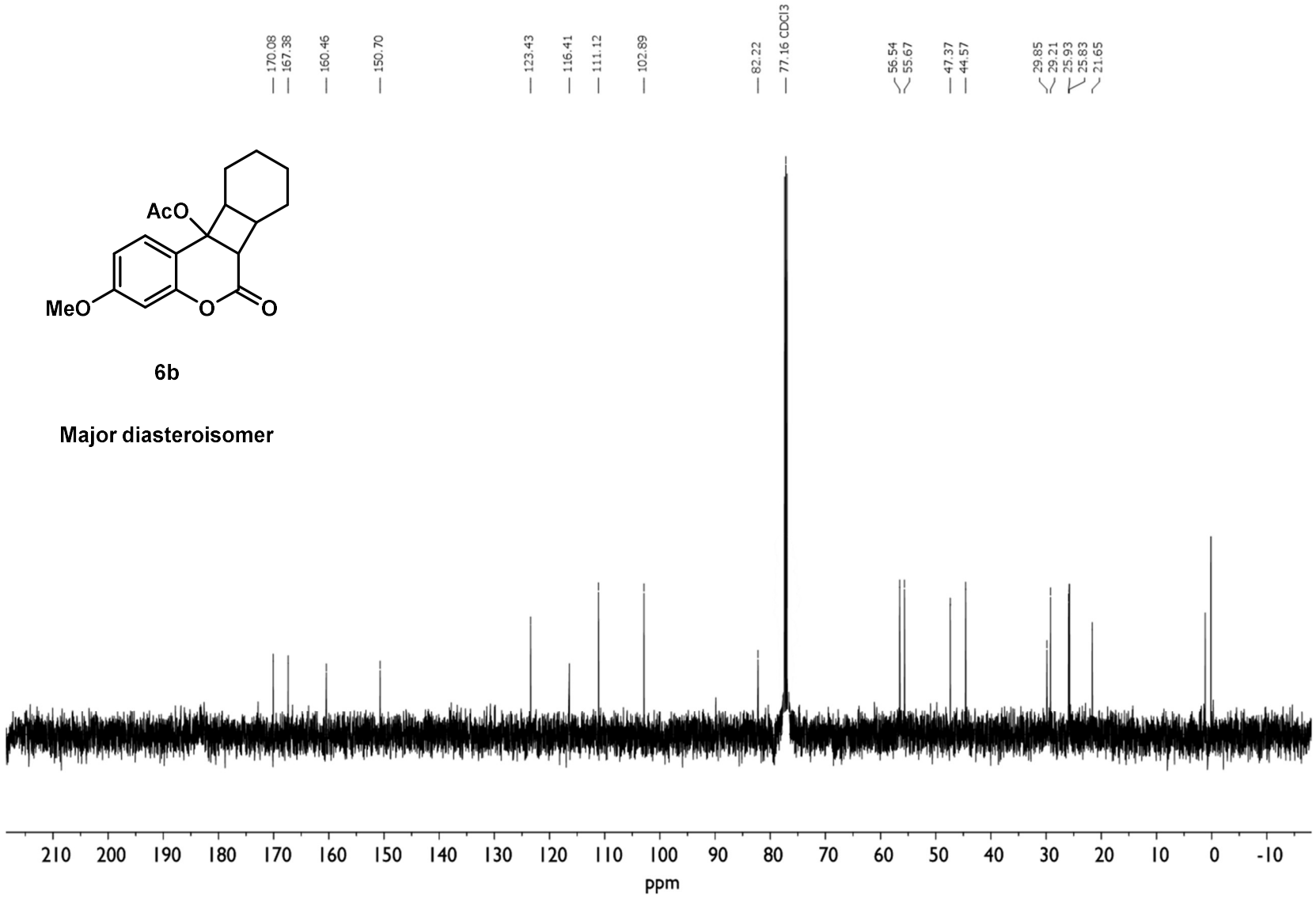


Figure S84 ^{13}C NMR of **6b**. Recorded at 151 MHz NMR.

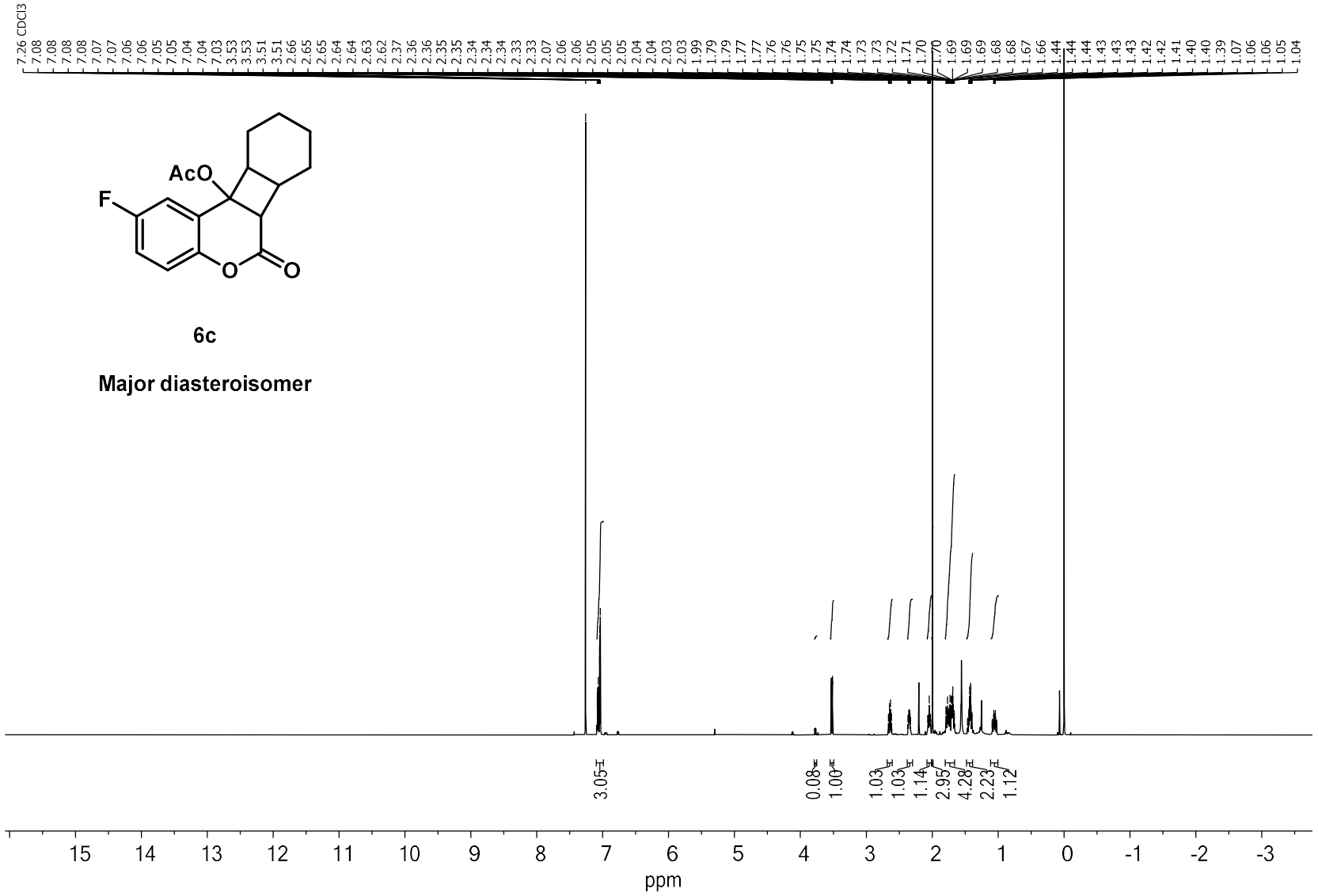


Figure S85 ^{1}H NMR of **6c**. Recorded at 600 MHz NMR.

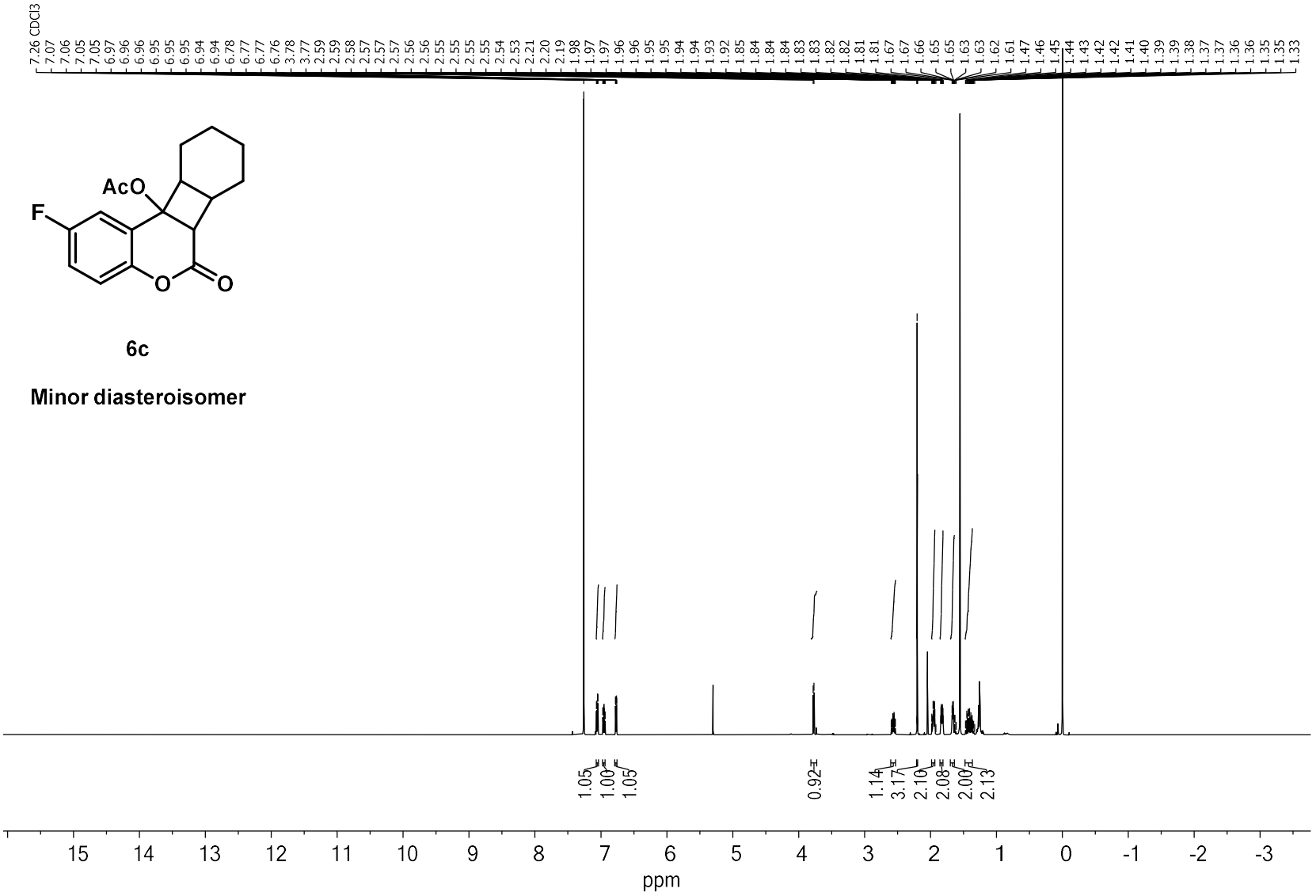


Figure S86 ^{1}H NMR of **6c**. Recorded at 600 MHz NMR.

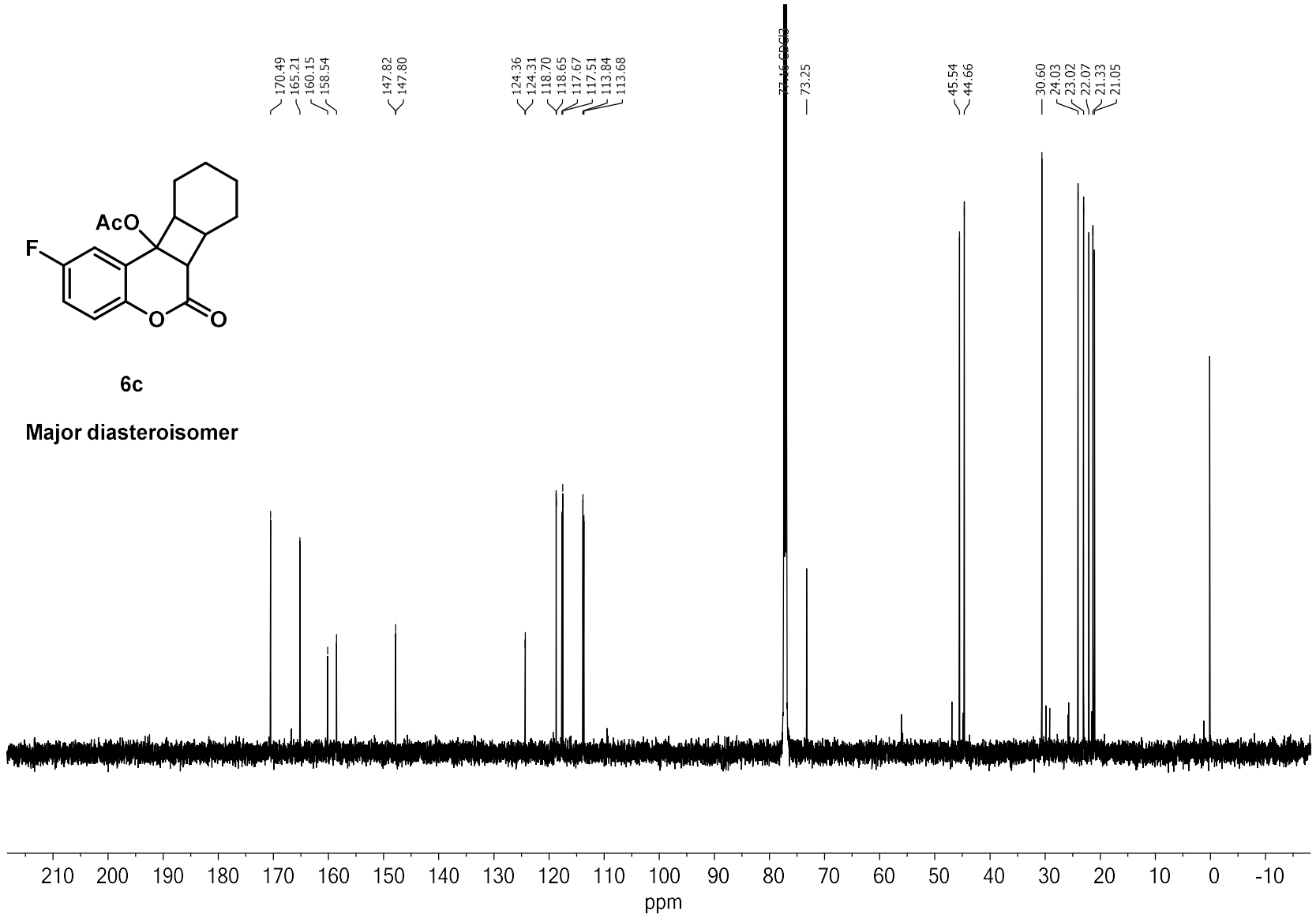


Figure S87 ^{13}C NMR of **6c**. Recorded at 151 MHz NMR.

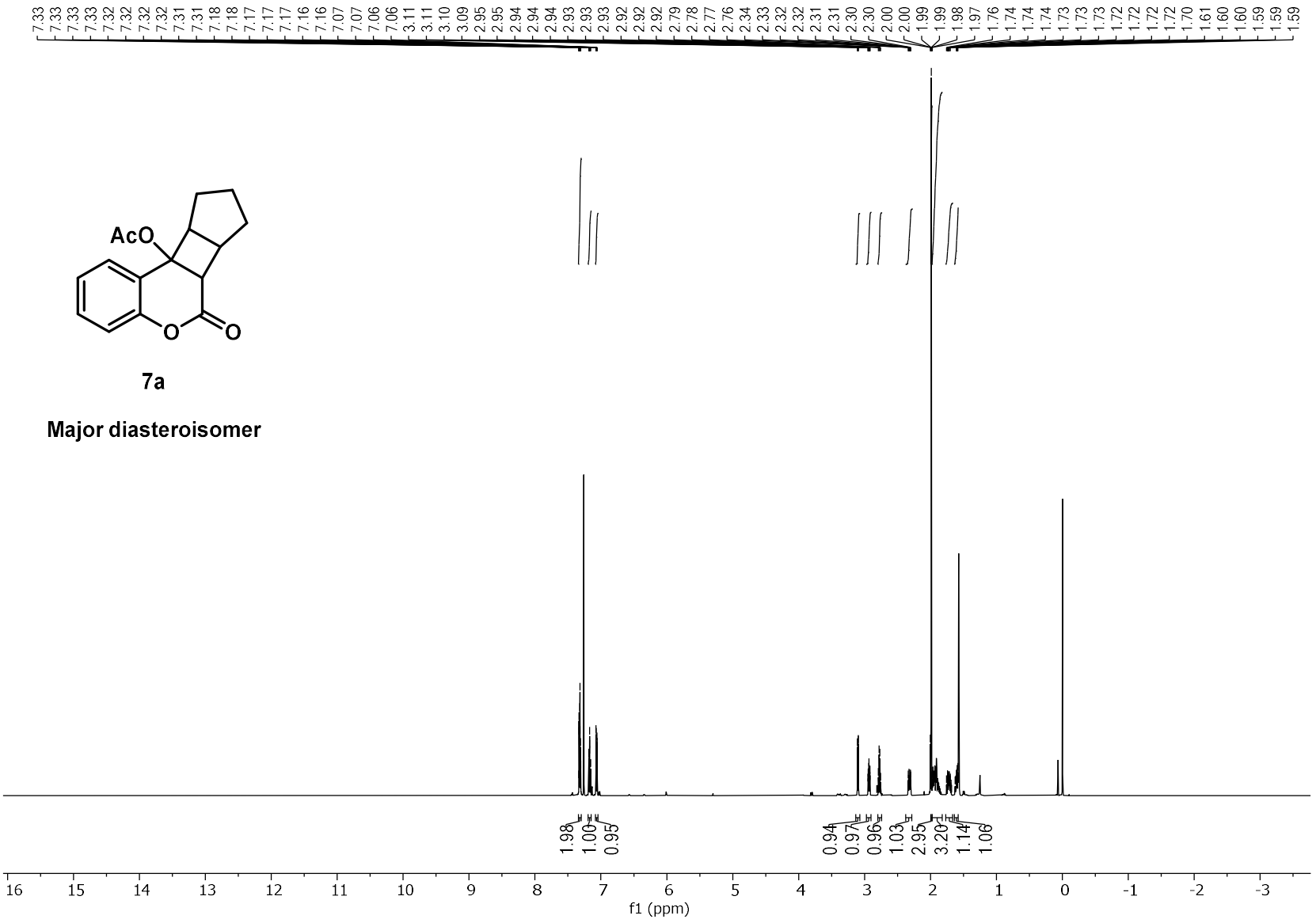


Figure S88 ^{1}H NMR of **7a**. Recorded at 600 MHz NMR.

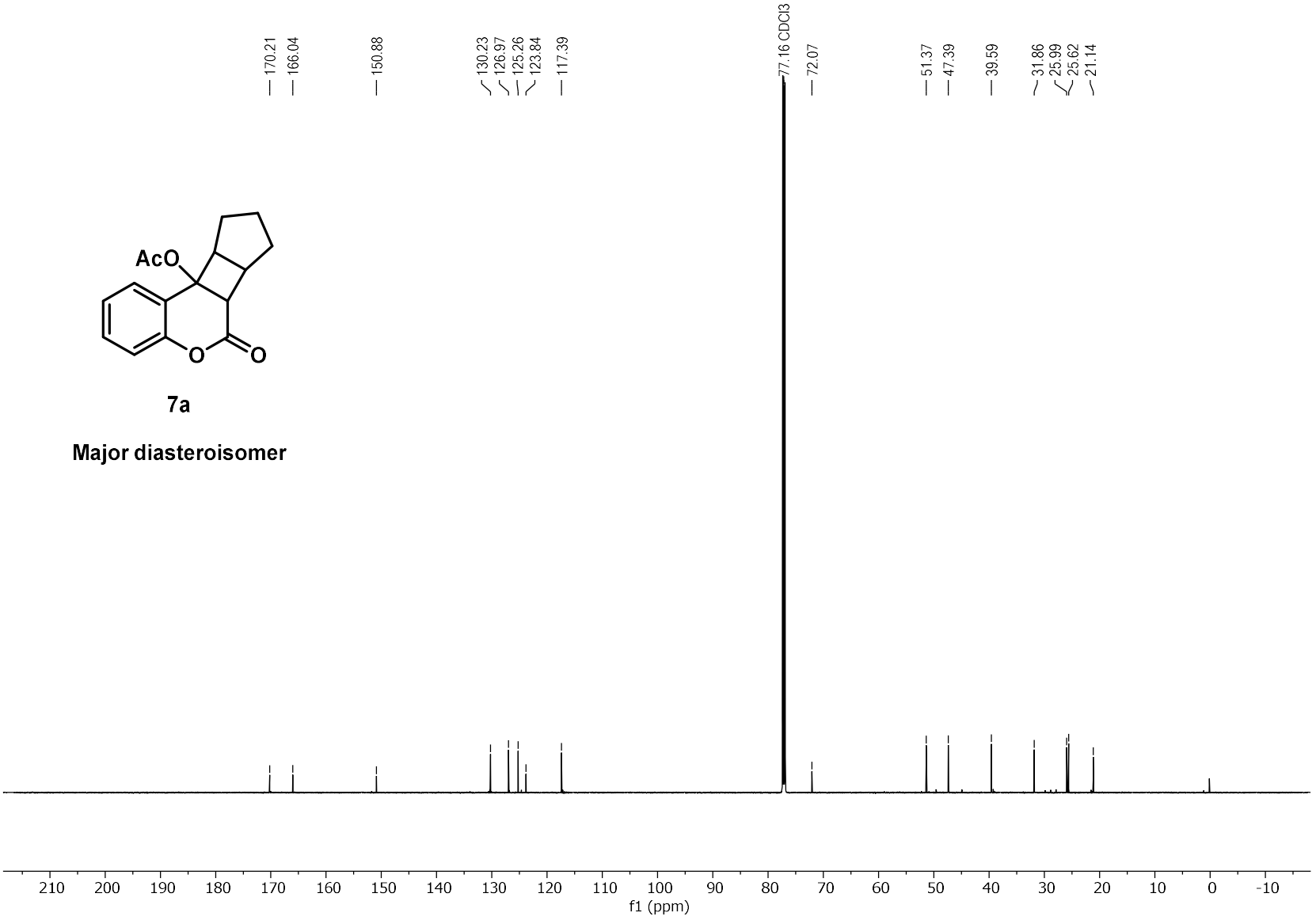


Figure S89 ^{13}C NMR of **7a**. Recorded at 151 MHz NMR.

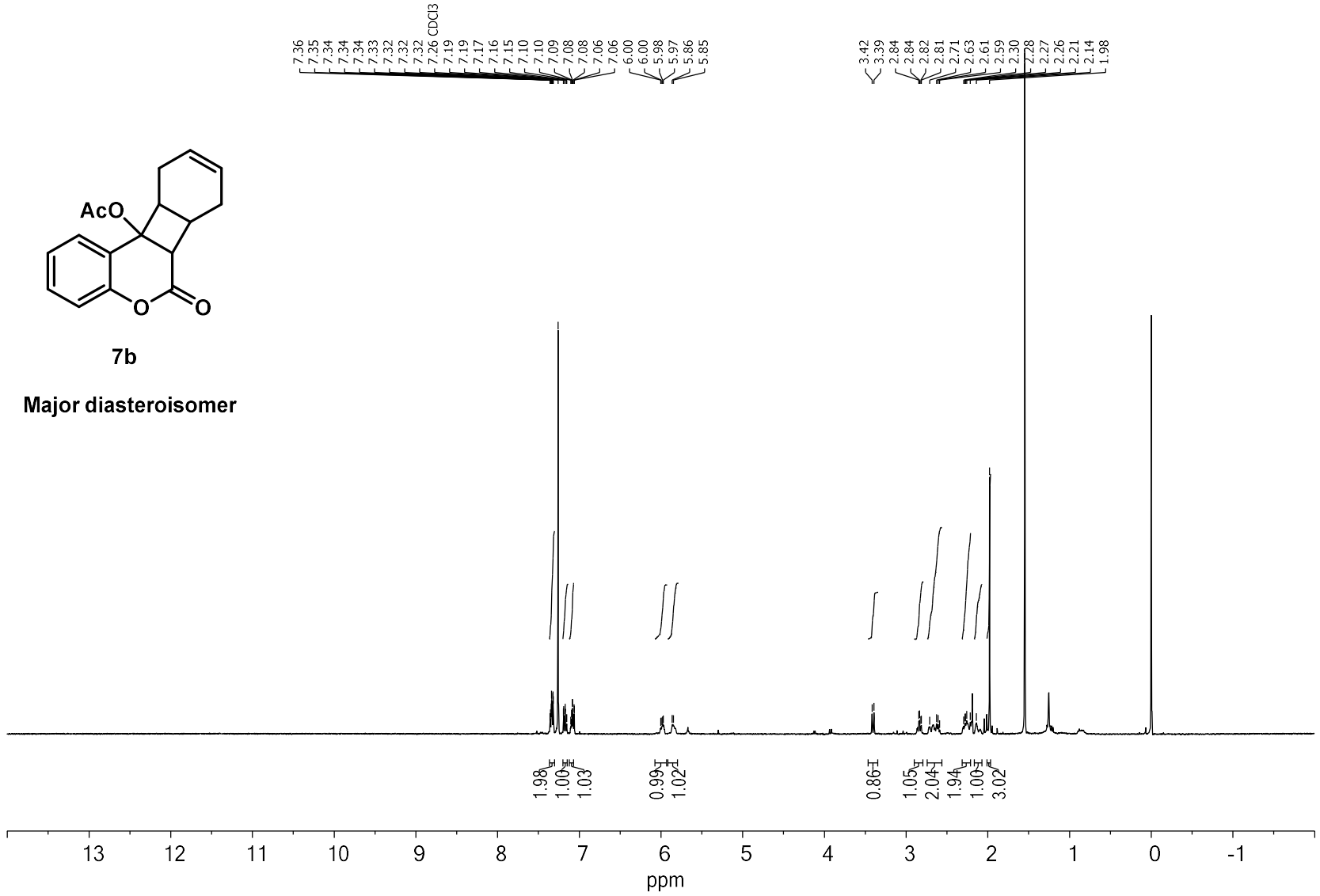


Figure S90 ^{1}H NMR of **7b**. Recorded at 600 MHz NMR.

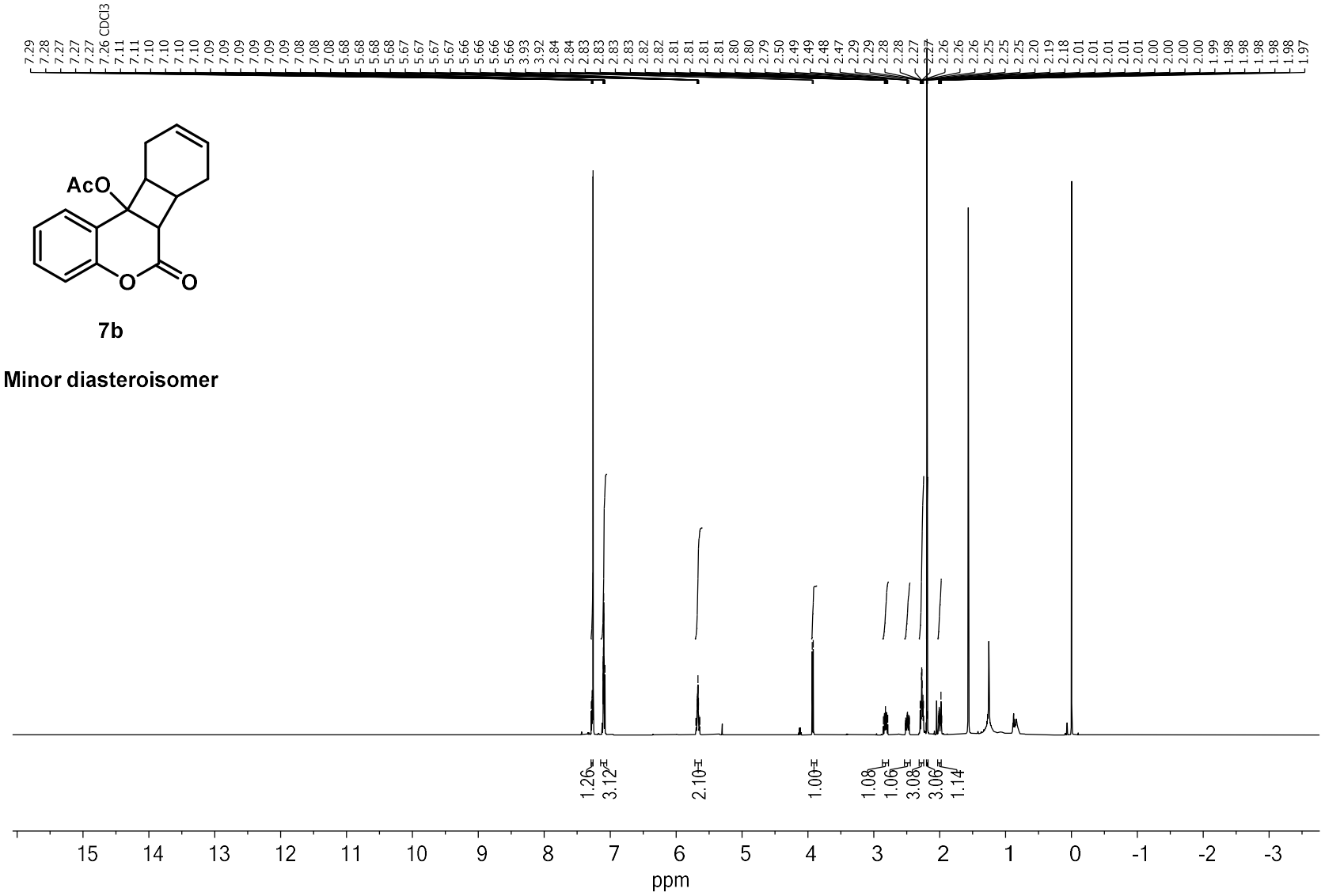


Figure S91 ^{1}H NMR of **7b**. Recorded at 600 MHz NMR.

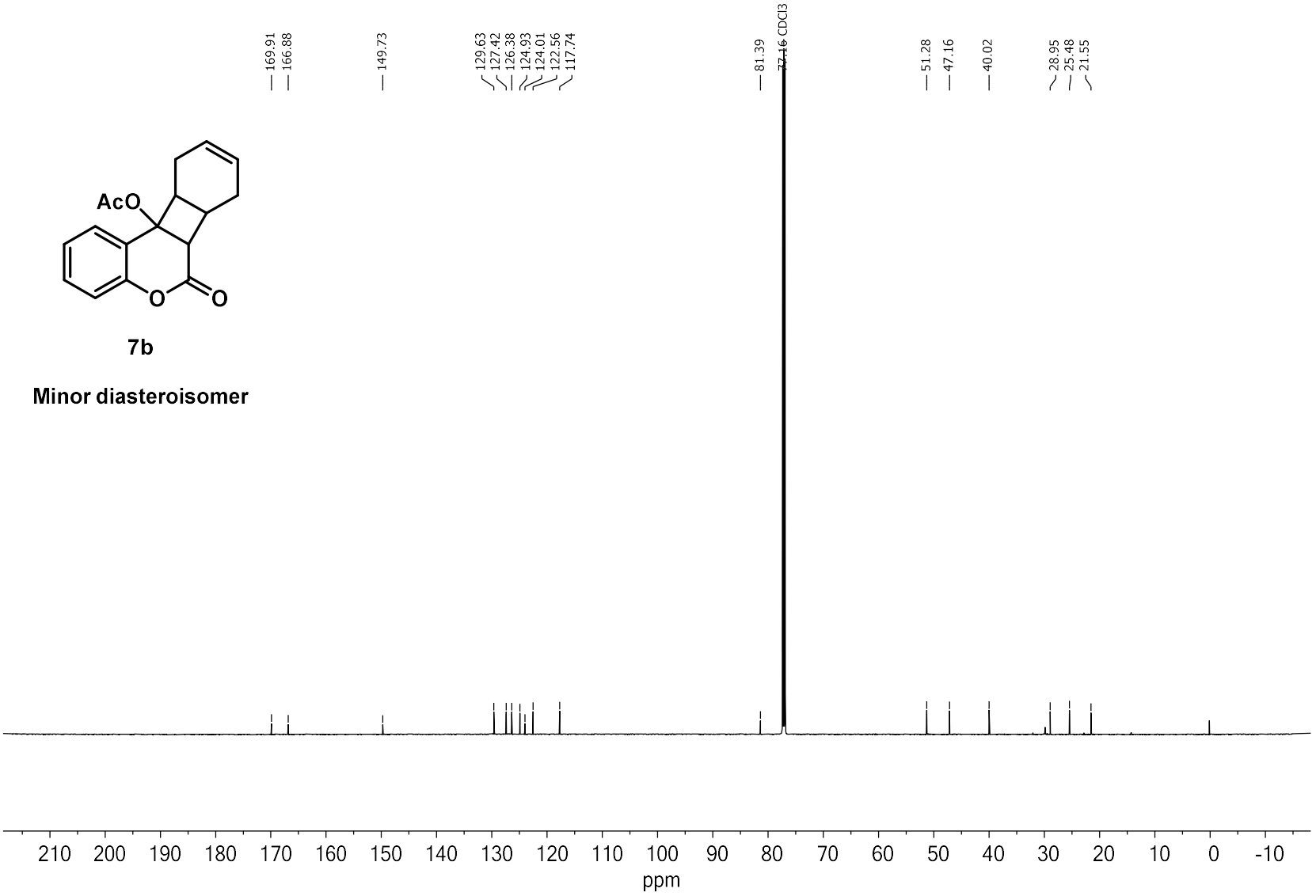


Figure S92 ^{13}C NMR of **7b**. Recorded at 151 MHz NMR.

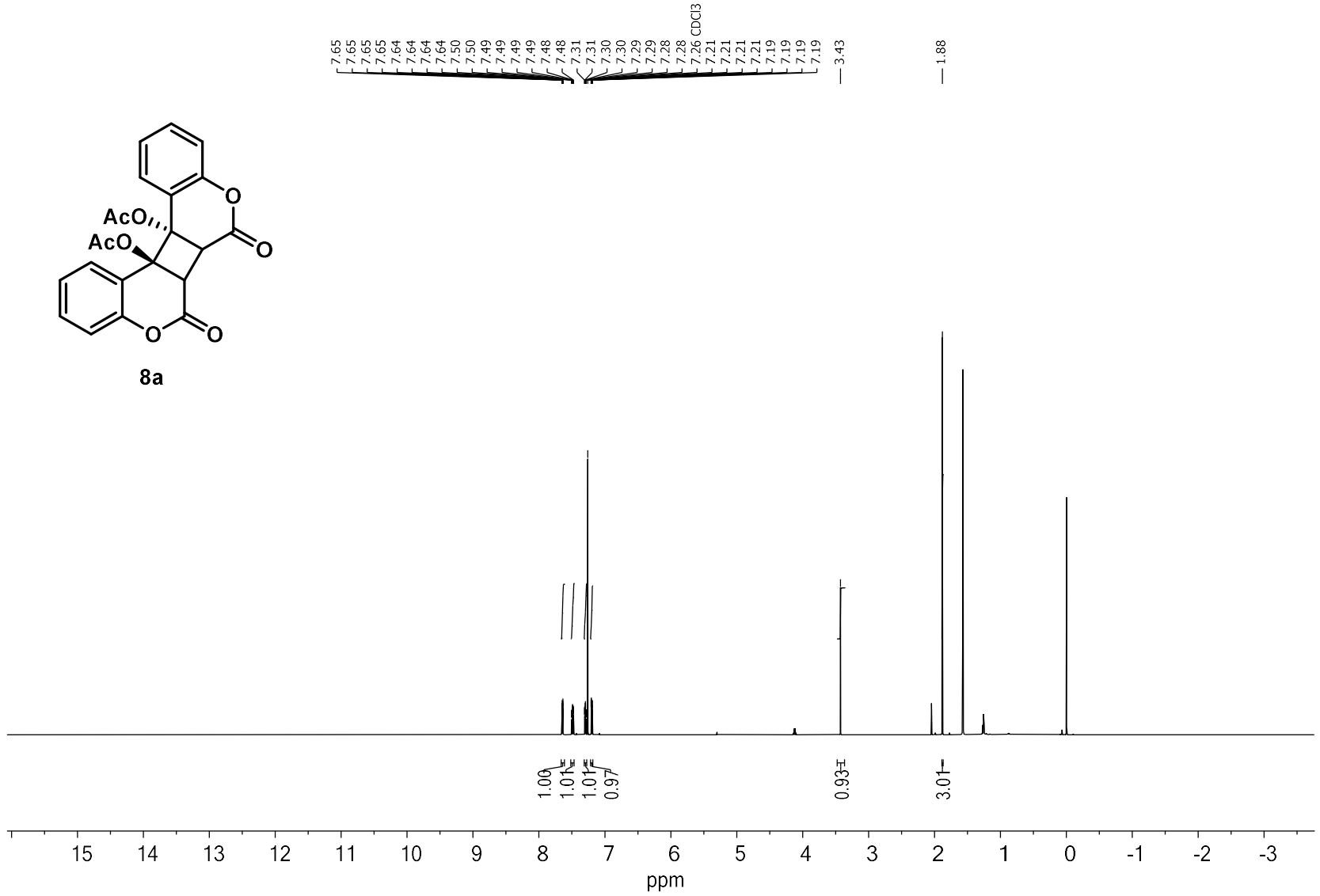


Figure S93 ^{1}H NMR of **8a**. Recorded at 600 MHz NMR.

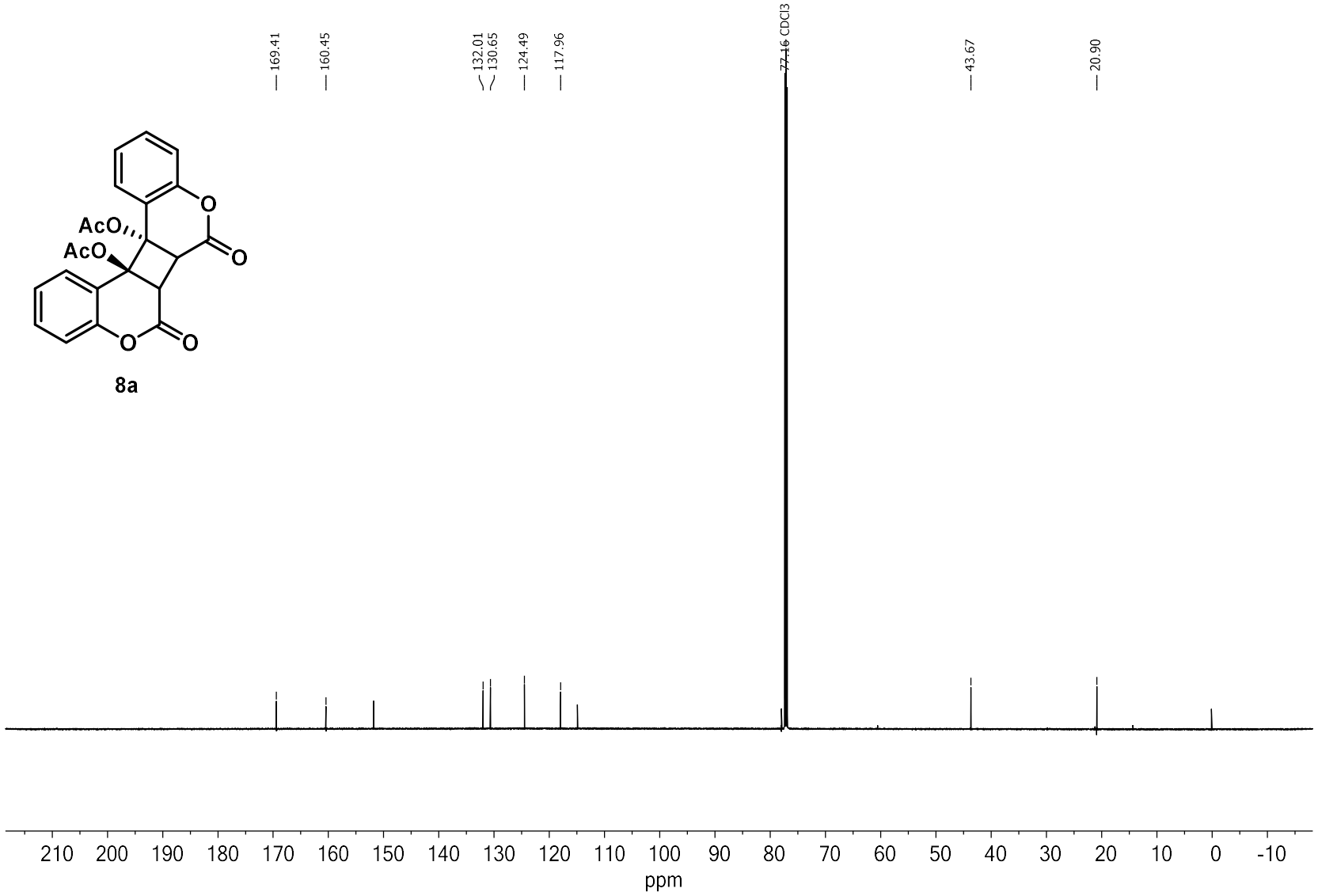


Figure S94 ^{13}C NMR of **8a**. Recorded at 151 MHz NMR.

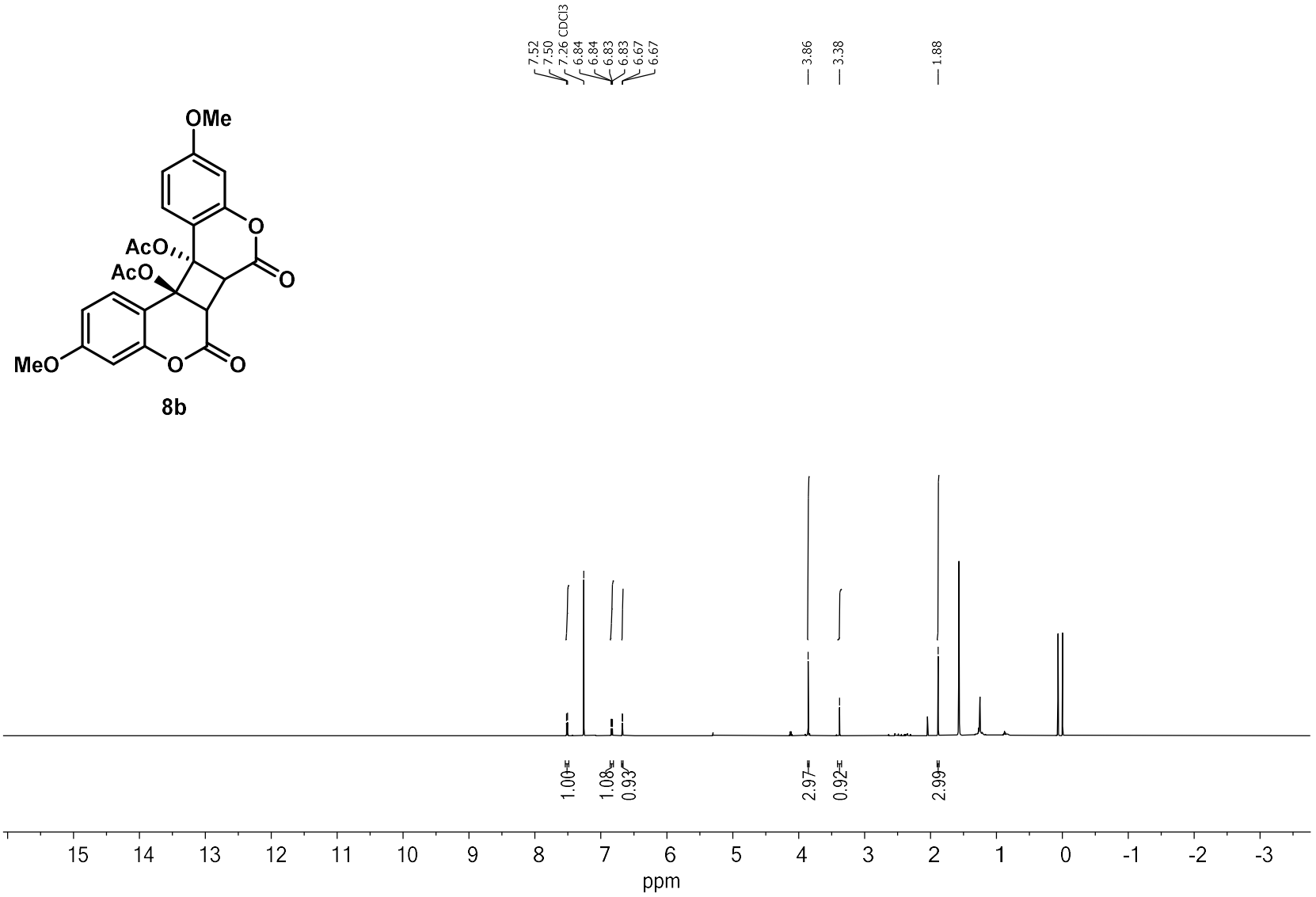


Figure S95 ^{1}H NMR of **8b**. Recorded at 600 MHz NMR.

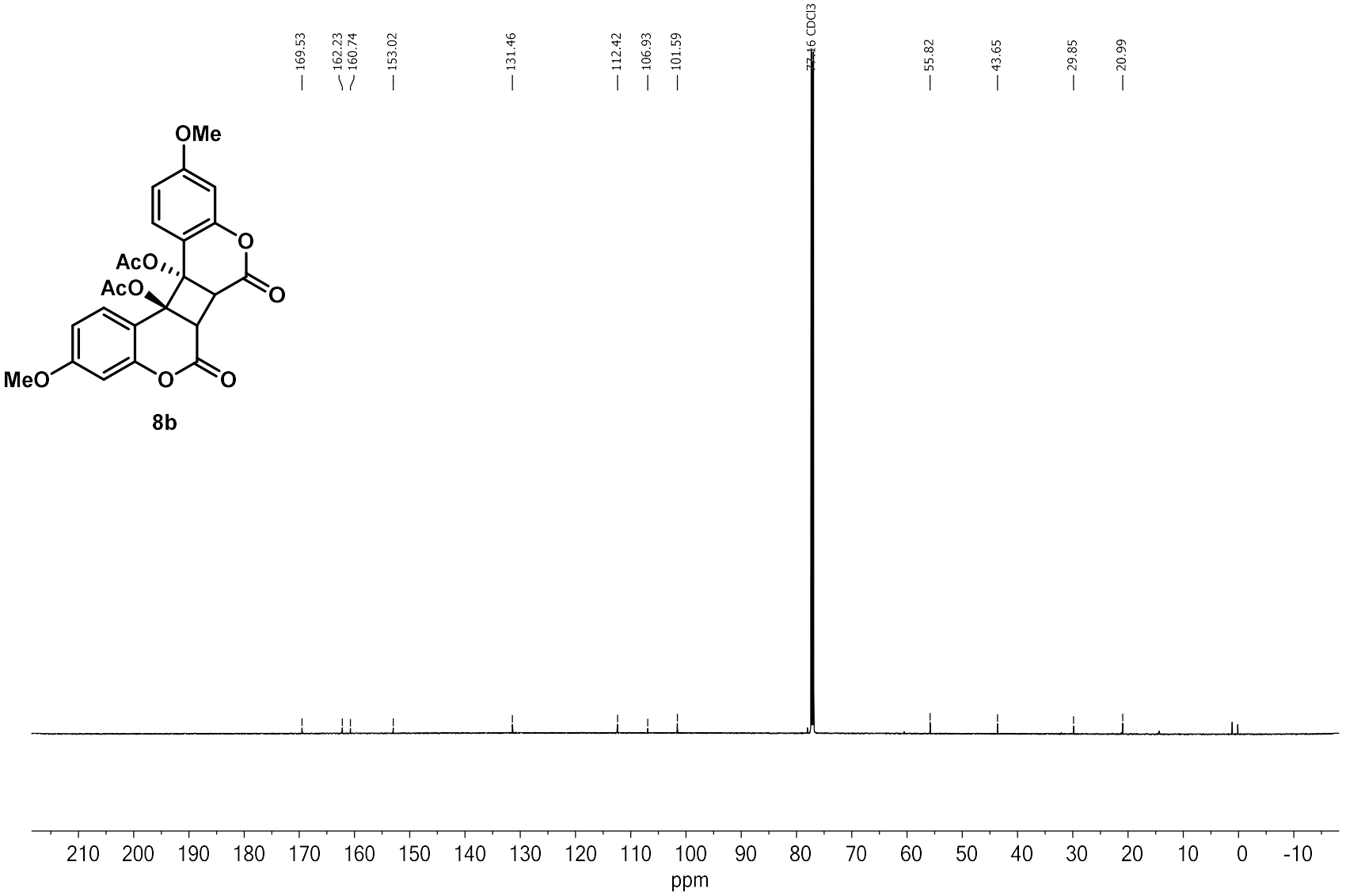


Figure S96 ^{13}C NMR of **8b**. Recorded at 151 MHz NMR.

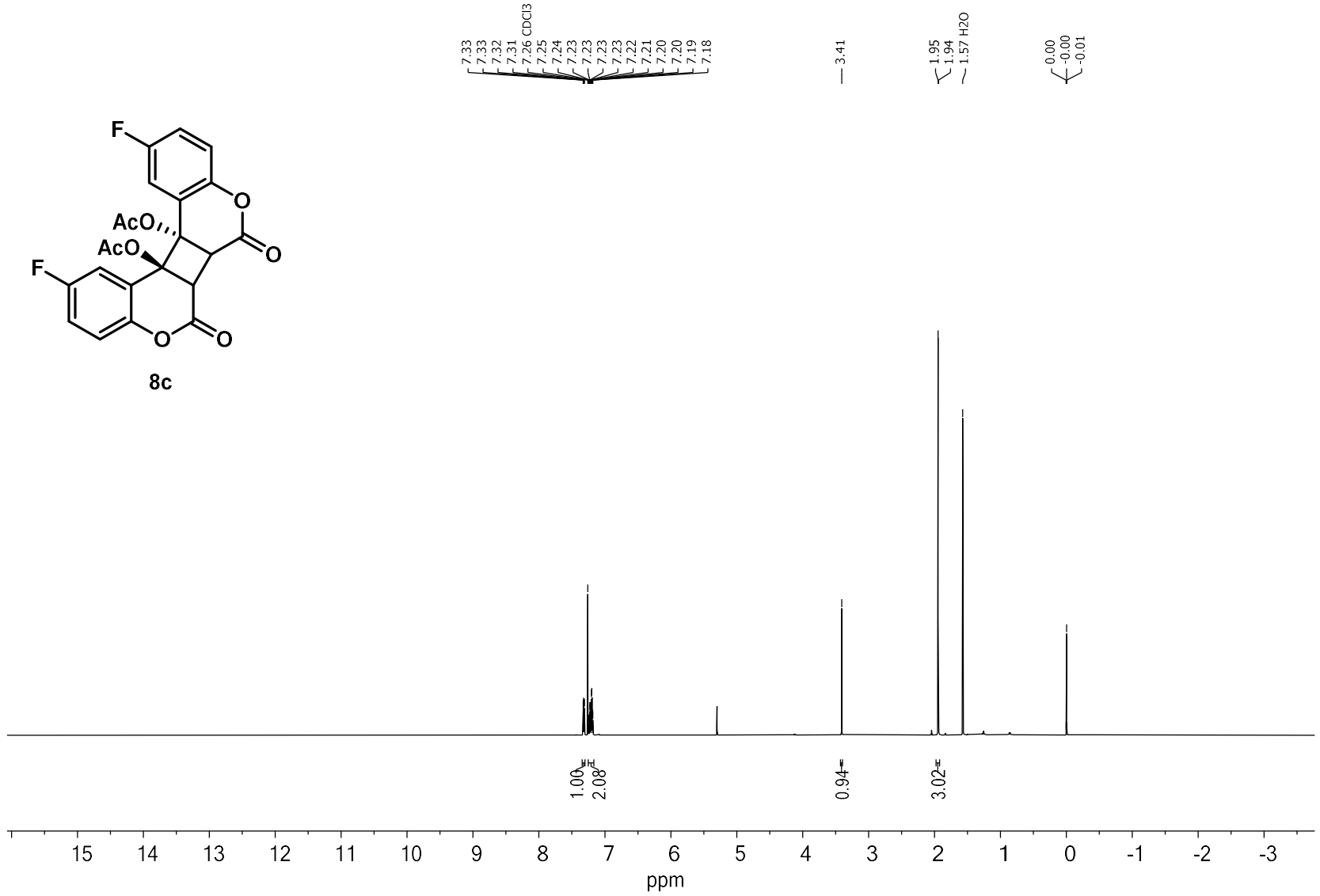


Figure S97 ^{1}H NMR of **8c**. Recorded at 600 MHz NMR.

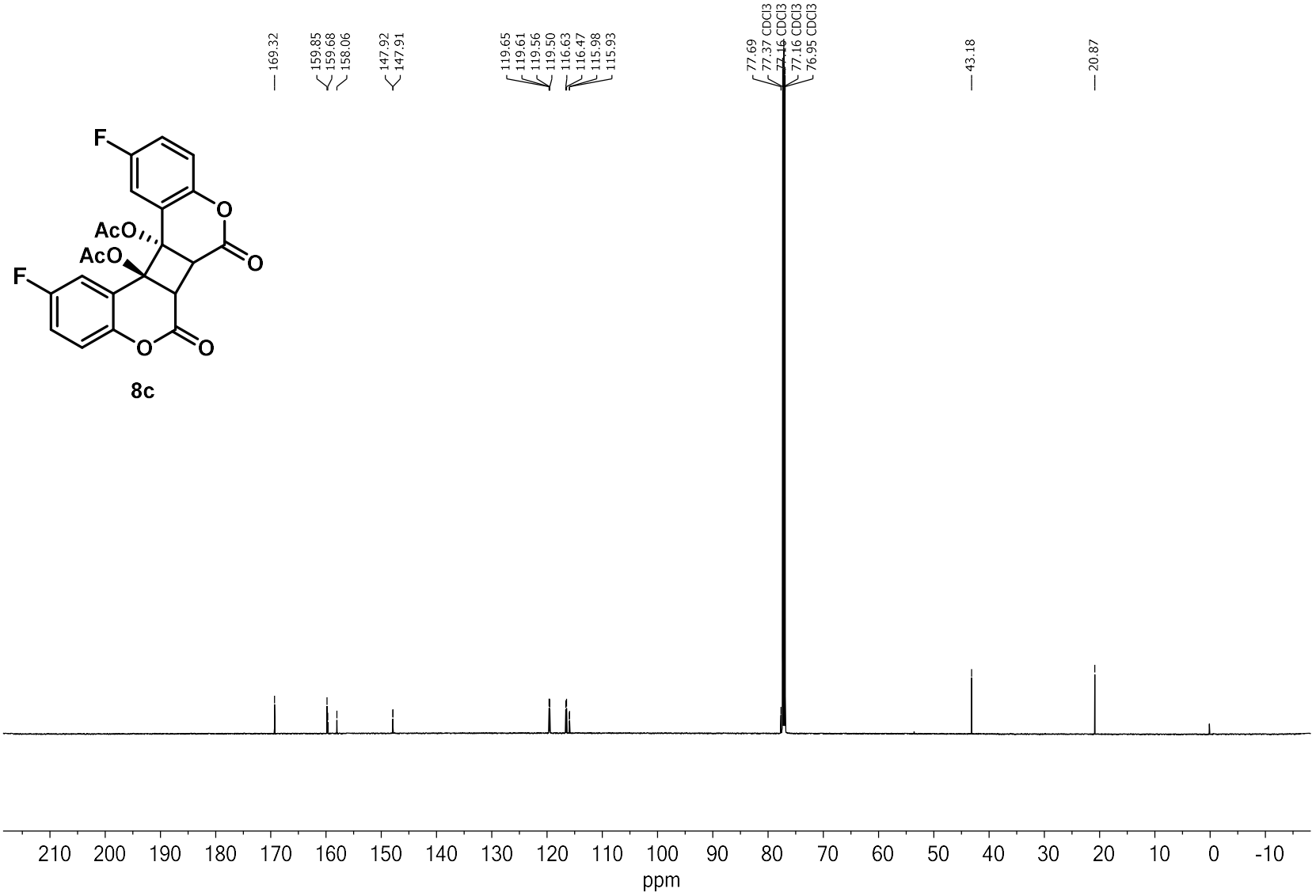


Figure S98 ^{13}C NMR of **8c**. Recorded at 151 MHz NMR.

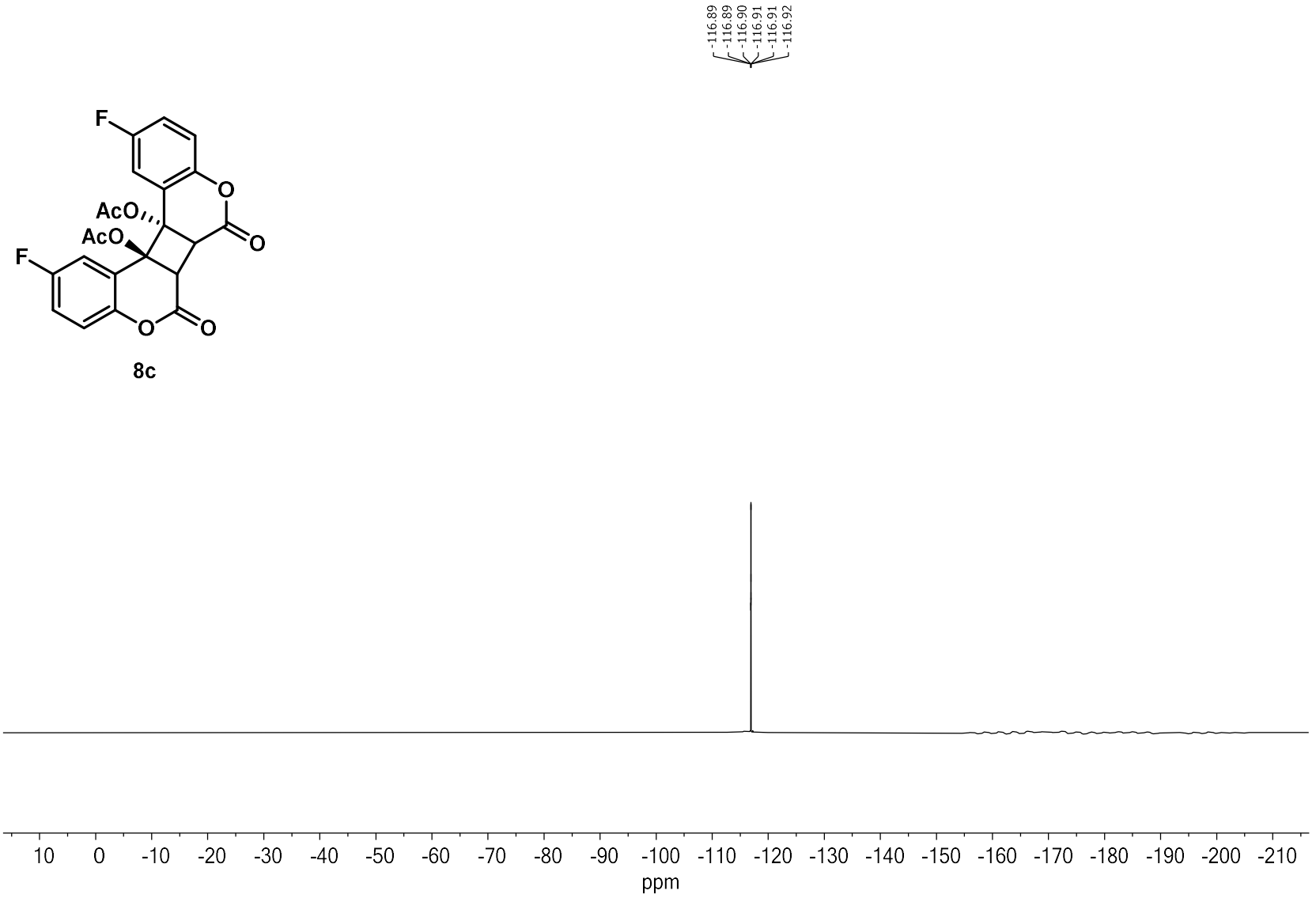


Figure S99 ^{19}F NMR of **8c**. Recorded at 565 MHz NMR.

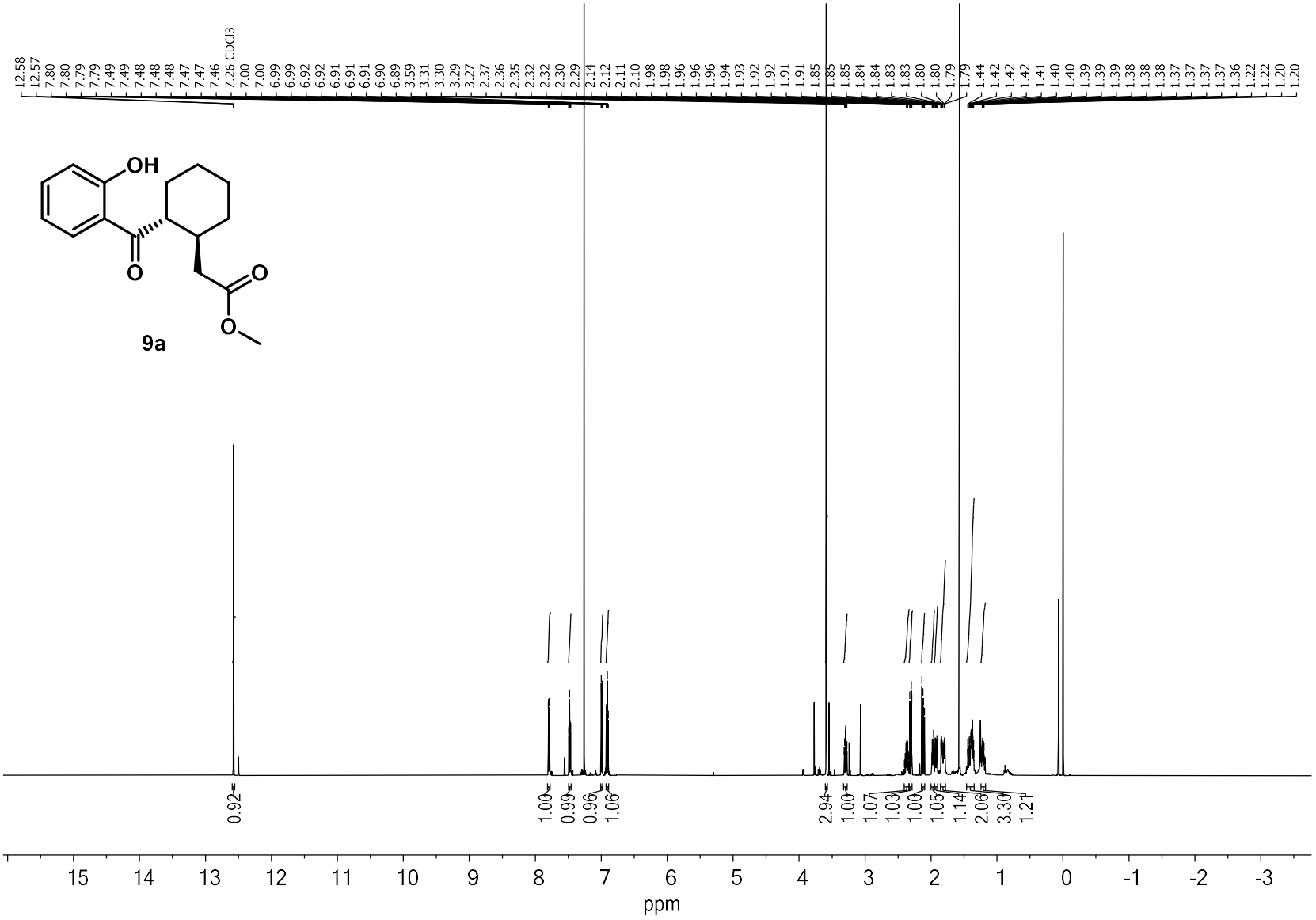


Figure S100 ^{1}H NMR of **9a**. Recorded at 600 MHz NMR.

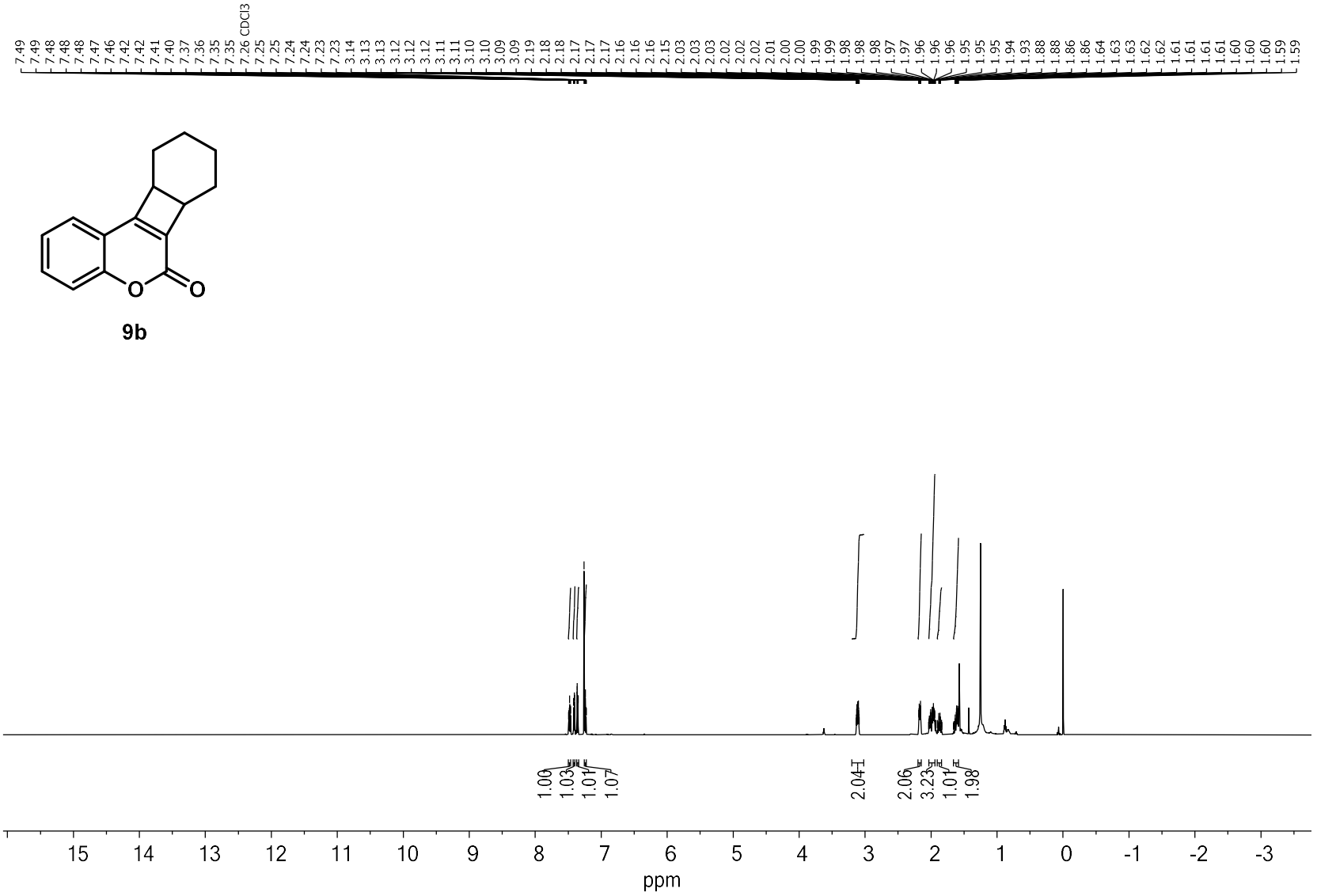


Figure S101 ^{1}H NMR of **9b**. Recorded at 600 MHz NMR.

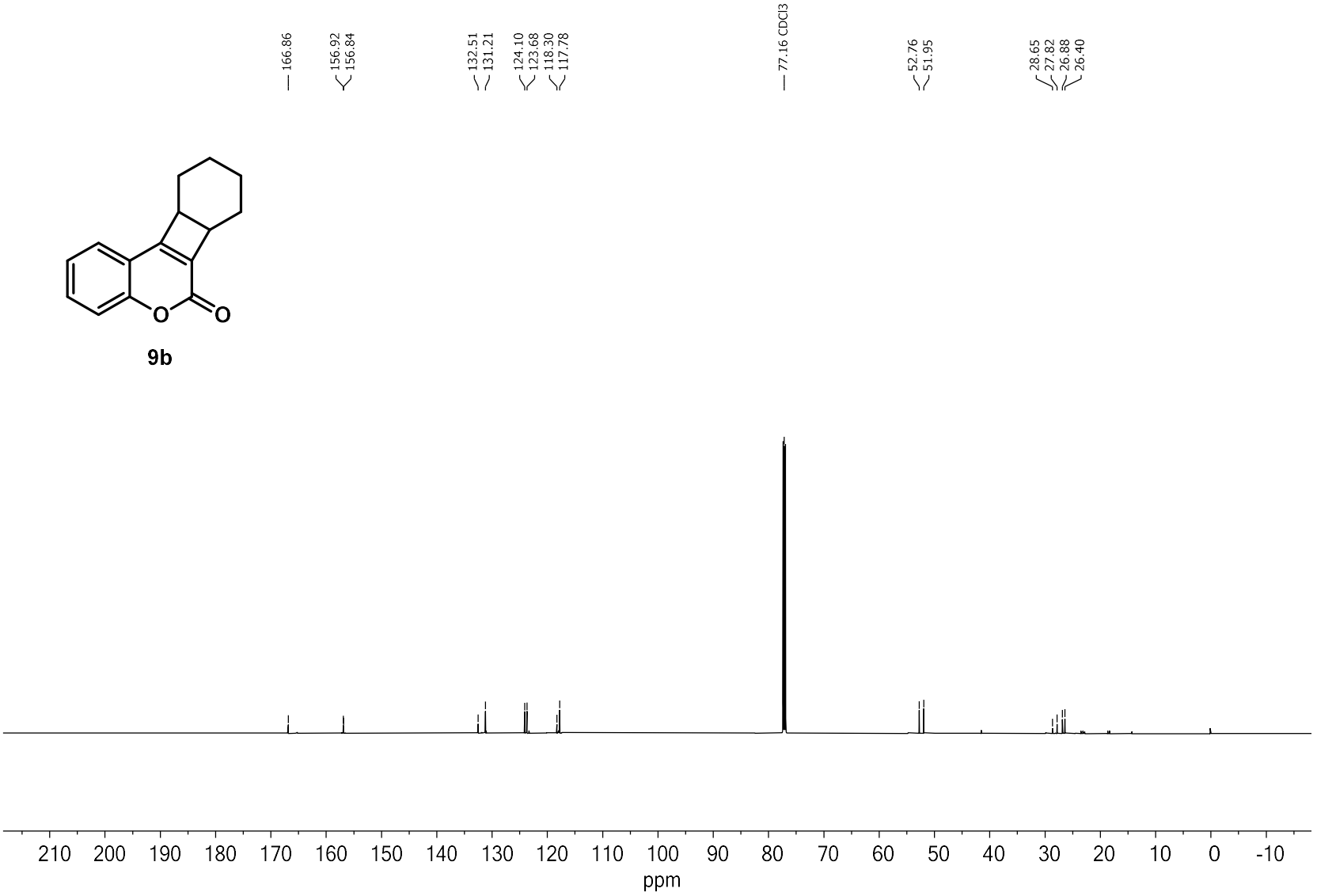
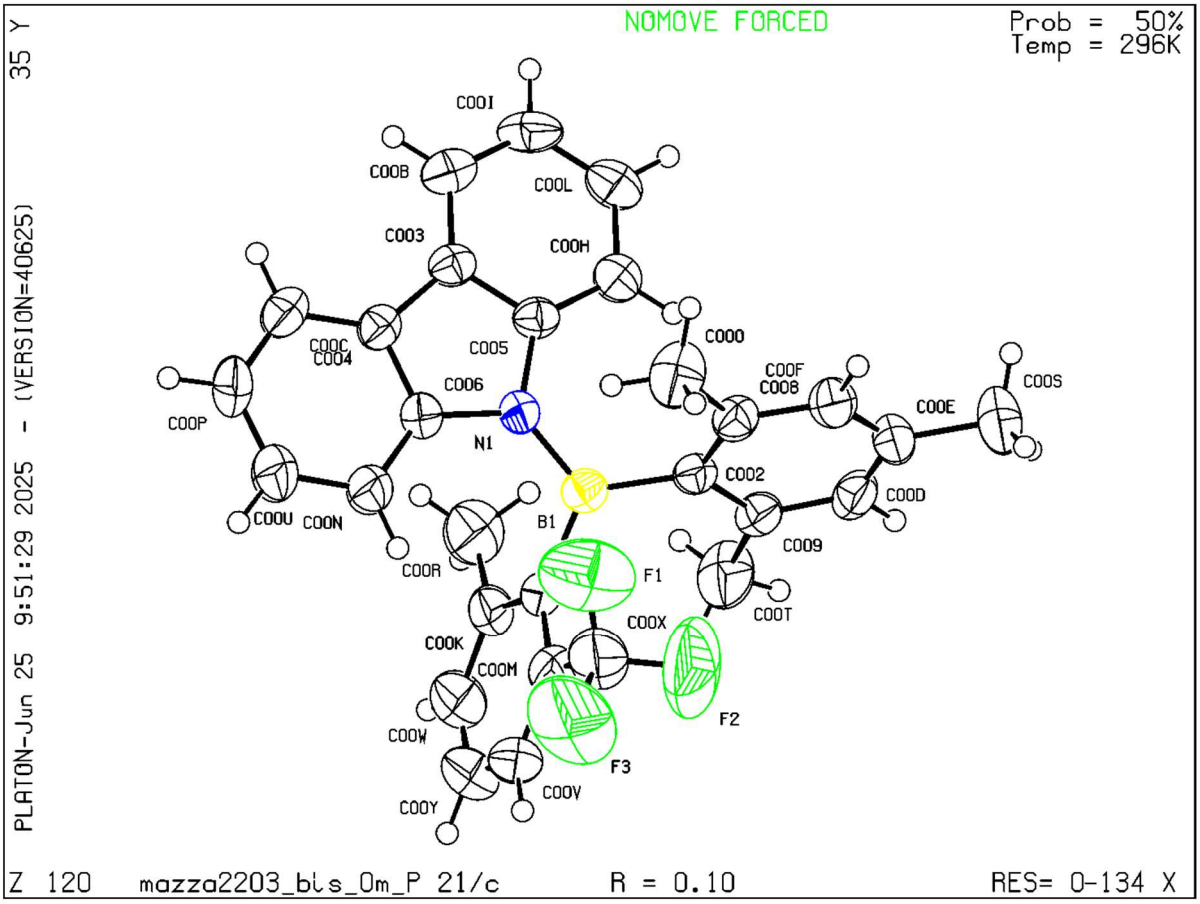


Figure S102 ^{13}C NMR of **9b**. Recorded at 151 MHz NMR.

9. X-Ray Analysis of C1, C2, 6a, 8c

9.1 X-Ray Crystallography of Photocatalysts

9.1.1 X-Ray Crystallography of C1



A specimen of $C_{29}H_{25}BF_3N$, approximate dimensions 0.220mm x 0.250mm x 0.300 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured(λ = 0.71073 Å). The total exposure time was 20.33 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 27037 reflections to a maximum θ angle of 25.00 (0.84Å resolution), of which 4179 were independent (average redundancy 6.470, completeness = 98.4%, R_{int}= 5.31%, R_{sig}=3.34%) and 3791(90.72%) were greater than $2\sigma(F^2)$. The final cell constants of a = 18.422(9) Å, b = 16.459(8) Å, c = 8.059(4) Å, β = 99.72(2)°, volume = 2408.(2) $Å^3$, are based upon the refinement of the XYZ-centroids of 9903 reflections above 20 σ(I) with 5.137° < 2θ < 56.68°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.879. The calculated minimum and maximum transmission coefficients (based on crystal size) are0.9740 and 0.9810. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z = 4 for the formula unit, $C_{29}H_{25}BF_3N$. The final anisotropic full-matrix least-squares refinement on F^2 with311 variables converged at R1 = 9.61%, for the observed data and wR2 = 24.46% for all data. The goodness-of-fit was 1.086. The largest peak in the final difference electron density synthesis was 0.275 $e^-/Å^3$ and the largest hole was -0.283 $e^-/Å^3$ with an RMS

deviation of 0.057 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.256 g/cm^3 and F(000), 952 e^-.

Sample and crystal data for compound C1

Identification code	mazza2203_bis_	
Chemical formula	$C_{29}H_{25}BF_3N$	
Formula weight	455.31 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.220 x 0.250 x 0.300 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 18.422(9) Å	α = 90°
	b = 16.459(8) Å	β = 99.72(2)°
	c = 8.059(4) Å	γ = 90°
Volume	2408.(2) $Å^3$	
Z	4	
Density (calculated)	1.256 g/cm^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	952	

Data collection and structure refinement for Compound C1.

Theta range for data collection	1.67 to 25.00°
Index ranges	-21<=h<=21, -19<=k<=19, -9<=l<=9
Reflections collected	27037
Independent reflections	4179 [R(int) = 0.0531]
Coverage of independent reflections	98.4%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9810 and 0.9740
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2017/1 (Sheldrick, 2017)

Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	4179 / 0 / 311	
Goodness-of-fit on F^2	1.086	
Δ/σ_{max}	0.044	
Final R indices	3791 data; I>2σ(I)	R1 = 0.0961, wR2 = 0.2420
	all data	R1 = 0.1013, wR2 = 0.2446
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0587P)^2+6.2251P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.275 and -0.283 eÅ^{-3}	
R.M.S. deviation from mean	0.057 eÅ^{-3}	

Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for Compound C1.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
N1	0.24457(16)	0.55726(19)	0.6009(4)	0.0403(7)
C002	0.2030(2)	0.4617(2)	0.3413(5)	0.0394(9)
C003	0.1841(2)	0.6550(2)	0.7326(5)	0.0395(8)
C004	0.2625(2)	0.6608(2)	0.7987(4)	0.0398(9)
C005	0.1748(2)	0.5927(2)	0.6129(5)	0.0393(8)
C006	0.2975(2)	0.6008(2)	0.7179(5)	0.0403(9)
C007	0.3254(2)	0.4291(3)	0.5833(5)	0.0516(11)
C008	0.1829(2)	0.5190(2)	0.2110(5)	0.0449(9)
C009	0.1729(2)	0.3823(2)	0.3138(5)	0.0451(9)
F1	0.3662(2)	0.5227(3)	0.3244(6)	0.1300(17)
C00B	0.1230(2)	0.6964(3)	0.7740(6)	0.0533(11)
C00C	0.3027(3)	0.7122(3)	0.9162(5)	0.0535(11)
C00D	0.1238(2)	0.3652(3)	0.1682(5)	0.0507(10)
C00E	0.1033(2)	0.4216(3)	0.0427(5)	0.0542(11)
C00F	0.1342(2)	0.4980(3)	0.0660(5)	0.0537(11)
B1	0.2574(2)	0.4859(3)	0.5069(6)	0.0413(10)
C00H	0.1047(2)	0.5705(3)	0.5335(6)	0.0529(11)
C00I	0.0542(3)	0.6755(3)	0.6924(7)	0.0653(13)

	x/a	y/b	z/c	U(eq)
F3	0.4607(2)	0.4526(4)	0.3140(6)	0.167(2)
C00K	0.3237(3)	0.3920(3)	0.7420(6)	0.0635(13)
C00L	0.0451(2)	0.6134(3)	0.5728(7)	0.0639(13)
C00M	0.3844(3)	0.4102(3)	0.5042(6)	0.0671(14)
C00N	0.3742(2)	0.5933(3)	0.7509(6)	0.0578(12)
C00O	0.2132(3)	0.6049(3)	0.2185(6)	0.0712(15)
C00P	0.3782(3)	0.7030(3)	0.9529(6)	0.0643(13)
F2	0.3548(3)	0.4084(4)	0.2129(5)	0.161(2)
C00R	0.2633(3)	0.4099(4)	0.8407(6)	0.0786(16)
C00S	0.0501(3)	0.4008(4)	0.8827(7)	0.0854(18)
C00T	0.1891(3)	0.3147(3)	0.4422(7)	0.0796(17)
C00U	0.4130(3)	0.6446(3)	0.8706(7)	0.0705(14)
C00V	0.4403(3)	0.3558(4)	0.5748(10)	0.100(2)
C00W	0.3779(4)	0.3375(4)	0.8080(8)	0.099(2)
C00X	0.3924(3)	0.4485(5)	0.3423(8)	0.095(2)
C00Y	0.4351(4)	0.3198(5)	0.7262(11)	0.118(3)

Bond lengths (Å) for Compound C1.

N1-C005	1.429(5)	N1-C006	1.429(5)
N1-B1	1.439(5)	C002-C008	1.413(5)
C002-C009	1.422(5)	C002-B1	1.578(6)
C003-C005	1.399(5)	C003-C00B	1.404(6)
C003-C004	1.455(5)	C004-C00C	1.386(6)
C004-C006	1.400(5)	C005-C00H	1.390(6)
C006-C00N	1.399(6)	C007-C00M	1.386(6)
C007-C00K	1.423(7)	C007-B1	1.600(6)
C008-C00F	1.391(6)	C008-C00O	1.518(6)
C009-C00D	1.384(6)	C009-C00T	1.514(6)
F1-C00X	1.312(8)	C00B-C00I	1.369(7)
C00B-H00B	0.93	C00C-C00P	1.380(6)
C00C-H00C	0.93	C00D-C00E	1.377(6)

C00D-H00D	0.93	C00E-C00F	1.380(6)
C00E-C00S	1.521(6)	C00F-H00F	0.93
C00H-C00L	1.387(6)	C00H-H00H	0.93
C00I-C00L	1.396(7)	C00I-H00I	0.93
F3-C00X	1.319(7)	C00K-C00W	1.380(7)
C00K-C00R	1.502(8)	C00L-H00L	0.93
C00M-C00V	1.409(8)	C00M-C00X	1.478(9)
C00N-C00U	1.387(6)	C00N-H00N	0.93
C00O-H00A	0.96	C00O-H00E	0.96
C00O-H00G	0.96	C00P-C00U	1.385(7)
C00P-H00P	0.93	F2-C00X	1.326(7)
C00R-H00*J*	0.96	C00R-H00K	0.96
C00R-H00M	0.96	C00S-H00O	0.96
C00S-H00Q	0.96	C00S-H00R	0.96
C00T-H00S	0.96	C00T-H00T	0.96
C00T-H00U	0.96	C00U-H00V	0.93
C00V-C00Y	1.374(11)	C00V-H00W	0.93
C00W-C00Y	1.366(11)	C00W-H00$	0.93
C00Y-H00Y	0.93		

Bond angles (°) for Compound C1.

C005-N1-C006	105.8(3)	C005-N1-B1	126.7(3)
C006-N1-B1	127.0(3)	C008-C002-C009	116.8(3)
C008-C002-B1	120.7(3)	C009-C002-B1	122.5(3)
C005-C003-C00B	120.6(4)	C005-C003-C004	107.4(3)
C00B-C003-C004	131.9(4)	C00C-C004-C006	120.8(4)
C00C-C004-C003	132.3(4)	C006-C004-C003	106.9(3)
C00H-C005-C003	120.4(4)	C00H-C005-N1	129.6(4)
C003-C005-N1	109.8(3)	C00N-C006-C004	120.3(4)
C00N-C006-N1	129.5(4)	C004-C006-N1	110.1(3)
C00M-C007-C00K	117.0(4)	C00M-C007-B1	125.4(4)
C00K-C007-B1	117.5(4)	C00F-C008-C002	120.7(4)

C00F-C008-C00O	116.4(4)	C002-C008-C00O	122.9(4)
C00D-C009-C002	120.0(4)	C00D-C009-C00T	117.1(4)
C002-C009-C00T	122.8(4)	C00I-C00B-C003	118.6(4)
C00I-C00B-H00B	120.7	C003-C00B-H00B	120.7
C00P-C00C-C004	118.9(4)	C00P-C00C-H00C	120.6
C004-C00C-H00C	120.6	C00E-C00D-C009	123.0(4)
C00E-C00D-H00D	118.5	C009-C00D-H00D	118.5
C00D-C00E-C00F	117.3(4)	C00D-C00E-C00S	121.9(5)
C00F-C00E-C00S	120.8(5)	C00E-C00F-C008	122.2(4)
C00E-C00F-H00F	118.9	C008-C00F-H00F	118.9
N1-B1-C002	120.9(3)	N1-B1-C007	117.5(3)
C002-B1-C007	121.5(3)	C00L-C00H-C005	118.2(4)
C00L-C00H-H00H	120.9	C005-C00H-H00H	120.9
C00B-C00I-C00L	120.6(4)	C00B-C00I-H00I	119.7
C00L-C00I-H00I	119.7	C00W-C00K-C007	120.1(6)
C00W-C00K-C00R	118.4(5)	C007-C00K-C00R	121.5(4)
C00H-C00L-C00I	121.5(4)	C00H-C00L-H00L	119.2
C00I-C00L-H00L	119.2	C007-C00M-C00V	122.2(6)
C007-C00M-C00X	120.8(5)	C00V-C00M-C00X	116.9(5)
C00U-C00N-C006	117.6(4)	C00U-C00N-H00N	121.2
C006-C00N-H00N	121.2	C008-C00O-H00A	109.5
C008-C00O-H00E	109.5	H00A-C00O-H00E	109.5
C008-C00O-H00G	109.5	H00A-C00O-H00G	109.5
H00E-C00O-H00G	109.5	C00C-C00P-C00U	120.3(4)
C00C-C00P-H00P	119.9	C00U-C00P-H00P	119.9
C00K-C00R-H00*J*	109.5	C00K-C00R-H00K	109.5
H00*J*-C00R-H00K	109.5	C00K-C00R-H00M	109.5
H00*J*-C00R-H00M	109.5	H00K-C00R-H00M	109.5
C00E-C00S-H00O	109.5	C00E-C00S-H00Q	109.5
H00O-C00S-H00Q	109.5	C00E-C00S-H00R	109.5
H00O-C00S-H00R	109.5	H00Q-C00S-H00R	109.5
C009-C00T-H00S	109.5	C009-C00T-H00T	109.5

H00S-C00T-H00T	109.5	C009-C00T-H00U	109.5
H00S-C00T-H00U	109.5	H00T-C00T-H00U	109.5
C00N-C00U-C00P	122.0(4)	C00N-C00U-H00V	119.0
C00P-C00U-H00V	119.0	C00Y-C00V-C00M	118.5(6)
C00Y-C00V-H00W	120.7	C00M-C00V-H00W	120.7
C00Y-C00W-C00K	121.3(7)	C00Y-C00W-H00$	119.3
C00K-C00W-H00$	119.3	F1-C00X-F3	106.1(7)
F1-C00X-F2	104.1(6)	F3-C00X-F2	106.0(5)
F1-C00X-C00M	113.9(5)	F3-C00X-C00M	114.5(6)
F2-C00X-C00M	111.4(7)	C00W-C00Y-C00V	120.7(6)
C00W-C00Y-H00Y	119.6	C00V-C00Y-H00Y	119.6

Torsion angles (°) for Compound C1.

C005-C003-C004-C00C	178.6(4)	C00B-C003-C004-C00C	-4.6(7)
C005-C003-C004-C006	-0.9(4)	C00B-C003-C004-C006	176.0(4)
C00B-C003-C005-C00H	-0.3(6)	C004-C003-C005-C00H	177.0(4)
C00B-C003-C005-N1	-176.5(3)	C004-C003-C005-N1	0.8(4)
C006-N1-C005-C00H	-176.1(4)	B1-N1-C005-C00H	-3.4(6)
C006-N1-C005-C003	-0.4(4)	B1-N1-C005-C003	172.4(4)
C00C-C004-C006-C00N	-2.0(6)	C003-C004-C006-C00N	177.5(4)
C00C-C004-C006-N1	-178.9(3)	C003-C004-C006-N1	0.7(4)
C005-N1-C006-C00N	-176.7(4)	B1-N1-C006-C00N	10.6(7)
C005-N1-C006-C004	-0.2(4)	B1-N1-C006-C004	-172.9(4)
C009-C002-C008-C00F	1.9(6)	B1-C002-C008-C00F	-179.1(4)
C009-C002-C008-C00O	-177.1(4)	B1-C002-C008-C00O	1.9(6)
C008-C002-C009-C00D	-2.9(6)	B1-C002-C009-C00D	178.2(4)
C008-C002-C009-C00T	-179.7(4)	B1-C002-C009-C00T	1.4(6)
C005-C003-C00B-C00I	-1.2(6)	C004-C003-C00B-C00I	-177.7(4)
C006-C004-C00C-C00P	-0.2(6)	C003-C004-C00C-C00P	-179.6(4)
C002-C009-C00D-C00E	1.9(6)	C00T-C009-C00D-C00E	178.9(5)
C009-C00D-C00E-C00F	0.3(6)	C009-C00D-C00E-C00S	179.1(4)
C00D-C00E-C00F-C008	-1.3(7)	C00S-C00E-C00F-C008	179.9(4)

C002-C008-C00F-C00E	0.2(6)	C00O-C008-C00F-C00E	179.3(4)
C005-N1-B1-C002	29.7(6)	C006-N1-B1-C002	-159.0(4)
C005-N1-B1-C007	-146.2(4)	C006-N1-B1-C007	25.0(6)
C008-C002-B1-N1	51.4(5)	C009-C002-B1-N1	-129.7(4)
C008-C002-B1-C007	-132.8(4)	C009-C002-B1-C007	46.1(5)
C00M-C007-B1-N1	-120.7(5)	C00K-C007-B1-N1	62.3(5)
C00M-C007-B1-C002	63.4(6)	C00K-C007-B1-C002	-113.7(4)
C003-C005-C00H-C00L	1.9(6)	N1-C005-C00H-C00L	177.2(4)
C003-C00B-C00I-C00L	1.1(7)	C00M-C007-C00K-C00W	-2.3(7)
B1-C007-C00K-C00W	175.0(5)	C00M-C007-C00K-C00R	178.3(5)
B1-C007-C00K-C00R	-4.4(7)	C005-C00H-C00L-C00I	-1.9(7)
C00B-C00I-C00L-C00H	0.4(8)	C00K-C007-C00M-C00V	0.9(7)
B1-C007-C00M-C00V	-176.1(5)	C00K-C007-C00M-C00X	-177.5(5)
B1-C007-C00M-C00X	5.5(7)	C004-C006-C00N-C00U	2.8(7)
N1-C006-C00N-C00U	179.0(4)	C004-C00C-C00P-C00U	1.4(7)
C006-C00N-C00U-C00P	-1.6(8)	C00C-C00P-C00U-C00N	-0.5(9)
C007-C00M-C00V-C00Y	0.7(9)	C00X-C00M-C00V-C00Y	179.2(6)
C007-C00K-C00W-C00Y	2.0(9)	C00R-C00K-C00W-C00Y	-178.6(6)
C007-C00M-C00X-F1	31.6(8)	C00V-C00M-C00X-F1	-146.9(5)
C007-C00M-C00X-F3	154.0(6)	C00V-C00M-C00X-F3	-24.5(9)
C007-C00M-C00X-F2	-85.7(7)	C00V-C00M-C00X-F2	95.8(6)
C00K-C00W-C00Y-C00V	-0.2(11)	C00M-C00V-C00Y-C00W	-1.1(11)

Anisotropic atomic displacement parameters (Å^2) for Compound C1.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	0.0352(16)	0.0451(18)	0.0390(17)	-0.0054(14)	0.0021(13)	0.0015(13)
C002	0.0374(19)	0.039(2)	0.042(2)	-0.0035(16)	0.0084(16)	0.0026(16)
C003	0.047(2)	0.0335(19)	0.040(2)	0.0061(16)	0.0108(16)	0.0031(16)
C004	0.051(2)	0.0362(19)	0.0327(18)	0.0021(15)	0.0088(16)	0.0007(16)
C005	0.041(2)	0.038(2)	0.040(2)	0.0034(16)	0.0105(16)	0.0037(16)
C006	0.040(2)	0.043(2)	0.0373(19)	-0.0005(16)	0.0052(16)	-0.0025(16)

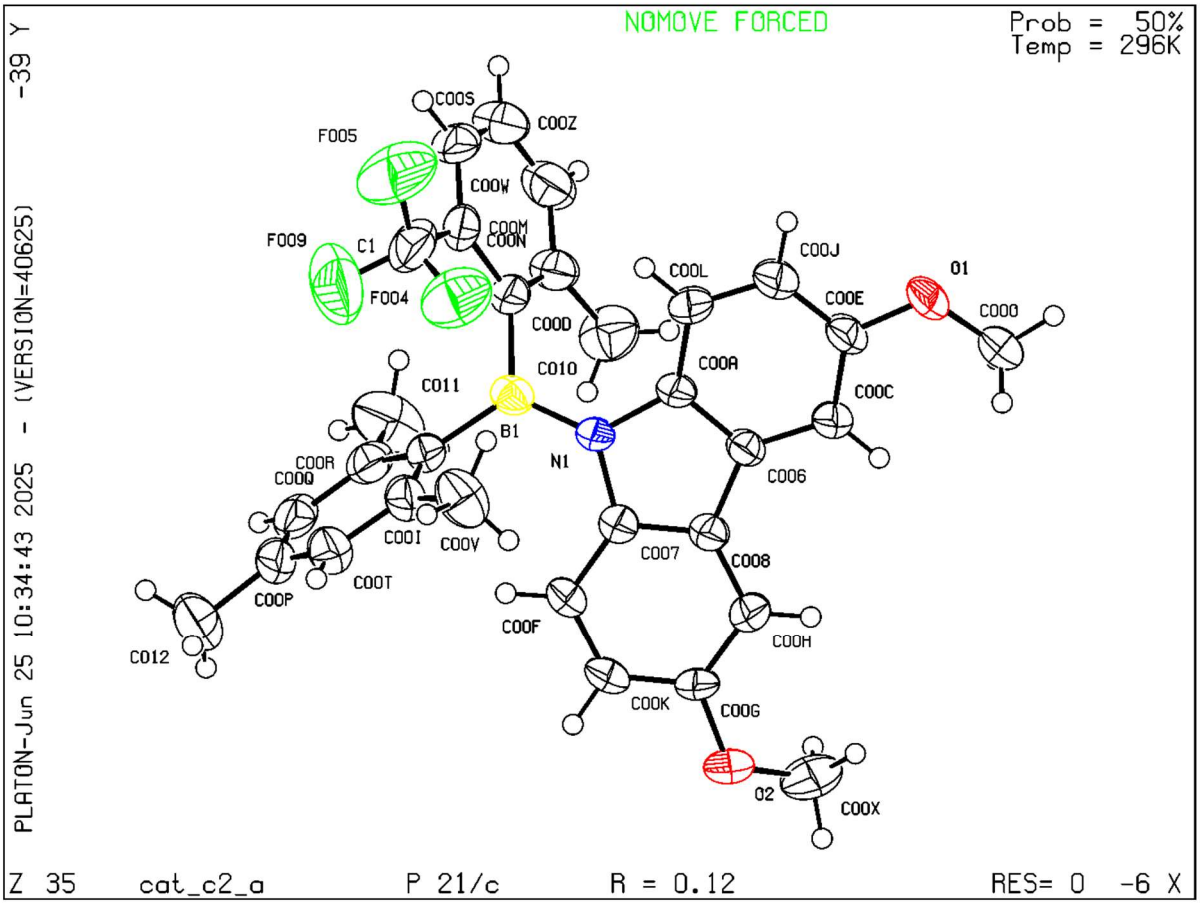
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C007	0.046(2)	0.054(2)	0.051(2)	-0.018(2)	-0.0053(19)	0.0092(19)
C008	0.051(2)	0.044(2)	0.041(2)	-0.0024(17)	0.0107(17)	0.0019(18)
C009	0.048(2)	0.039(2)	0.048(2)	-0.0039(17)	0.0095(18)	0.0010(17)
F1	0.121(3)	0.160(4)	0.126(3)	0.041(3)	0.073(3)	0.029(3)
C00B	0.062(3)	0.044(2)	0.057(3)	0.0010(19)	0.020(2)	0.008(2)
C00C	0.066(3)	0.043(2)	0.051(2)	-0.0097(19)	0.011(2)	-0.001(2)
C00D	0.049(2)	0.047(2)	0.058(3)	-0.018(2)	0.012(2)	-0.0077(19)
C00E	0.044(2)	0.069(3)	0.046(2)	-0.011(2)	-0.0025(19)	0.003(2)
C00F	0.062(3)	0.058(3)	0.040(2)	0.0011(19)	0.0044(19)	0.008(2)
B1	0.039(2)	0.043(2)	0.043(2)	-0.0004(19)	0.0122(19)	-0.0006(19)
C00H	0.043(2)	0.057(3)	0.058(3)	-0.007(2)	0.0064(19)	0.0004(19)
C00I	0.048(3)	0.061(3)	0.091(4)	0.000(3)	0.026(2)	0.017(2)
F3	0.070(2)	0.306(7)	0.138(4)	-0.019(4)	0.054(3)	0.015(3)
C00K	0.071(3)	0.055(3)	0.055(3)	-0.007(2)	-0.016(2)	0.012(2)
C00L	0.037(2)	0.077(3)	0.078(3)	-0.002(3)	0.008(2)	0.005(2)
C00M	0.050(3)	0.084(4)	0.065(3)	-0.036(3)	0.002(2)	0.012(2)
C00N	0.041(2)	0.066(3)	0.065(3)	-0.021(2)	0.005(2)	-0.001(2)
C00O	0.105(4)	0.049(3)	0.058(3)	0.010(2)	0.009(3)	-0.014(3)
C00P	0.065(3)	0.067(3)	0.055(3)	-0.018(2)	-0.008(2)	-0.012(2)
F2	0.159(4)	0.249(6)	0.072(3)	-0.061(3)	0.010(3)	-0.025(4)
C00R	0.103(4)	0.079(4)	0.052(3)	0.016(3)	0.009(3)	0.007(3)
C00S	0.075(4)	0.108(5)	0.063(3)	-0.020(3)	-0.017(3)	-0.004(3)
C00T	0.112(5)	0.042(3)	0.078(4)	0.007(2)	-0.004(3)	-0.015(3)
C00U	0.048(3)	0.079(3)	0.080(3)	-0.027(3)	-0.004(2)	-0.008(2)
C00V	0.059(3)	0.121(6)	0.109(5)	-0.056(5)	-0.014(3)	0.040(3)
C00W	0.110(5)	0.088(4)	0.081(4)	-0.009(3)	-0.030(4)	0.036(4)
C00X	0.052(3)	0.153(7)	0.083(4)	-0.035(4)	0.017(3)	0.015(4)
C00Y	0.102(5)	0.110(6)	0.118(6)	-0.032(5)	-0.049(5)	0.054(4)

Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for Compound C1.

	x/a	y/b	z/c	U(eq)

H00B	0.1290	0.7372	0.8550	0.064
H00C	0.2792	0.7521	0.9693	0.064
H00D	0.1038	0.3133	0.1544	0.061
H00F	0.1220	0.5368	-0.0180	0.064
H00H	0.0980	0.5281	0.4561	0.063
H00I	0.0131	0.7030	0.7168	0.078
H00L	-0.0021	0.6004	0.5183	0.077
H00N	0.3984	0.5552	0.6945	0.069
H00A	0.2432	0.6118	0.1328	0.107
H00E	0.2426	0.6143	0.3270	0.107
H00G	0.1732	0.6430	0.2003	0.107
H00P	0.4058	0.7362	1.0333	0.077
H00*J*	0.2607	0.3669	0.9200	0.118
H00K	0.2172	0.4140	0.7653	0.118
H00M	0.2735	0.4603	0.9001	0.118
H00O	0.0748	0.4058	-0.2125	0.128
H00Q	0.0090	0.4374	-0.1299	0.128
H00R	0.0330	0.3460	-0.1103	0.128
H00S	0.1604	0.2677	0.4030	0.119
H00T	0.1767	0.3323	0.5475	0.119
H00U	0.2406	0.3013	0.4575	0.119
H00V	0.4640	0.6397	0.8965	0.085
H00W	0.4797	0.3445	0.5201	0.12
H00$	0.3754	0.3123	0.9101	0.118
H00Y	0.4710	0.2830	0.7736	0.141

9.1.2 X-Ray Crystallography of C2



A specimen of $C_{31}H_{29}BF_3NO_2$, approximate dimensions 0.090 mm x 0.120 mm x 0.150 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The total exposure time was 20.33 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 27700 reflections to a maximum θ angle of 25.00° (0.84 Å resolution), of which 4640 were independent (average redundancy 5.970, completeness = 99.9%, R_{int} = 9.78%, R_{sig} = 6.53%) and 3365 (72.52%) were greater than $2\sigma(F^2)$. The final cell constants of a = 15.580(4) Å, b = 11.120(3) Å, c = 15.222(4) Å, β = 91.099(5)°, volume = 2636.7(10) $Å^3$, are based upon the refinement of the XYZ-centroids of 4630 reflections above 20 σ(I) with 4.500° < 2θ < 50.11°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.766. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9860 and 0.9920. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z = 4 for the formula unit, $C_{31}H_{29}BF_3NO_2$. The final anisotropic full-matrix least-squares refinement on $F^2$with 349 variables converged at R1 = 11.57%, for the observed data and wR2 = 25.94% for all data. The goodness-of-fit was 1.169. The largest peak in the final difference electron density synthesis was 0.239 $e^-/Å^3$ and the largest hole was -0.249 $e^-/Å^3$ with an RMS deviation of 0.057 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.298 g/cm^3 and F(000), 1080 e^-.

Sample and crystal data for C2.

Identification code	mazza2507ABS	
Chemical formula	$C_{31}H_{29}BF_3NO_2$	
Formula weight	515.36 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.090 x 0.120 x 0.150 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 15.580(4) Å	α = 90°
	b = 11.120(3) Å	β = 91.099(5)°
	c = 15.222(4) Å	γ = 90°
Volume	2636.7(10) $Å^3$	
Z	4	
Density (calculated)	1.298 g/cm^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	1080	

Data collection and structure refinement for C2.

Theta range for data collection	2.25 to 25.00°
Index ranges	-18<=h<=18, -13<=k<=13, -18<=l<=18
Reflections collected	27700
Independent reflections	4640 [R(int) = 0.0978]
Coverage of independent reflections	99.9%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9920 and 0.9860
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2017/1 (Sheldrick, 2017)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4640 / 0 / 349

Goodness-of-fit on F^2	1.169	
Final R indices	3365 data; I>2σ(I)	R1 = 0.1157, wR2 = 0.2407
	all data	R1 = 0.1504, wR2 = 0.2594
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0795P)^2+4.5259P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.239 and -0.249 eÅ^{-3}	
R.M.S. deviation from mean	0.057 eÅ^{-3}	

Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for C2.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
O1	0.3920(2)	0.7787(3)	0.6137(3)	0.0627(11)
N1	0.2735(2)	0.3452(3)	0.4794(2)	0.0399(9)
O2	0.5441(3)	0.0949(3)	0.6369(3)	0.0788(14)
F004	0.0479(2)	0.3866(4)	0.4556(3)	0.0970(13)
F005	0.9591(3)	0.4689(5)	0.3683(3)	0.1240(18)
C006	0.3727(3)	0.4589(4)	0.5568(3)	0.0382(11)
C007	0.3376(3)	0.2672(4)	0.5170(3)	0.0404(11)
C008	0.3994(3)	0.3349(4)	0.5610(3)	0.0384(11)
F009	0.0053(3)	0.2925(4)	0.3431(4)	0.1277(19)
C00A	0.2959(3)	0.4628(4)	0.5096(3)	0.0386(11)
C00B	0.1818(3)	0.1802(4)	0.4004(3)	0.0444(12)
C00C	0.4089(3)	0.5633(4)	0.5929(3)	0.0463(12)
C00D	0.1870(3)	0.4175(4)	0.3413(3)	0.0461(12)
C00E	0.3637(3)	0.6701(4)	0.5825(3)	0.0468(12)
C00F	0.3465(3)	0.1425(4)	0.5129(4)	0.0523(14)
C00G	0.4790(3)	0.1578(4)	0.5971(3)	0.0493(13)
C00H	0.4712(3)	0.2820(4)	0.6013(3)	0.0469(12)
C00I	0.1427(3)	0.1220(5)	0.4701(4)	0.0506(13)
C00J	0.2852(3)	0.6707(5)	0.5385(4)	0.0548(14)
C00K	0.4170(3)	0.0911(4)	0.5535(4)	0.0530(14)
C00L	0.2489(3)	0.5693(4)	0.5030(4)	0.0501(13)

	x/a	y/b	z/c	U(eq)
C00M	0.1018(3)	0.4521(5)	0.3216(4)	0.0531(14)
C00N	0.2502(4)	0.4732(5)	0.2912(4)	0.0551(14)
C00O	0.4770(4)	0.7844(5)	0.6472(4)	0.0612(15)
C00P	0.1280(4)	0.9381(5)	0.3868(5)	0.0661(17)
C00Q	0.1665(4)	0.9946(5)	0.3178(5)	0.0684(19)
C00R	0.1938(3)	0.1144(5)	0.3225(3)	0.0551(14)
C00S	0.0816(4)	0.5343(5)	0.2563(4)	0.0665(17)
C00T	0.1153(4)	0.0025(5)	0.4620(4)	0.0635(16)
C1	0.0298(4)	0.3997(7)	0.3705(5)	0.0721(18)
C00V	0.1300(4)	0.1782(6)	0.5592(4)	0.0723(18)
C00W	0.2284(5)	0.5555(5)	0.2265(4)	0.0722(17)
C00X	0.6239(4)	0.1492(6)	0.6497(5)	0.081(2)
B1	0.2139(3)	0.3145(5)	0.4107(4)	0.0417(13)
C00Z	0.1459(5)	0.5864(6)	0.2091(5)	0.0766(19)
C010	0.3445(4)	0.4463(6)	0.3034(4)	0.0770(19)
C011	0.2401(5)	0.1645(6)	0.2451(4)	0.095(2)
C012	0.1038(5)	0.8065(6)	0.3804(6)	0.106(3)

Bond lengths (Å) for C2.

O1-C00E	1.369(6)	O1-C00O	1.412(6)
N1-B1	1.426(7)	N1-C00A	1.427(6)
N1-C007	1.434(6)	O2-C00G	1.363(6)
O2-C00X	1.393(7)	F004-C1	1.327(7)
F005-C1	1.343(7)	C006-C00A	1.385(6)
C006-C00C	1.399(6)	C006-C008	1.441(6)
C007-C008	1.385(6)	C007-C00F	1.395(7)
C008-C00H	1.395(6)	F009-C1	1.317(8)
C00A-C00L	1.396(6)	C00B-C00I	1.394(7)
C00B-C00R	1.408(7)	C00B-B1	1.583(7)
C00C-C00E	1.388(6)	C00C-H00C	0.93
C00D-C00N	1.401(7)	C00D-C00M	1.408(7)

C00D-B1	1.608(7)	C00E-C00*J*	1.384(7)
C00F-C00K	1.374(7)	C00F-H00F	0.93
C00G-C00K	1.378(7)	C00G-C00H	1.388(7)
C00H-H00H	0.93	C00I-C00T	1.400(8)
C00I-C00V	1.509(8)	C00*J*-C00L	1.367(7)
C00*J*-H00*J*	0.93	C00K-H00K	0.93
C00L-H00L	0.93	C00M-C00S	1.383(8)
C00M-C1	1.478(9)	C00N-C00W	1.383(8)
C00N-C010	1.508(8)	C00O-H00A	0.96
C00O-H00B	0.96	C00O-H00D	0.96
C00P-C00T	1.368(9)	C00P-C00Q	1.373(9)
C00P-C012	1.513(8)	C00Q-C00R	1.400(8)
C00Q-H00Q	0.93	C00R-C011	1.501(8)
C00S-C00Z	1.372(9)	C00S-H00S	0.93
C00T-H00T	0.93	C00V-H00E	0.96
C00V-H00G	0.96	C00V-H00I	0.96
C00W-C00Z	1.351(9)	C00W-H00W	0.93
C00X-H00M	0.96	C00X-H00N	0.96
C00X-H00O	0.96	C00Z-H00Z	0.93
C010-H01A	0.96	C010-H01B	0.96
C010-H01C	0.96	C011-H01D	0.96
C011-H01E	0.96	C011-H01F	0.96
C012-H01G	0.96	C012-H01H	0.96
C012-H01I	0.96		

Bond angles (°) for C2.

C00E-O1-C00O	117.3(4)	B1-N1-C00A	127.4(4)
B1-N1-C007	125.9(4)	C00A-N1-C007	105.2(3)
C00G-O2-C00X	119.6(5)	C00A-C006-C00C	121.1(4)
C00A-C006-C008	107.4(4)	C00C-C006-C008	131.5(4)

C008-C007-C00F	119.5(4)	C008-C007-N1	109.7(4)
C00F-C007-N1	130.8(4)	C007-C008-C00H	121.8(4)
C007-C008-C006	107.5(4)	C00H-C008-C006	130.7(4)
C006-C00A-C00L	120.7(4)	C006-C00A-N1	110.0(4)
C00L-C00A-N1	129.0(4)	C00I-C00B-C00R	117.8(5)
C00I-C00B-B1	120.3(4)	C00R-C00B-B1	121.9(5)
C00E-C00C-C006	117.7(4)	C00E-C00C-H00C	121.2
C006-C00C-H00C	121.2	C00N-C00D-C00M	115.6(5)
C00N-C00D-B1	119.7(4)	C00M-C00D-B1	124.6(5)
O1-C00E-C00*J*	116.1(4)	O1-C00E-C00C	123.8(4)
C00*J*-C00E-C00C	120.2(4)	C00K-C00F-C007	118.3(5)
C00K-C00F-H00F	120.9	C007-C00F-H00F	120.9
O2-C00G-C00K	116.5(4)	O2-C00G-C00H	123.7(5)
C00K-C00G-C00H	119.8(4)	C00G-C00H-C008	118.1(5)
C00G-C00H-H00H	121.0	C008-C00H-H00H	121.0
C00B-C00I-C00T	120.7(5)	C00B-C00I-C00V	124.0(5)
C00T-C00I-C00V	115.3(5)	C00L-C00*J*-C00E	122.8(5)
C00L-C00*J*-H00*J*	118.6	C00E-C00*J*-H00*J*	118.6
C00F-C00K-C00G	122.6(5)	C00F-C00K-H00K	118.7
C00G-C00K-H00K	118.7	C00*J*-C00L-C00A	117.4(4)
C00*J*-C00L-H00L	121.3	C00A-C00L-H00L	121.3
C00S-C00M-C00D	122.4(6)	C00S-C00M-C1	117.2(5)
C00D-C00M-C1	120.4(5)	C00W-C00N-C00D	121.0(5)
C00W-C00N-C010	116.4(6)	C00D-C00N-C010	122.6(5)
O1-C00O-H00A	109.5	O1-C00O-H00B	109.5
H00A-C00O-H00B	109.5	O1-C00O-H00D	109.5
H00A-C00O-H00D	109.5	H00B-C00O-H00D	109.5
C00T-C00P-C00Q	118.2(6)	C00T-C00P-C012	121.4(7)
C00Q-C00P-C012	120.3(7)	C00P-C00Q-C00R	122.2(6)
C00P-C00Q-H00Q	118.9	C00R-C00Q-H00Q	118.9
C00Q-C00R-C00B	119.5(6)	C00Q-C00R-C011	117.6(6)
C00B-C00R-C011	122.7(5)	C00Z-C00S-C00M	119.8(6)

C00Z-C00S-H00S	120.1	C00M-C00S-H00S	120.1
C00P-C00T-C00I	121.5(6)	C00P-C00T-H00T	119.2
C00I-C00T-H00T	119.2	F009-C1-F004	105.4(6)
F009-C1-F005	106.1(5)	F004-C1-F005	104.2(6)
F009-C1-C00M	114.6(6)	F004-C1-C00M	112.7(5)
F005-C1-C00M	113.0(6)	C00I-C00V-H00E	109.5
C00I-C00V-H00G	109.5	H00E-C00V-H00G	109.5
C00I-C00V-H00I	109.5	H00E-C00V-H00I	109.5
H00G-C00V-H00I	109.5	C00Z-C00W-C00N	121.8(7)
C00Z-C00W-H00W	119.1	C00N-C00W-H00W	119.1
O2-C00X-H00M	109.5	O2-C00X-H00N	109.5
H00M-C00X-H00N	109.5	O2-C00X-H00O	109.5
H00M-C00X-H00O	109.5	H00N-C00X-H00O	109.5
N1-B1-C00B	119.9(4)	N1-B1-C00D	118.0(4)
C00B-B1-C00D	121.9(4)	C00W-C00Z-C00S	119.4(6)
C00W-C00Z-H00Z	120.3	C00S-C00Z-H00Z	120.3
C00N-C010-H01A	109.5	C00N-C010-H01B	109.5
H01A-C010-H01B	109.5	C00N-C010-H01C	109.5
H01A-C010-H01C	109.5	H01B-C010-H01C	109.5
C00R-C011-H01D	109.5	C00R-C011-H01E	109.5
H01D-C011-H01E	109.5	C00R-C011-H01F	109.5
H01D-C011-H01F	109.5	H01E-C011-H01F	109.5
C00P-C012-H01G	109.5	C00P-C012-H01H	109.5
H01G-C012-H01H	109.5	C00P-C012-H01I	109.5
H01G-C012-H01I	109.5	H01H-C012-H01I	109.5

Torsion angles (°) for C2.

B1-N1-C007-C008	161.7(4)	C00A-N1-C007-C008	-4.9(5)
B1-N1-C007-C00F	-16.2(8)	C00A-N1-C007-C00F	177.2(5)
C00F-C007-C008-C00H	0.4(8)	N1-C007-C008-C00H	-177.7(4)
C00F-C007-C008-C006	-178.4(5)	N1-C007-C008-C006	3.5(5)

C00A-C006-C008-C007	-0.6(5)	C00C-C006-C008-C007	177.1(5)
C00A-C006-C008-C00H	-179.2(5)	C00C-C006-C008-C00H	-1.6(9)
C00C-C006-C00A-C00L	-5.4(7)	C008-C006-C00A-C00L	172.5(5)
C00C-C006-C00A-N1	179.5(4)	C008-C006-C00A-N1	-2.6(5)
B1-N1-C00A-C006	-161.8(5)	C007-N1-C00A-C006	4.6(5)
B1-N1-C00A-C00L	23.6(8)	C007-N1-C00A-C00L	-170.0(5)
C00A-C006-C00C-C00E	2.3(7)	C008-C006-C00C-C00E	-175.1(5)
C00O-O1-C00E-C00*J*	-170.8(5)	C00O-O1-C00E-C00C	9.2(8)
C006-C00C-C00E-O1	-179.4(5)	C006-C00C-C00E-C00*J*	0.7(8)
C008-C007-C00F-C00K	0.2(8)	N1-C007-C00F-C00K	177.8(5)
C00X-O2-C00G-C00K	153.4(6)	C00X-O2-C00G-C00H	-28.9(9)
O2-C00G-C00H-C008	-177.1(5)	C00K-C00G-C00H-C008	0.5(8)
C007-C008-C00H-C00G	-0.7(8)	C006-C008-C00H-C00G	177.8(5)
C00R-C00B-C00I-C00T	-0.8(7)	B1-C00B-C00I-C00T	-179.0(5)
C00R-C00B-C00I-C00V	176.4(5)	B1-C00B-C00I-C00V	-1.8(8)
O1-C00E-C00*J*-C00L	179.5(5)	C00C-C00E-C00*J*-C00L	-0.6(9)
C007-C00F-C00K-C00G	-0.4(9)	O2-C00G-C00K-C00F	177.9(5)
C00H-C00G-C00K-C00F	0.1(9)	C00E-C00*J*-C00L-C00A	-2.4(8)
C006-C00A-C00L-C00*J*	5.4(8)	N1-C00A-C00L-C00*J*	179.4(5)
C00N-C00D-C00M-C00S	0.9(7)	B1-C00D-C00M-C00S	-174.6(5)
C00N-C00D-C00M-C1	-179.7(5)	B1-C00D-C00M-C1	4.7(8)
C00M-C00D-C00N-C00W	-0.7(8)	B1-C00D-C00N-C00W	175.1(5)
C00M-C00D-C00N-C010	-179.7(5)	B1-C00D-C00N-C010	-3.9(8)
C00T-C00P-C00Q-C00R	0.7(8)	C012-C00P-C00Q-C00R	-176.8(5)
C00P-C00Q-C00R-C00B	0.2(8)	C00P-C00Q-C00R-C011	176.3(6)
C00I-C00B-C00R-C00Q	-0.1(7)	B1-C00B-C00R-C00Q	178.1(4)
C00I-C00B-C00R-C011	-176.0(5)	B1-C00B-C00R-C011	2.2(8)
C00D-C00M-C00S-C00Z	-1.0(8)	C1-C00M-C00S-C00Z	179.6(6)
C00Q-C00P-C00T-C00I	-1.7(8)	C012-C00P-C00T-C00I	175.8(5)
C00B-C00I-C00T-C00P	1.8(8)	C00V-C00I-C00T-C00P	-175.7(5)
C00S-C00M-C1-F009	98.5(7)	C00D-C00M-C1-F009	-80.9(7)
C00S-C00M-C1-F004	-141.1(5)	C00D-C00M-C1-F004	39.5(8)

C00S-C00M-C1-F005	-23.3(8)	C00D-C00M-C1-F005	157.3(5)
C00D-C00N-C00W-C00Z	0.5(9)	C010-C00N-C00W-C00Z	179.6(6)
C00A-N1-B1-C00B	-166.4(4)	C007-N1-B1-C00B	30.0(7)
C00A-N1-B1-C00D	18.3(7)	C007-N1-B1-C00D	-145.4(5)
C00I-C00B-B1-N1	56.8(6)	C00R-C00B-B1-N1	-121.4(5)
C00I-C00B-B1-C00D	-128.1(5)	C00R-C00B-B1-C00D	53.8(7)
C00N-C00D-B1-N1	59.1(6)	C00M-C00D-B1-N1	-125.5(5)
C00N-C00D-B1-C00B	-116.2(5)	C00M-C00D-B1-C00B	59.2(7)
C00N-C00W-C00Z-C00S	-0.6(10)	C00M-C00S-C00Z-C00W	0.8(9)

Anisotropic atomic displacement parameters (Å^2) for C2.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.063(2)	0.0260(18)	0.098(3)	-0.0116(19)	-0.016(2)	0.0045(17)
N1	0.042(2)	0.028(2)	0.049(2)	-0.0028(17)	-0.0099(18)	0.0079(17)
O2	0.072(3)	0.044(2)	0.119(4)	0.010(2)	-0.043(3)	0.015(2)
F004	0.070(2)	0.123(4)	0.099(3)	0.014(3)	0.007(2)	0.017(2)
F005	0.060(2)	0.157(5)	0.154(4)	0.016(3)	-0.002(3)	0.041(3)
C006	0.036(2)	0.029(2)	0.049(3)	0.000(2)	0.001(2)	0.001(2)
C007	0.042(3)	0.036(3)	0.043(3)	-0.001(2)	-0.003(2)	0.002(2)
C008	0.041(3)	0.033(2)	0.041(3)	0.000(2)	0.000(2)	0.003(2)
F009	0.091(3)	0.100(4)	0.192(5)	-0.034(3)	0.000(3)	-0.033(3)
C00A	0.042(3)	0.029(2)	0.045(3)	-0.002(2)	-0.004(2)	0.008(2)
C00B	0.040(3)	0.037(3)	0.056(3)	-0.004(2)	-0.011(2)	0.004(2)
C00C	0.041(3)	0.034(3)	0.063(3)	0.001(2)	-0.009(2)	0.004(2)
C00D	0.049(3)	0.040(3)	0.049(3)	-0.006(2)	-0.013(2)	0.005(2)
C00E	0.049(3)	0.028(3)	0.063(3)	-0.006(2)	-0.001(2)	0.004(2)
C00F	0.057(3)	0.028(3)	0.071(4)	-0.005(2)	-0.014(3)	0.002(2)
C00G	0.048(3)	0.035(3)	0.064(3)	0.001(2)	-0.017(2)	0.015(2)
C00H	0.042(3)	0.043(3)	0.055(3)	-0.003(2)	-0.012(2)	0.006(2)
C00I	0.043(3)	0.044(3)	0.065(3)	-0.003(3)	-0.004(2)	-0.005(2)
C00*J*	0.053(3)	0.035(3)	0.076(4)	-0.005(3)	-0.008(3)	0.010(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C00K	0.059(3)	0.026(2)	0.073(4)	-0.002(2)	-0.009(3)	0.009(2)
C00L	0.039(3)	0.043(3)	0.068(3)	-0.003(3)	-0.011(2)	0.014(2)
C00M	0.047(3)	0.048(3)	0.064(3)	-0.012(3)	-0.017(3)	-0.001(3)
C00N	0.063(4)	0.043(3)	0.059(3)	0.003(3)	-0.004(3)	0.008(3)
C00O	0.072(4)	0.032(3)	0.079(4)	-0.007(3)	-0.013(3)	0.004(3)
C00P	0.049(3)	0.044(3)	0.104(5)	-0.009(4)	-0.026(3)	0.001(3)
C00Q	0.065(4)	0.053(4)	0.086(5)	-0.029(3)	-0.037(3)	0.026(3)
C00R	0.053(3)	0.055(3)	0.056(3)	-0.007(3)	-0.015(3)	0.014(3)
C00S	0.072(4)	0.049(3)	0.077(4)	-0.014(3)	-0.030(3)	0.026(3)
C00T	0.055(4)	0.048(3)	0.087(4)	0.004(3)	-0.009(3)	-0.007(3)
C1	0.048(4)	0.083(5)	0.084(5)	-0.014(4)	-0.022(3)	0.011(3)
C00V	0.085(5)	0.060(4)	0.073(4)	-0.002(3)	0.018(3)	-0.013(3)
C00W	0.094(5)	0.047(3)	0.075(4)	0.007(3)	-0.003(4)	-0.002(3)
C00X	0.052(4)	0.081(5)	0.109(5)	0.007(4)	-0.013(3)	0.030(3)
B1	0.035(3)	0.036(3)	0.053(3)	0.000(3)	0.006(2)	0.005(2)
C00Z	0.097(5)	0.048(4)	0.084(5)	0.009(3)	-0.017(4)	0.011(4)
C010	0.055(4)	0.091(5)	0.085(5)	0.013(4)	0.009(3)	0.001(3)
C011	0.154(7)	0.074(5)	0.060(4)	-0.005(4)	0.027(4)	0.016(5)
C012	0.089(5)	0.049(4)	0.179(8)	-0.014(5)	-0.032(5)	-0.007(4)

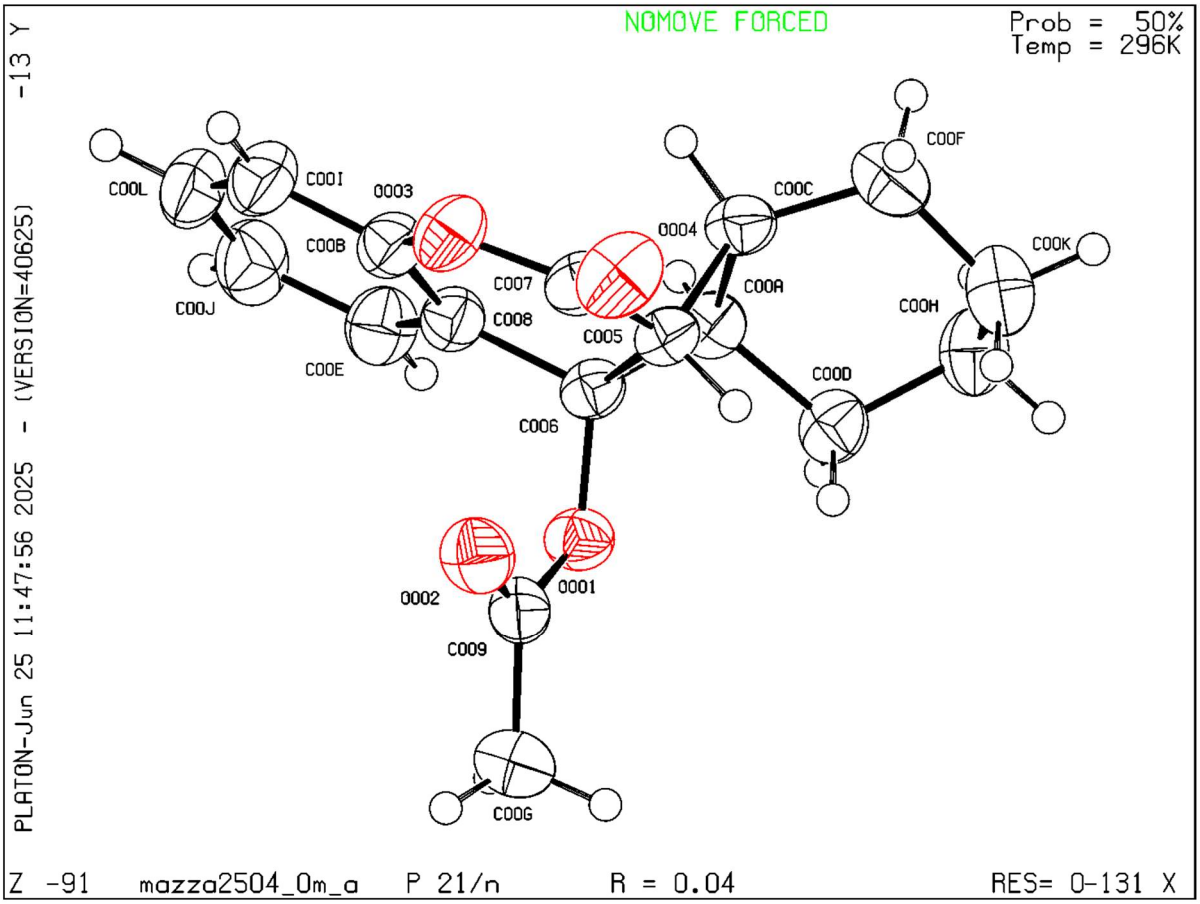
Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for C2.

	x/a	y/b	z/c	U(eq)
H00C	0.4615	0.5613	0.6229	0.056
H00F	0.3058	0.0955	0.4836	0.063
H00H	0.5126	0.3285	0.6301	0.056
H00*J*	0.2558	0.7432	0.5328	0.066
H00K	0.4232	0.0079	0.5513	0.064
H00L	0.1951	0.5713	0.4756	0.06
H00A	0.4834	0.7303	0.6960	0.092
H00B	0.4895	0.8650	0.6663	0.092
H00D	0.5161	0.7619	0.6020	0.092

	x/a	y/b	z/c	U(eq)
H00Q	0.1748	-0.0482	0.2661	0.082
H00S	0.0245	0.5541	0.2443	0.08
H00T	0.0879	-0.0339	0.5088	0.076
H00E	0.1824	0.1724	0.5933	0.108
H00G	0.0850	0.1367	0.5889	0.108
H00I	0.1147	0.2613	0.5521	0.108
H00W	0.2716	0.5906	0.1940	0.087
H00M	0.6446	0.1775	0.5944	0.121
H00N	0.6636	0.0918	0.6742	0.121
H00O	0.6184	0.2159	0.6893	0.121
H00Z	0.1328	0.6425	0.1656	0.092
H01A	0.3694	0.5020	0.3447	0.116
H01B	0.3725	0.4539	0.2480	0.116
H01C	0.3516	0.3658	0.3251	0.116
H01D	0.2996	0.1759	0.2605	0.143
H01E	0.2151	0.2403	0.2286	0.143
H01F	0.2352	0.1095	0.1967	0.143
H01G	0.0651	-0.2052	0.3313	0.159
H01H	0.0764	-0.2179	0.4334	0.159
H01I	0.1546	-0.2408	0.3723	0.159

9.2 X-Ray analysis of products

9.2.1 X-Ray Crystallography of product 6a-syn



A specimen of $C_{17}H_{18}O_4$, approximate dimensions 0.080 mm x 0.120 mm x 0.150 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The total exposure time was 20.33 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 19790 reflections to a maximum θ angle of 25.98° (0.81 Å resolution), of which 2872 were independent (average redundancy 6.891, completeness = 98.8%, R_{int} = 3.70%, R_{sig} = 2.37%) and 2621 (91.26%) were greater than $2\sigma(F^2)$. The final cell constants of a = 8.348(6) Å, b = 13.213(10) Å, c = 13.751(10) Å, β = 102.88(3)°, volume = 1478.6(19) $Å^3$, are based upon the refinement of the XYZ-centroids of 9984 reflections above 20 σ(I) with 5.004° < 2θ < 52.10°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.868. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9860 and 0.9930. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/n 1, with Z = 4 for the formula unit, $C_{17}H_{18}O_4$. The final anisotropic full-matrix least-squares refinement on F^2 with191 variables converged at R1 = 4.31%, for the observed data and wR2 = 10.74% for all data. The goodness-of-fit was 1.063. The largest peak in the final difference electron density synthesis was 0.244 $e^-/Å^3$ and the largest hole was -0.149 $e^-/Å^3$ with an RMS deviation of 0.030 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.286 g/cm^3 and F(000), 608 e^-.

Sample and crystal data for 6a.

Identification code	mazza2504	
Chemical formula	$C_{17}H_{18}O_4$	
Formula weight	286.31 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.080 x 0.120 x 0.150 mm	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 8.348(6) Å	α = 90°
	b = 13.213(10) Å	β = 102.88(3)°
	c = 13.751(10) Å	γ = 90°
Volume	1478.6(19) $Å^3$	
Z	4	
Density (calculated)	1.286 g/cm^3	
Absorption coefficient	0.091 mm^{-1}	
F(000)	608	

Data collection and structure refinement for 6a.

Theta range for data collection	2.94 to 25.98°
Index ranges	-10<=h<=10, -16<=k<=16, -16<=l<=16
Reflections collected	19790
Independent reflections	2872 [R(int) = 0.0370]
Coverage of independent reflections	98.8%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9930 and 0.9860
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2017/1 (Sheldrick, 2017)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	2872 / 0 / 191

Goodness-of-fit on F^2	1.063	
Final R indices	2621 data; I>2σ(I)	R1 = 0.0431, wR2 = 0.1054
	all data	R1 = 0.0465, wR2 = 0.1074
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0393P)^2+0.5214P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.244 and -0.149 eÅ^{-3}	
R.M.S. deviation from mean	0.030 eÅ^{-3}	

Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 6a.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
O001	0.52630(12)	0.26156(8)	0.57083(7)	0.0412(3)
O002	0.40172(14)	0.32447(9)	0.42228(8)	0.0521(3)
O003	0.73053(14)	0.36905(9)	0.36275(8)	0.0505(3)
O004	0.65456(16)	0.52231(9)	0.39154(9)	0.0598(3)
C005	0.69731(16)	0.40962(11)	0.53020(10)	0.0361(3)
C006	0.68202(16)	0.29743(11)	0.55489(10)	0.0361(3)
C007	0.68850(18)	0.43942(12)	0.42508(11)	0.0423(3)
C008	0.73957(17)	0.23068(11)	0.48110(11)	0.0402(3)
C009	0.39397(18)	0.28122(12)	0.49760(11)	0.0420(3)
C00A	0.81019(17)	0.31384(11)	0.65343(10)	0.0401(3)
C00B	0.76240(18)	0.26899(12)	0.39185(11)	0.0440(4)
C00C	0.87024(17)	0.40725(12)	0.60251(11)	0.0420(3)
C00D	0.7347(2)	0.34307(13)	0.74088(11)	0.0462(4)
C00E	0.7721(2)	0.12894(13)	0.50039(13)	0.0521(4)
C00F	0.9343(2)	0.49883(14)	0.66580(13)	0.0556(4)
C00G	0.2410(2)	0.24276(15)	0.52373(15)	0.0620(5)
C00H	0.8399(2)	0.41971(14)	0.80836(12)	0.0576(4)
C00I	0.8173(2)	0.20845(15)	0.32364(13)	0.0572(4)
C00*J*	0.8235(2)	0.06764(14)	0.43196(15)	0.0611(5)
C00K	0.8496(3)	0.51699(14)	0.75126(13)	0.0612(5)
C00L	0.8466(2)	0.10756(15)	0.34396(14)	0.0626(5)

Bond lengths (Å) for 6a.

O001-C009	1.344(2)	O001-C006	1.4456(19)
O002-C009	1.197(2)	O003-C007	1.363(2)
O003-C00B	1.390(2)	O004-C007	1.198(2)
C005-C007	1.484(2)	C005-C006	1.532(2)
C005-C00C	1.560(2)	C005-H005	0.98
C006-C008	1.502(2)	C006-C00A	1.543(2)
C008-C00B	1.379(2)	C008-C00E	1.385(2)
C009-C00G	1.491(2)	C00A-C00D	1.526(2)
C00A-C00C	1.556(2)	C00A-H00A	0.98
C00B-C00I	1.386(2)	C00C-C00F	1.517(2)
C00C-H00C	0.98	C00D-C00H	1.515(2)
C00D-H00B	0.97	C00D-H00D	0.97
C00E-C00*J*	1.381(3)	C00E-H00E	0.93
C00F-C00K	1.520(3)	C00F-H00F	0.97
C00F-H00G	0.97	C00G-H00H	0.96
C00G-H00I	0.96	C00G-H00*J*	0.96
C00H-C00K	1.518(3)	C00H-H00K	0.97
C00H-H00L	0.97	C00I-C00L	1.373(3)
C00I-H00M	0.93	C00*J*-C00L	1.372(3)
C00*J*-H00N	0.93	C00K-H00O	0.97
C00K-H00P	0.97	C00L-H00Q	0.93

Bond angles (°) for 6a.

C009-O001-C006	116.09(12)	C007-O003-C00B	121.84(12)
C007-C005-C006	118.94(12)	C007-C005-C00C	117.64(12)
C006-C005-C00C	87.15(10)	C007-C005-H005	110.4
C006-C005-H005	110.4	C00C-C005-H005	110.4
O001-C006-C008	110.11(12)	O001-C006-C005	118.22(11)
C008-C006-C005	111.31(12)	O001-C006-C00A	112.58(12)
C008-C006-C00A	114.33(12)	C005-C006-C00A	89.02(11)

O004-C007-O003	116.99(14)	O004-C007-C005	125.02(14)
O003-C007-C005	117.90(13)	C00B-C008-C00E	117.80(14)
C00B-C008-C006	120.93(14)	C00E-C008-C006	121.27(14)
O002-C009-O001	123.13(14)	O002-C009-C00G	125.84(15)
O001-C009-C00G	111.02(15)	C00D-C00A-C006	113.58(13)
C00D-C00A-C00C	112.63(13)	C006-C00A-C00C	86.92(11)
C00D-C00A-H00A	113.7	C006-C00A-H00A	113.7
C00C-C00A-H00A	113.7	C008-C00B-C00I	121.49(16)
C008-C00B-O003	123.35(13)	C00I-C00B-O003	115.16(15)
C00F-C00C-C00A	118.84(14)	C00F-C00C-C005	120.51(13)
C00A-C00C-C005	87.57(11)	C00F-C00C-H00C	109.4
C00A-C00C-H00C	109.4	C005-C00C-H00C	109.4
C00H-C00D-C00A	111.53(15)	C00H-C00D-H00B	109.3
C00A-C00D-H00B	109.3	C00H-C00D-H00D	109.3
C00A-C00D-H00D	109.3	H00B-C00D-H00D	108.0
C00*J*-C00E-C008	121.08(17)	C00*J*-C00E-H00E	119.5
C008-C00E-H00E	119.5	C00C-C00F-C00K	113.85(14)
C00C-C00F-H00F	108.8	C00K-C00F-H00F	108.8
C00C-C00F-H00G	108.8	C00K-C00F-H00G	108.8
H00F-C00F-H00G	107.7	C009-C00G-H00H	109.5
C009-C00G-H00I	109.5	H00H-C00G-H00I	109.5
C009-C00G-H00*J*	109.5	H00H-C00G-H00*J*	109.5
H00I-C00G-H00*J*	109.5	C00D-C00H-C00K	109.87(14)
C00D-C00H-H00K	109.7	C00K-C00H-H00K	109.7
C00D-C00H-H00L	109.7	C00K-C00H-H00L	109.7
H00K-C00H-H00L	108.2	C00L-C00I-C00B	119.57(17)
C00L-C00I-H00M	120.2	C00B-C00I-H00M	120.2
C00L-C00*J*-C00E	120.11(18)	C00L-C00*J*-H00N	119.9
C00E-C00*J*-H00N	119.9	C00H-C00K-C00F	110.73(16)
C00H-C00K-H00O	109.5	C00F-C00K-H00O	109.5
C00H-C00K-H00P	109.5	C00F-C00K-H00P	109.5
H00O-C00K-H00P	108.1	C00*J*-C00L-C00I	119.93(16)

C00*J*-C00L-H00Q	120.0	C00I-C00L-H00Q	120.0

Torsion angles (°) for 6a.

C009-O001-C006-C008	-75.54(15)	C009-O001-C006-C005	53.94(16)
C009-O001-C006-C00A	155.60(12)	C007-C005-C006-O001	-101.58(15)
C00C-C005-C006-O001	138.20(12)	C007-C005-C006-C008	27.33(17)
C00C-C005-C006-C008	-92.89(13)	C007-C005-C006-C00A	143.17(13)
C00C-C005-C006-C00A	22.94(10)	C00B-O003-C007-O004	-176.00(14)
C00B-O003-C007-C005	7.4(2)	C006-C005-C007-O004	158.77(15)
C00C-C005-C007-O004	-98.19(19)	C006-C005-C007-O003	-24.94(19)
C00C-C005-C007-O003	78.10(18)	O001-C006-C008-C00B	118.61(15)
C005-C006-C008-C00B	-14.49(19)	C00A-C006-C008-C00B	-113.49(15)
O001-C006-C008-C00E	-61.65(18)	C005-C006-C008-C00E	165.24(14)
C00A-C006-C008-C00E	66.25(19)	C006-O001-C009-O002	1.0(2)
C006-O001-C009-C00G	-178.66(13)	O001-C006-C00A-C00D	-29.96(17)
C008-C006-C00A-C00D	-156.59(13)	C005-C006-C00A-C00D	90.38(13)
O001-C006-C00A-C00C	-143.35(12)	C008-C006-C00A-C00C	90.02(14)
C005-C006-C00A-C00C	-23.01(10)	C00E-C008-C00B-C00I	-0.5(2)
C006-C008-C00B-C00I	179.24(14)	C00E-C008-C00B-O003	178.49(14)
C006-C008-C00B-O003	-1.8(2)	C007-O003-C00B-C008	6.3(2)
C007-O003-C00B-C00I	-174.69(14)	C00D-C00A-C00C-C00F	32.12(18)
C006-C00A-C00C-C00F	146.43(14)	C00D-C00A-C00C-C005	-91.71(14)
C006-C00A-C00C-C005	22.60(10)	C007-C005-C00C-C00F	93.47(17)
C006-C005-C00C-C00F	-145.13(14)	C007-C005-C00C-C00A	-144.15(13)
C006-C005-C00C-C00A	-22.76(10)	C006-C00A-C00D-C00H	-142.77(14)
C00C-C00A-C00D-C00H	-45.97(17)	C00B-C008-C00E-C00*J*	-0.9(2)
C006-C008-C00E-C00*J*	179.40(15)	C00A-C00C-C00F-C00K	-33.3(2)
C005-C00C-C00F-C00K	72.3(2)	C00A-C00D-C00H-C00K	63.01(19)
C008-C00B-C00I-C00L	1.3(3)	O003-C00B-C00I-C00L	-177.72(15)
C008-C00E-C00*J*-C00L	1.4(3)	C00D-C00H-C00K-C00F	-63.4(2)
C00C-C00F-C00K-C00H	47.8(2)	C00E-C00*J*-C00L-C00I	-0.5(3)
C00B-C00I-C00L-C00*J*	-0.8(3)		

Anisotropic atomic displacement parameters (Å^2) for 6a.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

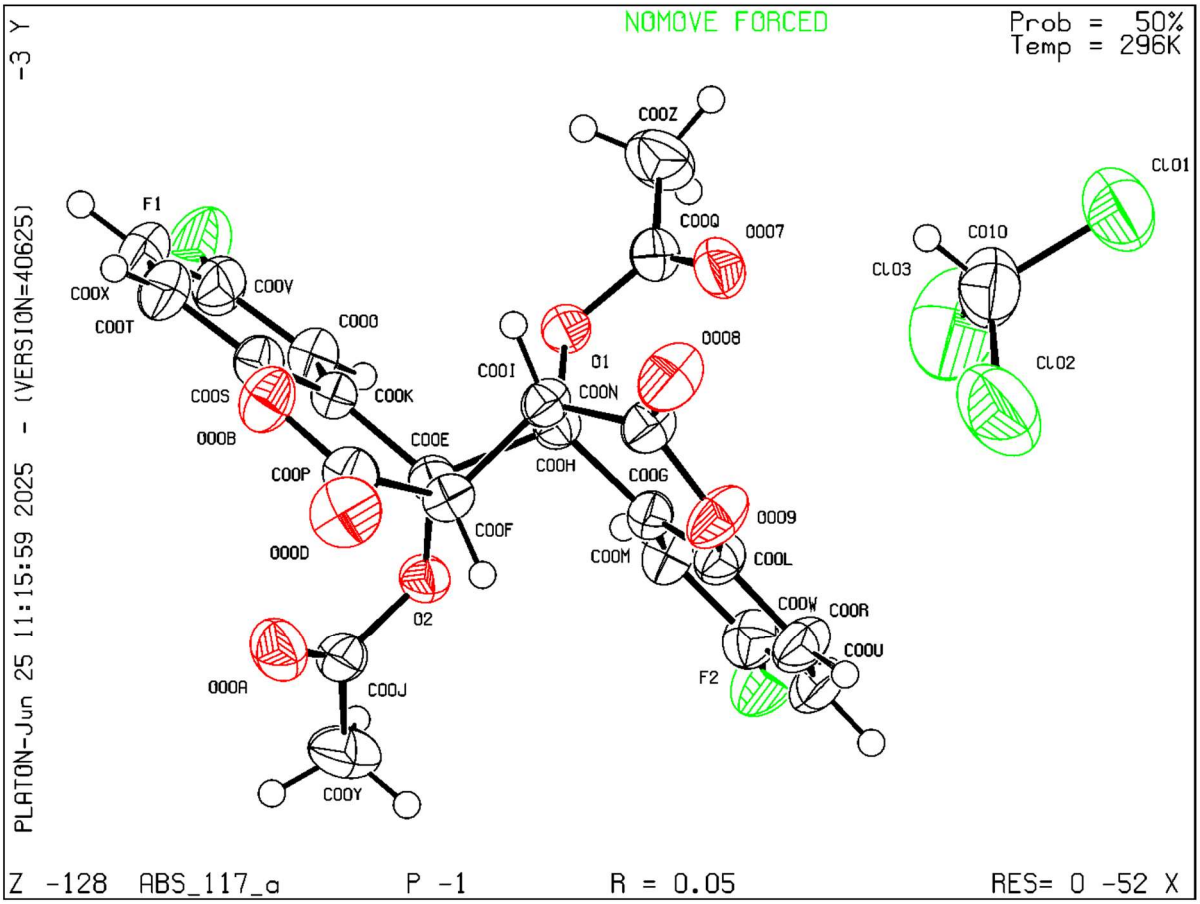
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O001	0.0393(5)	0.0467(6)	0.0386(5)	0.0048(4)	0.0105(4)	-0.0020(4)
O002	0.0490(6)	0.0625(7)	0.0407(6)	0.0030(5)	0.0015(5)	0.0006(5)
O003	0.0633(7)	0.0558(7)	0.0371(6)	0.0062(5)	0.0207(5)	0.0043(5)
O004	0.0773(8)	0.0542(7)	0.0520(7)	0.0192(6)	0.0234(6)	0.0127(6)
C005	0.0346(7)	0.0407(8)	0.0343(7)	0.0032(6)	0.0105(5)	0.0036(6)
C006	0.0356(7)	0.0404(8)	0.0329(7)	0.0044(6)	0.0091(5)	0.0027(6)
C007	0.0420(8)	0.0473(9)	0.0395(8)	0.0070(6)	0.0131(6)	0.0030(6)
C008	0.0374(7)	0.0445(8)	0.0379(7)	-0.0014(6)	0.0071(6)	0.0034(6)
C009	0.0411(8)	0.0420(8)	0.0423(8)	-0.0069(6)	0.0078(6)	-0.0002(6)
C00A	0.0384(7)	0.0432(8)	0.0367(7)	0.0044(6)	0.0044(6)	0.0068(6)
C00B	0.0409(8)	0.0526(9)	0.0391(8)	-0.0020(7)	0.0100(6)	0.0024(6)
C00C	0.0341(7)	0.0515(9)	0.0410(8)	0.0035(6)	0.0094(6)	0.0021(6)
C00D	0.0530(9)	0.0530(9)	0.0320(7)	0.0047(6)	0.0086(6)	0.0014(7)
C00E	0.0566(9)	0.0472(9)	0.0518(9)	0.0001(7)	0.0107(8)	0.0065(7)
C00F	0.0506(9)	0.0585(11)	0.0538(10)	0.0028(8)	0.0036(7)	-0.0115(8)
C00G	0.0454(9)	0.0688(12)	0.0727(12)	-0.0084(9)	0.0150(8)	-0.0109(8)
C00H	0.0702(11)	0.0631(11)	0.0364(8)	-0.0020(7)	0.0050(7)	0.0004(9)
C00I	0.0558(10)	0.0745(12)	0.0442(9)	-0.0096(8)	0.0174(8)	0.0022(9)
C00*J*	0.0614(11)	0.0482(10)	0.0710(12)	-0.0108(9)	0.0090(9)	0.0093(8)
C00K	0.0767(12)	0.0526(10)	0.0512(10)	-0.0076(8)	0.0078(9)	-0.0058(9)
C00L	0.0560(10)	0.0708(13)	0.0619(11)	-0.0247(9)	0.0153(8)	0.0068(9)

Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 6a.

	x/a	y/b	z/c	U(eq)
H005	0.6209	0.4503	0.5587	0.043
H00A	0.8918	0.2595	0.6690	0.048
H00C	0.9523	0.3855	0.5658	0.05
H00B	0.6262	0.3713	0.7155	0.055

	x/a	y/b	z/c	U(eq)
H00D	0.7227	0.2830	0.7791	0.055
H00E	0.7591	0.1015	0.5604	0.063
H00F	0.9203	0.5583	0.6234	0.067
H00G	1.0511	0.4901	0.6930	0.067
H00H	0.2063	0.2893	0.5686	0.093
H00I	0.2620	0.1778	0.5553	0.093
H00*J*	0.1561	0.2364	0.4642	0.093
H00K	0.9495	0.3925	0.8327	0.069
H00L	0.7928	0.4335	0.8654	0.069
H00M	0.8341	0.2360	0.2645	0.069
H00N	0.8426	-0.0008	0.4455	0.073
H00O	0.9102	0.5675	0.7961	0.073
H00P	0.7397	0.5428	0.7251	0.073
H00Q	0.8821	0.0663	0.2981	0.075

9.2.2 X-Ray Crystallography of product 8c



A specimen of $C_{22}H_{14}F_2O_8 \cdot CHCl_3$, approximate dimensions 0.600 mm x 0.800 mm x 1.000 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The total exposure time was 3.39 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 12822 reflections to a maximum θ angle of 25.00° (0.84 Å resolution), of which 4261 were independent (average redundancy 3.009, completeness = 99.4%, R_{int} = 4.88%, R_{sig} = 4.81%) and 3700 (86.83%) were greater than $2\sigma(F^2)$. The final cell constants of a = 10.346(3) Å, b = 10.817(3) Å, c = 12.515(3) Å, α = 111.880(5)°, β = 108.429(5)°, γ = 90.842(5)°, volume = 1219.0(5) $Å^3$, are based upon the refinement of the XYZ-centroids of 8423 reflections above 20 σ(I) with 4.551° < 2θ < 54.44°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.637. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6680 and 0.7790. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{23}H_{15}Cl_3F_2O_8$. The final anisotropic full-matrix least-squares refinement on F^2 with328 variables converged at R1 = 5.25%, for the observed data and wR2 = 13.88% for all data. The goodness-of-fit was 1.049. The largest peak in the final difference electron density synthesis was 0.477 $e^-/Å^3$ and the largest hole was -0.647 $e^-/Å^3$ with an RMS deviation of 0.051 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.536 g/cm^3 and F(000), 572 e^-.

Sample and crystal data for 8c.

Identification code	mazza2506ABS	
Chemical formula	$C_{23}H_{15}Cl_3F_2O_8$	
Formula weight	563.70 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.600 x 0.800 x 1.000 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.346(3) Å	α = 111.880(5)°
	b = 10.817(3) Å	β = 108.429(5)°
	c = 12.515(3) Å	γ = 90.842(5)°
Volume	1219.0(5) $Å^3$	
Z	2	
Density (calculated)	1.536 g/cm^3	
Absorption coefficient	0.438 mm^{-1}	
F(000)	572	

Data collection and structure refinement for 8c.

Theta range for data collection	1.87 to 25.00°
Index ranges	-12<=h<=12, -12<=k<=12, -14<=l<=14
Reflections collected	12822
Independent reflections	4261 [R(int) = 0.0488]
Coverage of independent reflections	99.4%
Absorption correction	Multi-Scan
Max. and min. transmission	0.7790 and 0.6680
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2017/1 (Sheldrick, 2017)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4261 / 0 / 328

Goodness-of-fit on F^2	1.049	
Final R indices	3700 data; I>2σ(I)	R1 = 0.0525, wR2 = 0.1333
	all data	R1 = 0.0592, wR2 = 0.1388
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0540P)^2+0.8956P]$ where $P=(F_o^2+2F_c^2)/3$	
Extinction coefficient	0.0150(40)	
Largest diff. peak and hole	0.477 and -0.647 eÅ^{-3}	
R.M.S. deviation from mean	0.051 eÅ^{-3}	

Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 8c.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Cl01	0.75740(13)	0.12995(14)	0.72861(11)	0.1025(4)
Cl02	0.61184(16)	0.27972(14)	0.59826(13)	0.1173(5)
Cl03	0.67621(16)	0.02285(14)	0.46602(12)	0.1259(5)
O1	0.86048(15)	0.21834(15)	0.27088(14)	0.0344(4)
O2	0.65594(15)	0.29671(15)	0.05143(13)	0.0344(4)
F2	0.35576(17)	0.99888(16)	0.08642(17)	0.0680(5)
O007	0.87926(19)	0.28448(19)	0.46802(16)	0.0480(5)
O008	0.8398(2)	0.6132(2)	0.55420(16)	0.0563(5)
O009	0.64327(17)	0.48527(18)	0.43058(16)	0.0487(5)
O00A	0.6661(2)	0.46521(19)	0.99058(18)	0.0534(5)
O00B	0.97110(18)	0.59619(17)	0.21196(17)	0.0485(5)
F1	0.0712(2)	0.09688(19)	0.9584(2)	0.0757(6)
O00D	0.8424(2)	0.73811(18)	0.2875(2)	0.0595(5)
C00E	0.7757(2)	0.3637(2)	0.15800(19)	0.0301(5)
C00F	0.7750(2)	0.5090(2)	0.2440(2)	0.0343(5)
C00G	0.6333(2)	0.2780(2)	0.25751(19)	0.0327(5)
C00H	0.7754(2)	0.3190(2)	0.26271(19)	0.0302(5)
C00I	0.8334(2)	0.4667(2)	0.35435(19)	0.0331(5)
C00*J*	0.6123(2)	0.3571(3)	0.9724(2)	0.0389(5)
C00K	0.9035(2)	0.3516(2)	0.12458(19)	0.0326(5)

	x/a	y/b	z/c	U(eq)
C00L	0.5738(2)	0.3632(2)	0.3353(2)	0.0375(5)
C00M	0.5582(2)	0.1536(2)	0.1734(2)	0.0391(5)
C00N	0.7785(2)	0.5270(2)	0.4564(2)	0.0393(5)
C00O	0.9320(2)	0.2256(2)	0.0592(2)	0.0394(5)
C00P	0.8610(2)	0.6242(2)	0.2486(2)	0.0399(5)
C00Q	0.9054(2)	0.2092(2)	0.3813(2)	0.0391(5)
C00R	0.4401(3)	0.3300(3)	0.3271(2)	0.0472(6)
C00S	0.9913(2)	0.4650(2)	0.1520(2)	0.0389(5)
C00T	0.1057(3)	0.4554(3)	0.1156(3)	0.0509(7)
C00U	0.3663(3)	0.2076(3)	0.2429(2)	0.0483(6)
C00V	0.0449(3)	0.2191(3)	0.0237(3)	0.0474(6)
C00W	0.4272(3)	0.1212(3)	0.1686(2)	0.0449(6)
C00X	0.1325(3)	0.3321(3)	0.0512(3)	0.0551(7)
C00Y	0.4905(3)	0.2712(3)	0.8659(3)	0.0581(7)
C00Z	0.9865(3)	0.0969(3)	0.3778(3)	0.0610(8)
C010	0.7292(4)	0.1674(4)	0.6005(3)	0.0757(10)

Bond lengths (Å) for 8c.

Cl01-C010	1.735(4)	Cl02-C010	1.731(4)
Cl03-C010	1.735(4)	O1-C00Q	1.353(3)
O1-C00H	1.423(3)	O2-C00*J*	1.348(3)
O2-C00E	1.431(2)	F2-C00W	1.354(3)
O007-C00Q	1.203(3)	O008-C00N	1.188(3)
O009-C00N	1.361(3)	O009-C00L	1.392(3)
O00A-C00*J*	1.197(3)	O00B-C00P	1.355(3)
O00B-C00S	1.391(3)	F1-C00V	1.355(3)
O00D-C00P	1.188(3)	C00E-C00K	1.502(3)
C00E-C00F	1.540(3)	C00E-C00H	1.557(3)
C00F-C00P	1.494(3)	C00F-C00I	1.560(3)
C00F-H00F	0.98	C00G-C00L	1.380(3)
C00G-C00M	1.385(3)	C00G-C00H	1.504(3)

C00H-C00I	1.548(3)	C00I-C00N	1.492(3)
C00I-H00I	0.98	C00*J*-C00Y	1.486(4)
C00K-C00S	1.380(3)	C00K-C00O	1.395(3)
C00L-C00R	1.386(3)	C00M-C00W	1.371(3)
C00M-H00M	0.93	C00O-C00V	1.369(3)
C00O-H00O	0.93	C00Q-C00Z	1.482(4)
C00R-C00U	1.367(4)	C00R-H00R	0.93
C00S-C00T	1.389(4)	C00T-C00X	1.362(4)
C00T-H00T	0.93	C00U-C00W	1.369(4)
C00U-H00U	0.93	C00V-C00X	1.375(4)
C00X-H00X	0.93	C00Y-H00A	0.96
C00Y-H00B	0.96	C00Y-H00C	0.96
C00Z-H00D	0.96	C00Z-H00E	0.96
C00Z-H00G	0.96	C010-H010	0.98

Bond angles (°) for 8c.

C00Q-O1-C00H	115.58(17)	C00*J*-O2-C00E	117.57(17)
C00N-O009-C00L	121.66(18)	C00P-O00B-C00S	122.41(18)
O2-C00E-C00K	110.66(17)	O2-C00E-C00F	118.36(17)
C00K-C00E-C00F	111.55(17)	O2-C00E-C00H	110.43(16)
C00K-C00E-C00H	116.34(17)	C00F-C00E-C00H	88.08(16)
C00P-C00F-C00E	120.20(19)	C00P-C00F-C00I	115.12(18)
C00E-C00F-C00I	88.11(16)	C00P-C00F-H00F	110.5
C00E-C00F-H00F	110.5	C00I-C00F-H00F	110.5
C00L-C00G-C00M	118.2(2)	C00L-C00G-C00H	121.1(2)
C00M-C00G-C00H	120.65(19)	O1-C00H-C00G	111.37(17)
O1-C00H-C00I	118.14(17)	C00G-C00H-C00I	111.46(17)
O1-C00H-C00E	112.57(17)	C00G-C00H-C00E	113.55(17)
C00I-C00H-C00E	87.93(15)	C00N-C00I-C00H	118.40(18)
C00N-C00I-C00F	115.38(19)	C00H-C00I-C00F	87.67(15)
C00N-C00I-H00I	111.1	C00H-C00I-H00I	111.1
C00F-C00I-H00I	111.1	O00A-C00*J*-O2	122.7(2)

O00A-C00*J*-C00Y	127.3(2)	O2-C00*J*-C00Y	110.0(2)
C00S-C00K-C00O	118.6(2)	C00S-C00K-C00E	120.7(2)
C00O-C00K-C00E	120.6(2)	C00G-C00L-C00R	121.8(2)
C00G-C00L-O009	123.5(2)	C00R-C00L-O009	114.7(2)
C00W-C00M-C00G	119.1(2)	C00W-C00M-H00M	120.4
C00G-C00M-H00M	120.4	O008-C00N-O009	117.8(2)
O008-C00N-C00I	125.8(2)	O009-C00N-C00I	116.22(19)
C00V-C00O-C00K	118.9(2)	C00V-C00O-H00O	120.6
C00K-C00O-H00O	120.6	O00D-C00P-O00B	118.8(2)
O00D-C00P-C00F	124.0(2)	O00B-C00P-C00F	117.1(2)
O007-C00Q-O1	122.2(2)	O007-C00Q-C00Z	126.7(2)
O1-C00Q-C00Z	111.1(2)	C00U-C00R-C00L	119.4(2)
C00U-C00R-H00R	120.3	C00L-C00R-H00R	120.3
C00K-C00S-C00T	121.3(2)	C00K-C00S-O00B	124.1(2)
C00T-C00S-O00B	114.6(2)	C00X-C00T-C00S	119.9(2)
C00X-C00T-H00T	120.1	C00S-C00T-H00T	120.1
C00R-C00U-C00W	118.7(2)	C00R-C00U-H00U	120.7
C00W-C00U-H00U	120.7	F1-C00V-C00O	118.9(2)
F1-C00V-C00X	118.6(2)	C00O-C00V-C00X	122.5(2)
F2-C00W-C00U	119.0(2)	F2-C00W-C00M	118.3(2)
C00U-C00W-C00M	122.7(2)	C00T-C00X-C00V	118.9(2)
C00T-C00X-H00X	120.6	C00V-C00X-H00X	120.6
C00*J*-C00Y-H00A	109.5	C00*J*-C00Y-H00B	109.5
H00A-C00Y-H00B	109.5	C00*J*-C00Y-H00C	109.5
H00A-C00Y-H00C	109.5	H00B-C00Y-H00C	109.5
C00Q-C00Z-H00D	109.5	C00Q-C00Z-H00E	109.5
H00D-C00Z-H00E	109.5	C00Q-C00Z-H00G	109.5
H00D-C00Z-H00G	109.5	H00E-C00Z-H00G	109.5
Cl02-C010-Cl03	111.7(2)	Cl02-C010-Cl01	109.8(2)
Cl03-C010-Cl01	111.6(2)	Cl02-C010-H010	107.9
Cl03-C010-H010	107.9	Cl01-C010-H010	107.9

Torsion angles (°) for 8c.

C00*J*-O2-C00E-C00K	-74.3(2)	C00*J*-O2-C00E-C00F	56.2(3)
C00*J*-O2-C00E-C00H	155.44(18)	O2-C00E-C00F-C00P	-108.2(2)
C00K-C00E-C00F-C00P	21.9(3)	C00H-C00E-C00F-C00P	139.6(2)
O2-C00E-C00F-C00I	133.63(18)	C00K-C00E-C00F-C00I	-96.27(18)
C00H-C00E-C00F-C00I	21.38(15)	C00Q-O1-C00H-C00G	-74.1(2)
C00Q-O1-C00H-C00I	56.8(2)	C00Q-O1-C00H-C00E	157.09(18)
C00L-C00G-C00H-O1	129.2(2)	C00M-C00G-C00H-O1	-51.3(3)
C00L-C00G-C00H-C00I	-5.1(3)	C00M-C00G-C00H-C00I	174.4(2)
C00L-C00G-C00H-C00E	-102.5(2)	C00M-C00G-C00H-C00E	77.0(3)
O2-C00E-C00H-O1	99.1(2)	C00K-C00E-C00H-O1	-28.1(2)
C00F-C00E-C00H-O1	-141.29(17)	O2-C00E-C00H-C00G	-28.6(2)
C00K-C00E-C00H-C00G	-155.83(18)	C00F-C00E-C00H-C00G	91.00(19)
O2-C00E-C00H-C00I	-141.20(17)	C00K-C00E-C00H-C00I	91.61(19)
C00F-C00E-C00H-C00I	-21.56(15)	O1-C00H-C00I-C00N	-106.4(2)
C00G-C00H-C00I-C00N	24.5(3)	C00E-C00H-C00I-C00N	139.0(2)
O1-C00H-C00I-C00F	135.87(18)	C00G-C00H-C00I-C00F	-93.27(19)
C00E-C00H-C00I-C00F	21.27(15)	C00P-C00F-C00I-C00N	95.3(2)
C00E-C00F-C00I-C00N	-142.01(19)	C00P-C00F-C00I-C00H	-144.23(19)
C00E-C00F-C00I-C00H	-21.52(15)	C00E-O2-C00*J*-O00A	-3.0(3)
C00E-O2-C00*J*-C00Y	178.0(2)	O2-C00E-C00K-C00S	123.0(2)
C00F-C00E-C00K-C00S	-11.0(3)	C00H-C00E-C00K-C00S	-110.0(2)
O2-C00E-C00K-C00O	-53.5(3)	C00F-C00E-C00K-C00O	172.50(19)
C00H-C00E-C00K-C00O	73.6(3)	C00M-C00G-C00L-C00R	-3.2(4)
C00H-C00G-C00L-C00R	176.3(2)	C00M-C00G-C00L-O009	174.1(2)
C00H-C00G-C00L-O009	-6.4(3)	C00N-O009-C00L-C00G	-2.5(4)
C00N-O009-C00L-C00R	175.0(2)	C00L-C00G-C00M-C00W	1.5(3)
C00H-C00G-C00M-C00W	-178.0(2)	C00L-O009-C00N-O008	-162.1(2)
C00L-O009-C00N-C00I	22.4(3)	C00H-C00I-C00N-O008	151.1(3)
C00F-C00I-C00N-O008	-107.0(3)	C00H-C00I-C00N-O009	-33.8(3)
C00F-C00I-C00N-O009	68.1(3)	C00S-C00K-C00O-C00V	-0.6(3)
C00E-C00K-C00O-C00V	175.9(2)	C00S-O00B-C00P-O00D	-172.2(2)

C00S-O00B-C00P-C00F	11.4(3)	C00E-C00F-C00P-O00D	160.9(2)
C00I-C00F-C00P-O00D	-95.7(3)	C00E-C00F-C00P-O00B	-22.8(3)
C00I-C00F-C00P-O00B	80.5(3)	C00H-O1-C00Q-O007	-2.6(3)
C00H-O1-C00Q-C00Z	177.0(2)	C00G-C00L-C00R-C00U	2.5(4)
O009-C00L-C00R-C00U	-175.0(2)	C00O-C00K-C00S-C00T	0.2(3)
C00E-C00K-C00S-C00T	-176.4(2)	C00O-C00K-C00S-O00B	177.2(2)
C00E-C00K-C00S-O00B	0.6(3)	C00P-O00B-C00S-C00K	-0.4(4)
C00P-O00B-C00S-C00T	176.8(2)	C00K-C00S-C00T-C00X	0.2(4)
O00B-C00S-C00T-C00X	-177.1(2)	C00L-C00R-C00U-C00W	-0.2(4)
C00K-C00O-C00V-F1	-178.9(2)	C00K-C00O-C00V-C00X	0.8(4)
C00R-C00U-C00W-F2	178.9(2)	C00R-C00U-C00W-C00M	-1.5(4)
C00G-C00M-C00W-F2	-179.5(2)	C00G-C00M-C00W-C00U	0.8(4)
C00S-C00T-C00X-C00V	-0.1(4)	F1-C00V-C00X-C00T	179.3(3)
C00O-C00V-C00X-C00T	-0.4(4)		

Anisotropic atomic displacement parameters (Å^2) for 8c.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl01	0.1165(9)	0.1324(10)	0.1035(8)	0.0793(8)	0.0558(7)	0.0496(7)
Cl02	0.1473(12)	0.1277(10)	0.1144(9)	0.0823(8)	0.0513(8)	0.0485(9)
Cl03	0.1351(11)	0.1106(9)	0.0964(8)	0.0010(7)	0.0450(8)	-0.0320(8)
O1	0.0351(8)	0.0366(8)	0.0359(8)	0.0164(7)	0.0155(7)	0.0113(6)
O2	0.0318(8)	0.0365(8)	0.0313(8)	0.0133(6)	0.0067(6)	0.0011(6)
F2	0.0559(10)	0.0502(9)	0.0775(12)	0.0020(8)	0.0262(9)	-0.0176(8)
O007	0.0558(11)	0.0575(11)	0.0401(9)	0.0249(9)	0.0219(8)	0.0139(9)
O008	0.0483(11)	0.0592(11)	0.0403(10)	-0.0035(9)	0.0167(8)	-0.0062(9)
O009	0.0369(9)	0.0509(10)	0.0435(10)	-0.0027(8)	0.0210(8)	-0.0008(8)
O00A	0.0593(12)	0.0530(11)	0.0565(11)	0.0323(9)	0.0186(9)	0.0061(9)
O00B	0.0483(10)	0.0381(9)	0.0612(11)	0.0184(8)	0.0237(9)	-0.0028(8)
F1	0.0861(13)	0.0649(11)	0.1019(14)	0.0303(10)	0.0683(12)	0.0324(10)
O00D	0.0660(13)	0.0338(10)	0.0744(13)	0.0174(9)	0.0238(11)	0.0052(9)
C00E	0.0278(10)	0.0305(11)	0.0295(10)	0.0111(9)	0.0081(8)	0.0013(8)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C00F	0.0297(11)	0.0342(11)	0.0374(12)	0.0129(9)	0.0111(9)	0.0047(9)
C00G	0.0308(11)	0.0375(12)	0.0313(11)	0.0140(9)	0.0125(9)	0.0045(9)
C00H	0.0282(10)	0.0316(11)	0.0307(11)	0.0113(9)	0.0110(9)	0.0055(8)
C00I	0.0290(11)	0.0352(11)	0.0320(11)	0.0100(9)	0.0108(9)	0.0027(9)
C00*J*	0.0357(12)	0.0494(14)	0.0359(12)	0.0184(11)	0.0161(10)	0.0135(11)
C00K	0.0296(11)	0.0389(12)	0.0318(11)	0.0161(9)	0.0113(9)	0.0052(9)
C00L	0.0331(12)	0.0425(13)	0.0346(12)	0.0108(10)	0.0141(9)	0.0048(10)
C00M	0.0396(13)	0.0367(12)	0.0412(13)	0.0123(10)	0.0185(10)	0.0033(10)
C00N	0.0360(12)	0.0398(12)	0.0354(12)	0.0071(10)	0.0134(10)	0.0029(10)
C00O	0.0394(12)	0.0409(13)	0.0403(12)	0.0160(10)	0.0174(10)	0.0055(10)
C00P	0.0424(13)	0.0318(12)	0.0418(13)	0.0142(10)	0.0105(10)	0.0024(10)
C00Q	0.0383(12)	0.0419(13)	0.0419(13)	0.0214(11)	0.0144(10)	0.0048(10)
C00R	0.0353(13)	0.0590(16)	0.0443(14)	0.0120(12)	0.0203(11)	0.0080(11)
C00S	0.0372(12)	0.0414(13)	0.0403(12)	0.0190(10)	0.0133(10)	0.0031(10)
C00T	0.0401(14)	0.0607(17)	0.0627(17)	0.0326(14)	0.0221(12)	0.0021(12)
C00U	0.0306(12)	0.0625(17)	0.0514(15)	0.0200(13)	0.0171(11)	0.0000(11)
C00V	0.0493(15)	0.0525(15)	0.0551(15)	0.0265(13)	0.0305(12)	0.0205(12)
C00W	0.0422(14)	0.0418(13)	0.0449(14)	0.0129(11)	0.0132(11)	-0.0047(11)
C00X	0.0442(15)	0.0744(19)	0.0700(18)	0.0411(16)	0.0346(14)	0.0194(14)
C00Y	0.0486(16)	0.0672(18)	0.0453(15)	0.0207(14)	0.0011(12)	0.0112(14)
C00Z	0.0667(19)	0.0603(18)	0.0661(18)	0.0373(15)	0.0207(15)	0.0264(15)
C010	0.077(2)	0.086(2)	0.071(2)	0.0344(19)	0.0313(18)	-0.0031(19)

Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 8c.

	x/a	y/b	z/c	U(eq)
H00F	0.6802	0.5270	0.2338	0.041
H00I	0.9344	0.4814	0.3852	0.04
H00M	0.5960	0.0929	0.1209	0.047
H00O	0.8752	0.1473	0.0401	0.047
H00R	0.4009	0.3905	0.3784	0.057
H00T	1.1638	0.5329	0.1351	0.061

	x/a	y/b	z/c	U(eq)
H00U	0.2766	0.1835	0.2362	0.058
H00X	1.2087	0.3245	0.0263	0.066
H00A	0.4097	0.2816	-0.1114	0.087
H00B	0.5045	0.1786	-0.1585	0.087
H00C	0.4788	0.2979	-0.2013	0.087
H00D	1.0342	0.1048	0.4600	0.091
H00E	1.0522	0.1005	0.3389	0.091
H00G	0.9257	0.0126	0.3322	0.091
H010	0.8166	0.2117	0.6077	0.091

10. DFT calculation for photocatalysts C1-C5.

10.1 Singlet and Triplet energies optimized geometries (SCF)

C1

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GS1-Singlet
# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                  1.18610400    0.35045500   -0.02433800
 C                 -1.36375300    0.92766600    0.10381500
 C                  3.10520400    1.62509400    0.01927600
 C                  3.44967600    0.30043100   -0.45399700
 F                 -1.12959000   -1.33236400   -2.05326600
 C                  1.72298200    1.62669100    0.26308400
 C                  2.26341700   -0.44922300   -0.46428100
 C                 -0.39160700   -1.58924900    0.66652000
 C                 -1.49616800    1.73543500   -1.04870500
 C                 -2.36069400    1.01058100    1.10086600
 C                  3.87089800    2.76416000    0.25845100
 H                  4.93795100    2.75856900    0.06600700
 C                 -3.42702500    1.89024100    0.94648200
 H                 -4.17375000    1.95731900    1.73276100
 C                  4.65212900   -0.26739900   -0.86849600
 H                  5.56698400    0.31443400   -0.85842900
 C                 -2.59530100    2.58133200   -1.17658200
 H                 -2.68951300    3.18717600   -2.07361900
 C                 -3.56869300    2.67969500   -0.19021300
 C                  1.09714100    2.75701300    0.78685300
 H                  0.03871200    2.76724400    1.00521700
 F                 -2.28367900   -3.15157600   -2.01305900
 B                 -0.16701600   -0.08329200    0.21346700
 C                  2.25776800   -1.76334600   -0.92815500
 H                  1.34867600   -2.34377800   -0.98300400
 C                  0.23817600   -2.02937000    1.84867200
 C                 -1.24707800   -2.48592400    0.00942800
 C                  3.24537700    3.89715000    0.75198000
 H                  3.82138000    4.79482800    0.94375400
 C                  4.65417700   -1.58439500   -1.29883300
 H                  5.57859300   -2.04672100   -1.62456500
 C                  1.87206400    3.88468900    1.01641400
 H                  1.39712600    4.77408400    1.41458400
 C                 -0.48353900    1.75392700   -2.17120700
 H                 -0.95649700    2.08313600   -3.09825200
 H                 -0.03033500    0.78114400   -2.35219700
 H                  0.32519600    2.45619900   -1.94600000
 F                 -3.05357400   -1.38069700   -1.06508000
 C                 -2.31285800    0.18250100    2.36332400
 H                 -3.06577900    0.52668500    3.07421800
 H                 -1.34131300    0.24014500    2.85837600
 H                 -2.50903800   -0.87158600    2.15089200
 C                 -4.75738800    3.58744500   -0.35933400
 H                 -5.58920300    3.04620100   -0.82126500
 H                 -4.51974700    4.43780200   -1.00178200
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 H                -5.10649200    3.96736200    0.60319100
 C                 1.20159800   -1.15955800    2.62216500
 H                 1.32991400   -1.54148500    3.63595100
 H                 0.87099200   -0.12135000    2.69553400
 H                 2.18446200   -1.14901200    2.14126200
 C                 3.46400800   -2.31788700   -1.33132300
 H                 3.47714400   -3.34150700   -1.68769800
 C                -1.48977900   -3.76580800    0.49398100
 H                -2.14439200   -4.43790500   -0.04518900
 C                -1.93022500   -2.08871400   -1.27069300
 C                -0.02481500   -3.30993700    2.33276000
 H                 0.45462600   -3.63444600    3.25039300
 C                -0.87994500   -4.17517700    1.66860800
 H                -1.06623100   -5.16793200    2.06036600


GS2-Singlet
# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                 0.63072600   -0.71347900   -0.16394000
 C                -1.88890100   -0.00663200   -0.17986900
 C                 1.61440100   -2.76904200    0.16794700
 C                 2.50774100   -1.96115300   -0.63625200
 F                 0.55058400    0.68892900    2.33708700
 C                 0.48498500   -1.98229400    0.43575400
 C                 1.88941700   -0.71236500   -0.80674300
 C                 0.14089000    1.84195300   -0.25766500
 C                -2.82291100    0.65621000    0.64625300
 C                -2.37260000   -0.94490300   -1.12210000
 C                 1.71305400   -4.06264700    0.67612500
 H                 2.58665900   -4.67011000    0.46772100
 C                -3.73650200   -1.21426900   -1.19330400
 H                -4.09272200   -1.93162800   -1.92760300
 C                 3.75033000   -2.22344100   -1.20815600
 H                 4.22460800   -3.18884300   -1.07092400
 C                -4.17576800    0.33792600    0.55930500
 H                -4.87796700    0.83951100    1.21922800
 C                -4.65498300   -0.59500000   -0.35351800
 C                -0.54124600   -2.45963800    1.24826000
 H                -1.40135800   -1.85022300    1.48823500
 F                 2.58133600    0.97592700    1.66518800
 B                -0.35408100    0.33818400   -0.16705700
 C                 2.49489100    0.27733700   -1.57863300
 H                 2.03103300    1.23992400   -1.73863400
 C                -0.24751600    2.65078700   -1.34301200
 C                 0.94375500    2.42019000    0.73905000
 C                 0.67909500   -4.55231300    1.45722400
 H                 0.73434900   -5.55617800    1.86183000
 C                 4.36348100   -1.23242400   -1.95723200
 H                 5.33111300   -1.41439700   -2.40993500
 C                -0.43210600   -3.75108800    1.74206800
 H                -1.22504000   -4.14223600    2.36926300
 C                -2.41377100    1.70757100    1.65040700
 H                -1.99161200    2.58524200    1.15431100
 H                -1.66150800    1.33552200    2.34613900
 H                -3.27650200    2.03536500    2.23244700
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F	1.67078400	2.40596200	2.99137900
C	-1.47684000	-1.68288100	-2.09276500
H	-2.05693100	-2.03123800	-2.94896600
H	-1.02440400	-2.55961900	-1.61992400
H	-0.65972000	-1.06717900	-2.47164400
C	-6.12646000	-0.89412200	-0.45970400
H	-6.59533200	-0.25173400	-1.21187600
H	-6.63676900	-0.71782500	0.48933800
H	-6.29955600	-1.93021900	-0.75838000
C	-1.09721400	2.10538600	-2.46455100
H	-1.15751400	2.82091400	-3.28573900
H	-2.11202900	1.88921700	-2.12251300
H	-0.68477700	1.17551200	-2.86524500
C	3.73387900	0.00259400	-2.13944100
H	4.22024300	0.76711000	-2.73454900
C	1.35439100	3.74709000	0.66987800
H	1.96511200	4.16953200	1.45701900
C	1.43203300	1.62471600	1.92419100
C	0.18082600	3.97545600	-1.40598000
H	-0.11393100	4.58613400	-2.25290500
C	0.97276000	4.52596900	-0.40987300
H	1.29087600	5.55968600	-0.47272100

GS1-triplet
freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3
N	1.25913500	0.05241400	0.06233600
C	-1.11568100	1.14920500	-0.04491100
C	3.38148200	0.90979200	0.16547700
C	3.39965200	-0.27992900	-0.68602800
F	-1.81340100	-1.24666800	-1.92375100
C	2.03839600	1.05561100	0.59022000
C	2.06510100	-0.75237900	-0.71161800
C	-0.71166500	-1.51844600	0.77985000
C	-0.88813000	1.95310800	-1.18705200
C	-2.10067600	1.59045600	0.87666000
C	4.33291900	1.81079100	0.58033900
H	5.36718300	1.72363500	0.27060300
C	-2.79502900	2.77435000	0.65224200
H	-3.53658900	3.09602400	1.37986800
C	4.37465900	-0.94250900	-1.39273900
H	5.40351400	-0.60378200	-1.38989900
C	-1.60423200	3.13328700	-1.37780100
H	-1.41442700	3.72630200	-2.26943900
C	-2.56420000	3.56624100	-0.47052700
C	1.63328500	2.09490700	1.43035600
H	0.59815100	2.19165300	1.73092400
F	-3.40257400	-2.62176600	-1.48442600
B	-0.26509900	-0.12623600	0.27261400
C	1.68937300	-1.87831100	-1.44588400
H	0.66063600	-2.21287800	-1.45561600
C	-0.00215800	-2.20601200	1.81550100
C	-1.85323000	-2.20053200	0.26104700
C	3.93156700	2.85977300	1.42587400
H	4.66973300	3.57908500	1.75962100

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 C                  4.00426600   -2.08044000   -2.13064800
 H                  4.76188200   -2.61407700   -2.69181300
 C                  2.60881200    2.99611700    1.84193200
 H                  2.33519500    3.81778800    2.49171800
 C                  0.10702500    1.54921500   -2.24759500
 H                 -0.08283500    2.08270900   -3.18136000
 H                  0.05050800    0.47729100   -2.45066700
 H                  1.13742800    1.77547900   -1.95104500
 F                 -3.44809400   -0.65227100   -0.63666600
 C                 -2.41020900    0.80853900    2.12852800
 H                 -3.04212800    1.38889700    2.80468400
 H                 -1.49488000    0.52712400    2.65811600
 H                 -2.93152400   -0.12328900    1.89251600
 C                 -3.35266400    4.82864600   -0.70446800
 H                 -4.33172800    4.60352500   -1.14031800
 H                 -2.83304000    5.50091700   -1.39097700
 H                 -3.52934100    5.36550800    0.23119800
 C                  1.18874000   -1.58054500    2.49711600
 H                  1.42549700   -2.11024700    3.42162100
 H                  0.99044800   -0.53315200    2.74668900
 H                  2.08771000   -1.60186800    1.87297100
 C                  2.68757700   -2.53450100   -2.15807900
 H                  2.43677300   -3.41192000   -2.74072600
 C                 -2.28231400   -3.42608600    0.76541000
 H                 -3.15506300   -3.90528700    0.34145700
 C                 -2.61622200   -1.67402900   -0.92421000
 C                 -0.44178400   -3.43415300    2.28706100
 H                  0.10724300   -3.91255000    3.09290800
 C                 -1.58369100   -4.05091500    1.78318500
 H                 -1.91798400   -5.00378800    2.17569000


GS2-triplet
# freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3
 N                 -0.56868500   -0.68504500    0.20077700
 C                  1.92980000    0.09256300    0.28454000
 C                 -1.53477500   -2.70470900   -0.27188400
 C                 -2.25049300   -2.10044500    0.85118000
 F                 -2.71912300    0.45582000   -1.21925500
 C                 -0.51712200   -1.78049600   -0.62053000
 C                 -1.60875400   -0.86622600    1.09391800
 C                 -0.17947900    1.92572900    0.11430800
 C                  2.87486400    0.70034700   -0.58124400
 C                  2.40816900   -0.90895300    1.16664200
 C                 -1.65493000   -3.88545600   -0.96338200
 H                 -2.42204900   -4.60897600   -0.71565400
 C                  3.74952800   -1.27870400    1.16005300
 H                  4.09001400   -2.03985700    1.85825800
 C                 -3.31685000   -2.48529500    1.62937500
 H                 -3.82577500   -3.42689600    1.46262000
 C                  4.21119100    0.30540500   -0.55487600
 H                  4.91346900    0.78361800   -1.23356300
 C                  4.67306800   -0.68789200    0.30221700
 C                  0.38612100   -2.02941500   -1.65928400
 H                  1.15736400   -1.31114700   -1.90292300
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F	-2.57363200	2.02595400	-2.67608300
B	0.41923400	0.50480700	0.21585000
C	-2.01854200	-0.00370200	2.10690900
H	-1.51739500	0.94295400	2.26310400
C	0.36814000	2.96819300	0.93271200
C	-1.28535100	2.30817300	-0.70429100
C	-0.75066900	-4.13851500	-2.00986200
H	-0.83254100	-5.06572500	-2.56425900
C	-3.73582200	-1.62243800	2.65600100
H	-4.57554300	-1.90961600	3.27737200
C	0.24885500	-3.22639000	-2.34866600
H	0.92785300	-3.45564000	-3.16017500
C	2.47308400	1.76898900	-1.56932500
H	2.26849900	2.72343400	-1.07356300
H	1.55756600	1.49605200	-2.09928200
H	3.26653700	1.93612400	-2.30124200
F	-0.92391100	0.67645100	-2.40174800
C	1.49772400	-1.56755400	2.17418000
H	2.07652700	-2.06169400	2.95704300
H	0.85811500	-2.32907400	1.71511000
H	0.83896400	-0.83397800	2.64876400
C	6.11404900	-1.12718900	0.28721800
H	6.76984800	-0.32759500	-0.06482800
H	6.25489400	-1.98535500	-0.37854400
H	6.44731400	-1.42911800	1.28321500
C	1.52344800	2.70871600	1.86657200
H	1.66335900	3.55181600	2.54637000
H	2.46179300	2.54657600	1.32942300
H	1.35056400	1.80458400	2.45873800
C	-3.09726100	-0.40753500	2.88896500
H	-3.44664000	0.23573000	3.68686400
C	-1.84302400	3.58393800	-0.66154100
H	-2.68267400	3.82503400	-1.30071400
C	-1.86409400	1.37813000	-1.73077400
C	-0.19831800	4.23419300	0.94301300
H	0.22779800	4.99130000	1.59482100
C	-1.31069400	4.55454200	0.16761600
H	-1.74441500	5.54667500	0.20356900

C2

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GS1-conf1 sym
# freq wb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                  0.61108800    0.14614400    0.02286300
 C                 -1.89517500    0.88519200   -0.06350400
 C                  2.60860400    1.30749300   -0.00025500
 C                  2.89455900   -0.09351300   -0.23977600
 F                 -1.69276600   -1.65840800   -1.90548400
 C                  1.21697500    1.42223000    0.14458700
 C                  1.66424600   -0.76873200   -0.21688500
 C                 -1.11546200   -1.59227400    0.86553100
 C                 -1.92985800    1.53441000   -1.31863800
 C                 -2.92058500    1.16689400    0.86575800
 C                  3.43857100    2.41344400    0.11150500
 H                  4.51338100    2.33231400    0.00043300
 C                 -3.91745400    2.08322700    0.54652000
 H                 -4.68641900    2.30392900    1.28166700
 C                  4.08204000   -0.76945500   -0.47717700
 H                  5.03609800   -0.25617900   -0.49723700
 C                 -2.96291300    2.42276400   -1.60944900
 H                 -2.98140500    2.90510500   -2.58302000
 C                 -3.96268600    2.71727400   -0.69097800
 C                  0.65425100    2.65571100    0.44513500
 H                 -0.41045200    2.77244000    0.58983800
 F                 -2.95164900   -3.39464100   -1.69994500
 B                 -0.77018300   -0.17202700    0.23822600
 C                  1.61800800   -2.13099700   -0.48022400
 H                  0.68454400   -2.67353400   -0.51447000
 C                 -0.57980600   -1.90673300    2.13187300
 C                 -1.98814800   -2.52055500    0.27885300
 C                  2.87026800    3.65404700    0.38174600
 C                  4.03850400   -2.14194200   -0.70293200
 C                  1.48424800    3.76615300    0.55268400
 H                  1.03273400    4.72312500    0.77688200
 C                 -0.87500700    1.33952900   -2.38390700
 H                 -1.29146900    1.55474300   -3.36976400
 H                 -0.46955300    0.32994900   -2.40204400
 H                 -0.03741400    2.02525800   -2.22144600
 F                 -3.66651400   -1.47682500   -1.03812800
 C                 -2.97909500    0.51460600    2.22695800
 H                 -3.72855100    1.00240200    2.85250600
 H                 -2.02401300    0.56928900    2.75300400
 H                 -3.24691500   -0.54206600    2.14578000
 C                 -5.07913800    3.66695600   -1.03404700
 H                 -5.93397500    3.12051800   -1.44505700
 H                 -4.76391000    4.39738800   -1.78200900
 H                 -5.42771800    4.20521500   -0.14994400
 C                  0.39664300   -0.99984400    2.84382300
 H                  0.43770200   -1.24330000    3.90651500
 H                  0.14015400    0.05735500    2.75149100
 H                  1.40358000   -1.12021000    2.43262800
 C                  2.80826600   -2.81231000   -0.71028800
 H                  2.76142000   -3.87500300   -0.90626400
 C                 -2.33670000   -3.70979400    0.90905900
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 H                 -3.00245200   -4.41001400    0.42180000
 C                 -2.57632400   -2.26170700   -1.08127300
 C                 -0.94804700   -3.09533100    2.76018900
 H                 -0.54002800   -3.32080800    3.74001300
 C                 -1.81857400   -3.99296400    2.16203900
 H                 -2.08802500   -4.91305500    2.66667200
 O                  5.23593900   -2.74593600   -0.91960500
 O                  3.73596200    4.69744700    0.47219900
 C                  3.21156600    5.98111100    0.75371500
 H                  2.70746500    6.00405600    1.72581300
 H                  4.06577800    6.65487700    0.77760100
 H                  2.51540400    6.30945600   -0.02544000
 C                  5.24912600   -4.13851400   -1.16992600
 H                  4.68853200   -4.38811900   -2.07705900
 H                  6.29420000   -4.40766200   -1.30976900
 H                  4.84232600   -4.70181300   -0.32330200

GS1-conf2 asym
# freq wb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                  0.58298300    0.01000800    0.03599600
 C                 -1.81354400    1.05169200   -0.05027700
 C                  2.70370500    0.92190900    0.02232100
 C                  2.81600800   -0.49780500   -0.24209200
 F                 -1.91660900   -1.44808600   -1.94361400
 C                  1.33645900    1.20131500    0.17842800
 C                  1.51939400   -1.01826400   -0.22247800
 C                 -1.35341000   -1.51991200    0.82989700
 C                 -1.76109400    1.72317200   -1.29305600
 C                 -2.80508900    1.43622000    0.87864000
 C                  3.66073800    1.91951400    0.14573200
 H                  4.71784800    1.71367500    0.02567600
 C                 -3.68531600    2.46842900    0.57046300
 H                 -4.42886200    2.76477700    1.30513900
 C                  3.92623600   -1.30429000   -0.50008500
 H                  4.91736500   -0.87027800   -0.50857500
 C                 -2.67941300    2.73277400   -1.57264800
 H                 -2.63317000    3.23139700   -2.53704200
 C                 -3.64604600    3.12510200   -0.65526500
 C                  0.92695900    2.48767400    0.50455600
 H                 -0.11545400    2.72771500    0.65944600
 F                 -3.38345500   -3.01803600   -1.78483000
 B                 -0.82913000   -0.14118100    0.23612400
 C                  1.30721700   -2.36796700   -0.50878000
 H                  0.31571500   -2.79515800   -0.54430400
 C                 -0.87068800   -1.92830900    2.09059300
 C                 -2.33251500   -2.31678000    0.21811700
 C                  3.24608900    3.21410800    0.43934500
 C                  3.71211400   -2.65259400   -0.74804500
 C                  1.88418800    3.48872900    0.62349200
 H                  1.55203300    4.48890200    0.86689100
 C                 -0.72947400    1.42326300   -2.35668700
 H                 -1.11278100    1.69900900   -3.34093700
 H                 -0.44284500    0.37407300   -2.38843100
 H                  0.18042400    2.00562800   -2.18059900
 F                 -3.85863300   -1.04181300   -1.08079200
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 C                 -2.94870500    0.77320000    2.22835600
 H                 -3.63241800    1.34075500    2.86189700
 H                 -1.99557200    0.69856500    2.75549200
 H                 -3.34713400   -0.23992200    2.12928100
 C                 -4.64127400    4.20429900   -0.98839200
 H                 -5.54210600    3.77001700   -1.43354600
 H                 -4.22954500    4.91681800   -1.70619500
 H                 -4.94754600    4.75152500   -0.09424600
 C                  0.20610600   -1.16731500    2.82837600
 H                  0.20454100   -1.43380900    3.88636300
 H                  0.08710500   -0.08454800    2.75493400
 H                  1.19389600   -1.40736300    2.42323400
 C                  2.40485800   -3.16879300   -0.75605200
 H                  2.27466600   -4.22173600   -0.97505500
 C                 -2.83250600   -3.46655300    0.81853600
 H                 -3.57753900   -4.06570300    0.31166800
 C                 -2.87435200   -1.95532500   -1.13794700
 C                 -1.38999800   -3.07533400    2.68893700
 H                 -1.02000500   -3.37356700    3.66437300
 C                 -2.36259100   -3.84183200    2.06633900
 H                 -2.74888200   -4.73227100    2.54769800
 O                  4.69368900   -3.55358200   -1.00732300
 O                  4.23072200    4.14552600    0.53890900
 C                  3.86430100    5.47870800    0.83953800
 H                  3.37358000    5.54936300    1.81617000
 H                  4.79246200    6.04629800    0.86370900
 H                  3.20631400    5.89671400    0.07020500
 C                  6.02968700   -3.08852200   -1.02732500
 H                  6.32252200   -2.67381200   -0.05667000
 H                  6.64756300   -3.95646500   -1.24838200
 H                  6.17730900   -2.33197200   -1.80556500

GS1-conf3 asym
# freq wb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                  0.57118100    0.14017800    0.07023000
 C                 -1.86845300    1.08097100   -0.02564900
 C                  2.64826700    1.14311200    0.05576300
 C                  2.82598600   -0.26966700   -0.20990400
 F                 -1.83981000   -1.42154900   -1.93268500
 C                  1.27671500    1.36014700    0.21178200
 C                  1.54753900   -0.85008400   -0.19038800
 C                 -1.30350400   -1.47025100    0.84928400
 C                 -1.83913800    1.75493200   -1.26717500
 C                 -2.88738600    1.41421100    0.89452400
 C                  3.57462500    2.18109000    0.17924900
 H                  4.62982400    1.97926600    0.05004000
 C                 -3.81568200    2.40012500    0.57888600
 H                 -4.57979100    2.65823200    1.30690200
 C                  3.95694500   -1.03116900   -0.46751900
 H                  4.94801300   -0.59340400   -0.48564500
 C                 -2.80613600    2.71637100   -1.55529800
 H                 -2.77639400    3.21697100   -2.51927700
 C                 -3.79901000    3.05878100   -0.64696800
 C                  0.80809000    2.63333200    0.54192100
 H                 -0.24385900    2.82732000    0.69712600
```

F	-3.25186300	-3.04223600	-1.78617300
B	-0.83435000	-0.06780700	0.26442100
C	1.39569800	-2.20029000	-0.47614000
H	0.42335600	-2.66935000	-0.51197600
C	-0.81433600	-1.86189100	2.11264200
C	-2.24030800	-2.30728900	0.22518400
C	3.09983100	3.45027300	0.47536800
C	3.80663500	-2.39157100	-0.71706200
C	1.72247900	3.66138400	0.66012800
H	1.38961900	4.66269900	0.90571600
C	-0.78577900	1.50960400	-2.32359800
H	-1.18227800	1.74875200	-3.31221500
H	-0.43117500	0.48115500	-2.34236500
H	0.08339700	2.15250300	-2.15202800
F	-3.80070200	-1.08477800	-1.08301500
C	-3.00878100	0.74323700	2.24238100
H	-3.73239900	1.26921200	2.86737000
H	-2.05925700	0.72486500	2.78108500
H	-3.34491700	-0.29169600	2.13839100
C	-4.84513500	4.08694000	-0.98534700
H	-5.75291700	3.60173200	-1.35777100
H	-4.49406800	4.77184700	-1.75972600
H	-5.12374600	4.67236900	-0.10621800
C	0.22113100	-1.05644500	2.86196100
H	0.22657300	-1.33045500	3.91801600
H	0.05107200	0.01996700	2.79570000
H	1.22116600	-1.24660200	2.46049700
C	2.52860600	-2.96620100	-0.72668800
H	2.39935200	-4.01853600	-0.94032000
C	-2.69368000	-3.48096300	0.81652100
H	-3.40696300	-4.11045900	0.30083700
C	-2.78493500	-1.96319500	-1.13432600
C	-1.28716000	-3.03341900	2.70182800
H	-0.91341500	-3.31858300	3.67975500
C	-2.21871100	-3.84010100	2.06717500
H	-2.56946600	-4.74875000	2.54168800
O	4.95281700	-3.08183400	-0.95363900
O	3.88067900	4.55159300	0.61847900
C	5.27655800	4.39857300	0.44690100
H	5.51819800	4.04541200	-0.56146700
H	5.70858200	5.38620600	0.59501500
H	5.69603700	3.70619200	1.18482600
C	4.85711900	-4.46690700	-1.22704200
H	4.27313900	-4.65710200	-2.13383100
H	5.87742500	-4.81333400	-1.37922800
H	4.41323500	-5.01147200	-0.38681100

GS1-conf4 sym

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# freq wb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)
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0 1

N	0.52867400	0.04676500	0.06140500
C	-1.85103800	1.12633600	-0.02472200
C	2.65698700	0.92983400	0.07167600
C	2.75301400	-0.48347600	-0.22463600
F	-1.97417600	-1.33593500	-1.96394700

C	1.29920900	1.22149500	0.23212400
C	1.44945200	-0.98857900	-0.21797800
C	-1.43555600	-1.46863600	0.81170000
C	-1.77269600	1.82430700	-1.25159600
C	-2.84697000	1.50674200	0.90134500
C	3.64011200	1.91201400	0.21906200
H	4.68297600	1.65584300	0.08586400
C	-3.70505200	2.56139400	0.60709000
H	-4.45151200	2.85457000	1.34005800
C	3.85302800	-1.29981600	-0.49892000
H	4.85059900	-0.88064400	-0.49691000
C	-2.67048100	2.85547200	-1.51856400
H	-2.60461700	3.37484600	-2.47074000
C	-3.63994300	3.24480200	-0.60284700
C	0.90264100	2.51108000	0.59270600
H	-0.13663300	2.76062700	0.75338500
F	-3.46241000	-2.88947600	-1.84792200
B	-0.88814300	-0.08656700	0.24787100
C	1.21996100	-2.32913800	-0.53320800
H	0.22303500	-2.74258600	-0.57828200
C	-0.96794500	-1.90765000	2.06778300
C	-2.41962600	-2.24079400	0.17675300
C	3.23677200	3.19841700	0.54404700
C	3.62110600	-2.63910500	-0.77627500
C	1.87311400	3.48275600	0.73438200
H	1.59718400	4.49523100	1.00348400
C	-0.73430500	1.52978200	-2.31029200
H	-1.09635300	1.84601600	-3.29035500
H	-0.47573600	0.47449100	-2.37098600
H	0.18856400	2.08122800	-2.10448600
F	-3.91809500	-0.92124900	-1.10942400
C	-3.01835400	0.81603900	2.23383100
H	-3.70181100	1.37985700	2.87093400
H	-2.07363000	0.71522100	2.77160500
H	-3.43060400	-0.18838800	2.10686700
C	-4.61154000	4.34949600	-0.92161700
H	-5.52031300	3.94094500	-1.37494300
H	-4.18322400	5.06406300	-1.62750300
H	-4.90825200	4.88929300	-0.01975800
C	0.11219300	-1.17462600	2.82868300
H	0.10392500	-1.46790300	3.87952000
H	0.00195600	-0.08935500	2.78284400
H	1.09971400	-1.41219000	2.42155800
C	2.30714500	-3.13857400	-0.79659100
H	2.16396400	-4.18492300	-1.03787500
C	-2.93894400	-3.39549800	0.75057800
H	-3.68737700	-3.97501700	0.22619000
C	-2.94530500	-1.84621400	-1.17634400
C	-1.50658300	-3.05930300	2.63951500
H	-1.14829200	-3.38120100	3.61176600
C	-2.48385600	-3.80093900	1.99443700
H	-2.88525900	-4.69555300	2.45524500
O	4.59111900	-3.54738900	-1.05405400
O	4.07788800	4.25094500	0.71227500
C	5.46274000	4.02475100	0.53456700
H	5.68368800	3.68241700	-0.48229800
H	5.94929000	4.98299900	0.70494600

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 H                  5.84354900    3.29288300    1.25524900
 C                  5.93300800   -3.09999800   -1.06204600
 H                  6.22934500   -2.70956500   -0.08237800
 H                  6.53991400   -3.97116900   -1.30016800
 H                  6.09224900   -2.32928400   -1.82401400


GS2-conf1 sym
# freq wb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                 -0.29715800    0.24709700   -0.11889700
 C                  2.22698100   -0.32852200   -0.49474300
 C                 -1.36248300    2.29117100    0.02608000
 C                 -2.33054000    1.30339900   -0.40887200
 F                  0.34332400   -0.71308500    2.51305400
 C                 -0.14354800    1.61815200    0.19324000
 C                 -1.65946200    0.07125300   -0.46980000
 C                  0.36153900   -2.25824600    0.09275100
 C                  3.34020000   -0.78389400    0.24656900
 C                  2.46634700    0.44022900   -1.65734000
 C                 -1.47582200    3.64813000    0.29218900
 H                 -2.41298300    4.17772000    0.16805200
 C                  3.77281700    0.75395800   -2.02536700
 H                  3.93812800    1.33923800   -2.92586100
 C                 -3.67255300    1.41036800   -0.74229000
 H                 -4.19658200    2.35772000   -0.69691600
 C                  4.62811900   -0.42739100   -0.14319400
 H                  5.47125000   -0.76752500    0.45169500
 C                  4.86820900    0.34210800   -1.27686600
 C                  0.96507100    2.29816900    0.67759600
 H                  1.90656300    1.79516500    0.84934900
 F                 -1.73998600   -1.24736700    2.33968700
 B                  0.74585300   -0.73592500   -0.14224700
 C                 -2.33695400   -1.06127200   -0.90029200
 H                 -1.85131800   -2.02316100   -0.97811800
 C                  0.59059600   -3.21082200   -0.91902900
 C                 -0.18576900   -2.70823100    1.30531800
 C                 -0.35434800    4.33840300    0.74091800
 C                 -4.35583400    0.26942300   -1.15045500
 C                  0.85584000    3.65922600    0.93829400
 H                  1.72737000    4.18327300    1.30684900
 C                  3.19472500   -1.64485200    1.47876100
 H                  2.71596200   -2.59831200    1.24256900
 H                  2.58787100   -1.15895400    2.24337000
 H                  4.17275800   -1.85936000    1.91234900
 F                 -0.44020300   -2.37395800    3.63394500
 C                  1.36328000    0.95207300   -2.55746200
 H                  1.74895400    1.12503800   -3.56377500
 H                  0.96724100    1.90205000   -2.18627100
 H                  0.52009600    0.26489500   -2.63545300
 C                  6.27288900    0.67964800   -1.70033300
 H                  6.69832000   -0.13029500   -2.30139400
 H                  6.92368800    0.82236400   -0.83486900
 H                  6.29790600    1.58838400   -2.30511100
 C                  1.15887800   -2.81080000   -2.25832400
 H                  1.13057500   -3.64912900   -2.95575900
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 H                  2.19472400   -2.47649400   -2.16532400
 H                  0.59126200   -1.98956000   -2.70418100
 C                 -3.68383200   -0.95666800   -1.23068700
 H                 -4.20250500   -1.84874700   -1.55502700
 C                 -0.50205800   -4.04676200    1.51438700
 H                 -0.91493900   -4.36629900    2.46236800
 C                 -0.50111700   -1.76234600    2.43760900
 C                  0.25944300   -4.54674700   -0.70049800
 H                  0.42925200   -5.26915700   -1.49199800
 C                 -0.28052900   -4.96853700    0.50504200
 H                 -0.52638500   -6.01236100    0.65924200
 O                 -0.52880600    5.66584700    0.97473500
 O                 -5.66853400    0.44099900   -1.45862400
 C                  0.57464100    6.41385800    1.44835000
 H                  1.40473400    6.40021800    0.73388100
 H                  0.21728300    7.43541700    1.56230400
 H                  0.92313000    6.04394900    2.41856400
 C                 -6.41069600   -0.68750500   -1.87907000
 H                 -6.43963400   -1.46003000   -1.10320700
 H                 -7.42128200   -0.32920600   -2.06515100
 H                 -6.00427700   -1.11380000   -2.80262000


GS2-conf2 asym
# freq wb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                 -0.33754200    0.05523600   -0.14804000
 C                  2.22125900    0.48601500   -0.47647200
 C                 -2.10076900    1.53199700    0.03634800
 C                 -2.61411600    0.26613400   -0.44524300
 F                  0.57185600   -0.66534500    2.47761300
 C                 -0.71758800    1.36995600    0.20631300
 C                 -1.52815600   -0.60986400   -0.53008900
 C                  1.21751400   -2.02136900    0.02891500
 C                  3.41328500    0.46237000    0.28134400
 C                  2.16748600    1.32514400   -1.61372100
 C                 -2.72434900    2.73440800    0.34018800
 H                 -3.79186200    2.87198600    0.21499600
 C                  3.26209500    2.12245500   -1.94003800
 H                  3.20608900    2.75567300   -2.82132200
 C                 -3.90566100   -0.12918300   -0.79980500
 H                 -4.72465100    0.57358200   -0.72019600
 C                  4.47493300    1.29315700   -0.06622800
 H                  5.37536300    1.27890800    0.54157100
 C                  4.42094400    2.13280100   -1.17370500
 C                  0.04522400    2.40474500    0.72979500
 H                  1.10652900    2.29310900    0.90343000
 F                 -1.15820300   -1.92928400    2.22258000
 B                  1.00049500   -0.46143500   -0.16807200
 C                 -1.71891700   -1.90574000   -1.01216400
 H                 -0.90185600   -2.60561800   -1.11179200
 C                  1.81665200   -2.78814300   -0.98928000
 C                  0.85463300   -2.67719400    1.21681500
 C                 -1.95345400    3.78393300    0.82862900
 C                 -4.09239700   -1.42648700   -1.25386200
 C                 -0.57633700    3.61157200    1.02770000
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 H                  0.02683500    4.41608000    1.42629800
 C                  3.58943800   -0.43073000    1.48645100
 H                  3.53030400   -1.48624200    1.20966800
 H                  2.82332800   -0.25063800    2.24098000
 H                  4.56291100   -0.26011200    1.94886200
 F                  0.43343600   -2.53075900    3.54076300
 C                  0.96601200    1.40896100   -2.52935200
 H                  1.27106800    1.75357700   -3.51905800
 H                  0.23033200    2.12052200   -2.14281800
 H                  0.45229900    0.45480300   -2.65146900
 C                  5.59773900    2.99142400   -1.55357700
 H                  6.29271400    2.43184300   -2.18775200
 H                  6.15033700    3.31917000   -0.67043600
 H                  5.28095100    3.87531600   -2.11096700
 C                  2.22757700   -2.16720100   -2.30180400
 H                  2.52679000   -2.93616300   -3.01542900
 H                  3.06517700   -1.47863100   -2.16833700
 H                  1.40886100   -1.59905600   -2.75114800
 C                 -2.99630200   -2.29903900   -1.35982500
 H                 -3.17752200   -3.30158000   -1.72831200
 C                  1.06673500   -4.04033300    1.39519800
 H                  0.78487500   -4.51742500    2.32474800
 C                  0.18017500   -1.95066200    2.35419900
 C                  2.01303400   -4.15514100   -0.80188800
 H                  2.46378100   -4.73791400   -1.59830200
 C                  1.64547400   -4.78198000    0.37898400
 H                  1.81110500   -5.84471400    0.50900200
 O                 -2.62204300    4.93642800    1.09820500
 O                 -5.28930300   -1.94806000   -1.62810000
 C                 -1.88805600    6.03368700    1.60690300
 H                 -1.11382300    6.35865900    0.90360200
 H                 -2.60803200    6.83822100    1.74355800
 H                 -1.42695400    5.79554500    2.57140800
 C                 -6.42886700   -1.11470500   -1.54053900
 H                 -6.33340400   -0.23770700   -2.18998800
 H                 -7.27038500   -1.71846400   -1.87435300
 H                 -6.60531500   -0.78660600   -0.51040200


GS2-conf3 asym
# freq wb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                 -0.29661100    0.15628200   -0.10723100
 C                  2.27328200    0.50221500   -0.45297800
 C                 -2.00197000    1.69556300    0.08669300
 C                 -2.56740400    0.45078300   -0.39134100
 F                  0.61525600   -0.59591400    2.50657600
 C                 -0.63161900    1.48284600    0.24775700
 C                 -1.51056900   -0.47020400   -0.48243900
 C                  1.18818200   -1.97152100    0.05298000
 C                  3.46996900    0.43687300    0.29536500
 C                  2.23825600    1.34721800   -1.58671500
 C                 -2.59310700    2.92323800    0.39445600
 H                 -3.65836900    3.05775600    0.26045600
 C                  3.35539400    2.11044800   -1.91824200
 H                  3.31294400    2.74896100   -2.79640600
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C	-3.86350800	0.09533300	-0.73668500
H	-4.68495500	0.79875000	-0.66777800
C	4.55497200	1.23465400	-0.05720900
H	5.45903100	1.18914100	0.54360300
C	4.51952600	2.08059200	-1.16066800
C	0.17603900	2.49338200	0.77144800
H	1.23335700	2.34351500	0.94000600
F	-1.14899500	-1.81892400	2.28964600
B	1.02334200	-0.40416800	-0.13758300
C	-1.75244300	-1.75249000	-0.95636700
H	-0.96303200	-2.48297900	-1.05853000
C	1.74055400	-2.75661500	-0.97769000
C	0.82390600	-2.61702700	1.24572200
C	-1.77979300	3.93696900	0.87929600
C	-4.10766100	-1.19750700	-1.18739000
C	-0.40520400	3.70957300	1.06970800
H	0.19348000	4.51874900	1.47036600
C	3.62687500	-0.46536200	1.49634800
H	3.52283800	-1.51721600	1.21907800
H	2.87874700	-0.25646600	2.26149500
H	4.61230400	-0.33381200	1.94599200
F	0.45433800	-2.45532800	3.57723600
C	1.03381700	1.47245800	-2.49374700
H	1.34265800	1.81474100	-3.48307800
H	0.32128400	2.20243900	-2.09836400
H	0.49250000	0.53408900	-2.61884200
C	5.72013300	2.90337200	-1.54519100
H	6.39867800	2.32111200	-2.17674500
H	6.28214400	3.21942300	-0.66371300
H	5.42833600	3.79333800	-2.10646900
C	2.13915100	-2.14721300	-2.29919300
H	2.42611100	-2.92218700	-3.01129400
H	2.98032900	-1.46036400	-2.18178900
H	1.31542700	-1.58016100	-2.74154100
C	-3.05148400	-2.11107400	-1.29875300
H	-3.22803000	-3.11639100	-1.65674200
C	0.99329000	-3.98696400	1.41868400
H	0.71217500	-4.45581000	2.35270700
C	0.19103300	-1.87161000	2.39457600
C	1.89497900	-4.12954800	-0.79543200
H	2.31104000	-4.72568000	-1.60079900
C	1.52906800	-4.74571800	0.39173200
H	1.66246500	-5.81344500	0.51792000
O	-2.21376600	5.17949600	1.21363500
O	-5.39866400	-1.48293100	-1.50369900
C	-3.59002600	5.46393700	1.05294300
H	-4.20842500	4.81241400	1.67984500
H	-3.72319000	6.49697100	1.36790100
H	-3.89912300	5.36200100	0.00694300
C	-5.70299100	-2.78503300	-1.96523400
H	-5.45979500	-3.54386800	-1.21380800
H	-6.77550000	-2.79475400	-2.14945300
H	-5.17571600	-3.01380000	-2.89766200

GS2-conf4 sym

freq wb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1

N	-0.28241200	0.03936100	-0.11113900
C	2.17910400	0.86320300	-0.42782300
C	-2.23827500	1.23469500	0.11317300
C	-2.56228500	-0.07148200	-0.41863800
F	0.75431800	-0.63589600	2.48341700
C	-0.85290100	1.26830400	0.28738100
C	-1.36052500	-0.77861400	-0.52599400
C	1.56654900	-1.78596200	-0.01969300
C	3.36598800	0.99567900	0.32693900
C	1.98809500	1.72536000	-1.53253700
C	-3.04431200	2.32376300	0.45600300
H	-4.11534800	2.26970600	0.31132100
C	2.94447000	2.69324500	-1.83077100
H	2.78494500	3.34242400	-2.68740500
C	-3.78189600	-0.63660100	-0.79939600
H	-4.69471800	-0.06374700	-0.70217900
C	4.28426000	1.99236500	0.00889300
H	5.18056700	2.09487800	0.61431400
C	4.09333700	2.85384400	-1.06639400
C	-0.24577600	2.38735700	0.85915000
H	0.81982300	2.42429300	1.03796800
F	-0.76788600	-2.13715900	2.19239900
B	1.11859100	-0.26922800	-0.15359400
C	-1.36035400	-2.07071900	-1.05424300
H	-0.45053900	-2.64197500	-1.16936800
C	2.25476400	-2.41701100	-1.07416700
C	1.32078800	-2.53358900	1.14357000
C	-2.43159600	3.44821800	0.98870000
C	-3.77689500	-1.92913000	-1.30191100
C	-1.03984000	3.46626600	1.19185800
H	-0.60126600	4.35462900	1.63018600
C	3.68394500	0.09830200	1.49921900
H	3.76581100	-0.94629700	1.18918500
H	2.91279200	0.14813400	2.26854200
H	4.63202200	0.38766600	1.95523100
F	0.91376000	-2.53863000	3.47474800
C	0.78165300	1.65502500	-2.44282800
H	1.02149600	2.08164000	-3.41839100
H	-0.05453700	2.22564300	-2.02779300
H	0.42477600	0.63682700	-2.60177500
C	5.12103100	3.89737400	-1.41450600
H	5.90110700	3.47057000	-2.05294100
H	5.60780100	4.28784800	-0.51817100
H	4.67144000	4.73255300	-1.95533800
C	2.53914100	-1.69479900	-2.36804300
H	2.96346400	-2.37701600	-3.10589700
H	3.24114800	-0.87161100	-2.21770000
H	1.62671200	-1.27074500	-2.79628200
C	-2.56592900	-2.63105900	-1.42764500
H	-2.59917700	-3.63551500	-1.83220200
C	1.73298600	-3.85668700	1.26468100
H	1.53652500	-4.40648800	2.17586700
C	0.56015500	-1.96006300	2.31346800
C	2.65355200	-3.74587900	-0.94346000
H	3.17256200	-4.22499200	-1.76701000

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 C                  2.40019000   -4.46489800    0.21474900
 H                  2.72238600   -5.49570400    0.30045000
 O                 -3.08578600    4.57878700    1.36068100
 O                 -4.88422600   -2.60333100   -1.70731600
 C                 -4.48883200    4.61798900    1.18721300
 H                 -4.98663400    3.84253600    1.77955200
 H                 -4.80881200    5.59742300    1.53709500
 H                 -4.76408700    4.50287700    0.13310700
 C                 -6.13239800   -1.94673300   -1.60186900
 H                 -6.16070000   -1.04083300   -2.21728800
 H                 -6.87613600   -2.65200900   -1.96731700
 H                 -6.36029800   -1.68716300   -0.56229300


GS1-conf1 sym
# freq uwb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3
 N                  0.67053900   -0.04943700    0.15293300
 C                 -1.53860800    1.24450400   -0.39522000
 C                  2.88708600    0.53409300    0.11715800
 C                  2.76200200   -0.84802100   -0.33859600
 F                 -2.49161100   -1.52395500   -1.53777900
 C                  1.56464000    0.96224400    0.39924600
 C                  1.37341700   -1.13828100   -0.29481900
 C                 -1.49756700   -1.09041800    1.18436100
 C                 -1.18225300    1.64722900   -1.70511200
 C                 -2.48453000    2.04617000    0.29525900
 C                  3.94668500    1.38177900    0.29842200
 H                  4.97021200    1.09240100    0.09521900
 C                 -3.01584500    3.18444600   -0.30209600
 H                 -3.73504000    3.78327500    0.25210900
 C                  3.65765500   -1.79376100   -0.75876300
 H                  4.72398000   -1.61100400   -0.80561600
 C                 -1.73559200    2.79434400   -2.27059200
 H                 -1.45402400    3.07045900   -3.28424500
 C                 -2.65205600    3.58442700   -1.58595000
 C                  1.30657000    2.25050300    0.86797100
 H                  0.29239200    2.57030500    1.06972200
 F                 -4.26251700   -2.49483700   -0.80839000
 B                 -0.86431800    0.02751400    0.32266700
 C                  0.88328400   -2.38494700   -0.68675900
 H                 -0.17825400   -2.59192600   -0.65926000
 C                 -0.90137300   -1.52071100    2.41373200
 C                 -2.70737800   -1.75830800    0.82450000
 C                  3.68786300    2.68781800    0.77233900
 C                  3.16393600   -3.05928400   -1.15018100
 C                  2.37800800    3.10954900    1.05267500
 H                  2.18986500    4.11145600    1.41195700
 C                 -0.22856100    0.83416200   -2.54707800
 H                 -0.33243700    1.08837900   -3.60421800
 H                 -0.41897200   -0.23552600   -2.43314800
 H                  0.81661500    1.01339700   -2.27159900
 F                 -4.05841600   -0.37103800   -0.59070900
 C                 -2.92962100    1.70221300    1.69469300
 H                 -3.50132100    2.52237300    2.13533200
 H                 -2.07329800    1.48372600    2.33998500
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 H                -3.55881600    0.80785100    1.70053700
 C                -3.21654500    4.84030000   -2.19799900
 H                -4.26244300    4.98480000   -1.91553600
 H                -3.15901300    4.81089100   -3.28858300
 H                -2.66313200    5.72414700   -1.86276800
 C                 0.34883100   -0.86863800    2.94953600
 H                 0.49676500   -1.12634900    3.99997200
 H                 0.28448900    0.22158400    2.87151200
 H                 1.24777800   -1.17892100    2.40792500
 C                 1.78840700   -3.34166400   -1.11533200
 H                 1.41948800   -4.31041500   -1.42104100
 C                -3.30162900   -2.71882500    1.64058400
 H                -4.22097300   -3.19633200    1.32749500
 C                -3.36660300   -1.52593500   -0.50715500
 C                -1.50580100   -2.49096100    3.19850600
 H                -1.03858000   -2.76943600    4.13877200
 C                -2.70970700   -3.09006900    2.83464900
 H                -3.17225300   -3.83588900    3.47004200
 O                 4.10060600   -3.92988700   -1.54398800
 O                 4.77377400    3.45618200    0.92114000
 C                 4.61930800    4.78752400    1.39854100
 H                 4.18152400    4.79500900    2.40038800
 H                 5.62255800    5.20419500    1.43610400
 H                 4.00241200    5.37832500    0.71618500
 C                 3.70428100   -5.23021500   -1.96512500
 H                 3.04807300   -5.17475700   -2.83780700
 H                 4.62357400   -5.74508000   -2.23210600
 H                 3.20468400   -5.76792300   -1.15487000


GS1-conf2 asym
# freq uwb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3
 N                 0.61591300   -0.10735600    0.15179300
 C                -1.59620600    1.18680300   -0.38097000
 C                 2.82517300    0.51908800    0.15187000
 C                 2.71922700   -0.84675900   -0.35081800
 F                -2.53644400   -1.53064000   -1.62276200
 C                 1.50327200    0.92119000    0.44225500
 C                 1.33023500   -1.15576600   -0.32362600
 C                -1.55723400   -1.19855500    1.11975900
 C                -1.23009100    1.63548100   -1.67273700
 C                -2.54872900    1.96197300    0.32966700
 C                 3.87823000    1.37300400    0.36384500
 H                 4.90480400    1.10035900    0.15240800
 C                -3.08169400    3.11694900   -0.23366000
 H                -3.80204000    3.69805800    0.33769400
 C                 3.64050500   -1.76281700   -0.79789400
 H                 4.69529500   -1.52434600   -0.81505200
 C                -1.78488200    2.79807300   -2.20416300
 H                -1.49104500    3.11345300   -3.20277700
 C                -2.71414200    3.55796600   -1.50269800
 C                 1.22842300    2.18213900    0.94942900
 H                 0.21079200    2.48601800    1.15867300
 F                -4.30290500   -2.54291000   -0.94084900
 B                -0.92138700   -0.04994800    0.30323700
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C	0.85657000	-2.40736500	-0.76752800
H	-0.20196200	-2.62949000	-0.75338800
C	-0.96913400	-1.66755600	2.33932800
C	-2.76140000	-1.85948800	0.72777200
C	3.60514100	2.65784900	0.87910900
C	3.16118200	-3.01511200	-1.23387800
C	2.29323700	3.05119800	1.16748800
H	2.08880500	4.03747100	1.55982200
C	-0.25710100	0.86190800	-2.52964900
H	-0.34581200	1.15581500	-3.57781400
H	-0.44169200	-0.21267000	-2.46034900
H	0.78186700	1.03831500	-2.22973900
F	-4.11624200	-0.42787700	-0.63789600
C	-2.99584400	1.57439700	1.71714400
H	-3.57401200	2.37783300	2.17966000
H	-2.14068200	1.34194300	2.35908100
H	-3.61978200	0.67662300	1.69435700
C	-3.32956000	4.79499600	-2.10402100
H	-4.28821000	4.56378500	-2.58048500
H	-2.68072700	5.23204900	-2.86667000
H	-3.52025200	5.55461300	-1.34154300
C	0.27035100	-1.02429200	2.91020700
H	0.40047700	-1.30357600	3.95750700
H	0.20495600	0.06707600	2.85345900
H	1.17975300	-1.32075100	2.37840800
C	1.77687600	-3.31666500	-1.21654200
H	1.47195800	-4.29335600	-1.56955900
C	-3.35557100	-2.85188100	1.50478400
H	-4.27012800	-3.32275100	1.16847300
C	-3.41558500	-1.58019700	-0.59722400
C	-1.57346100	-2.66850600	3.08423700
H	-1.11262800	-2.97630300	4.01854500
C	-2.77025300	-3.26246300	2.68920600
H	-3.23282700	-4.03346500	3.29375900
O	3.94474100	-3.99252400	-1.68733600
O	4.68595800	3.43572900	1.05705700
C	4.50733100	4.74606800	1.57644500
H	4.06477300	4.71516400	2.57629900
H	5.50278300	5.17963000	1.63306700
H	3.88284400	5.35027100	0.91215500
C	5.35432200	-3.79129100	-1.74588500
H	5.76171600	-3.60511100	-0.74905200
H	5.76501700	-4.71633600	-2.14133900
H	5.60110000	-2.96411000	-2.41605000

GS1-conf3 asym

freq uwb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	0.62060400	0.02961100	0.18292500
C	-1.64273800	1.22697200	-0.35168400
C	2.80116900	0.71316800	0.19455800
C	2.75526700	-0.65449000	-0.31257000
F	-2.46954300	-1.52270100	-1.59227800
C	1.45100900	1.06146800	0.47342300
C	1.39051000	-1.01907700	-0.29989900

C	-1.50406400	-1.15675500	1.14903500
C	-1.29050600	1.69026900	-1.64200400
C	-2.62441200	1.96606700	0.35821400
C	3.82393600	1.60286200	0.42021400
H	4.84953900	1.33366600	0.20768800
C	-3.19564200	3.10306200	-0.20341700
H	-3.93720000	3.65734900	0.36742000
C	3.70965100	-1.53464900	-0.75552200
H	4.76464100	-1.29077000	-0.77985300
C	-1.88408400	2.83445200	-2.17192700
H	-1.59983900	3.16169200	-3.16950400
C	-2.84012000	3.56009000	-1.47059100
C	1.12087800	2.32909000	0.99291800
H	0.08981400	2.59003500	1.19253200
F	-4.18901600	-2.61431800	-0.91332600
B	-0.91796900	0.01936500	0.33392900
C	0.97336200	-2.26663900	-0.74007700
H	-0.07554000	-2.53256900	-0.73460200
C	-0.89694300	-1.60482000	2.36729700
C	-2.68194100	-1.86386200	0.75770600
C	3.48765000	2.86967000	0.93899200
C	3.29199000	-2.80770500	-1.19987600
C	2.14260400	3.21369800	1.21841700
H	1.94937300	4.20284700	1.61309400
C	-0.29207000	0.95039900	-2.49963800
H	-0.40784600	1.22311500	-3.55094800
H	-0.42380300	-0.13031300	-2.41110900
H	0.74150400	1.17942900	-2.21722600
F	-4.09882900	-0.49343900	-0.60788500
C	-3.06026000	1.55843000	1.74337100
H	-3.67580100	2.33492100	2.20358700
H	-2.19838200	1.36419400	2.38919600
H	-3.64280800	0.63345000	1.71718400
C	-3.49585200	4.77778400	-2.06874500
H	-4.45995600	4.52162700	-2.52076500
H	-2.87393000	5.22163400	-2.84957200
H	-3.68561600	5.54026100	-1.30879100
C	0.32083900	-0.91997400	2.93610100
H	0.47679100	-1.21490100	3.97552400
H	0.20725700	0.16858900	2.90413700
H	1.23422500	-1.16718500	2.38623400
C	1.93765300	-3.16159700	-1.19260900
H	1.62262200	-4.13626200	-1.53770700
C	-3.23868200	-2.87703800	1.53581300
H	-4.13507000	-3.38196600	1.19993300
C	-3.34628500	-1.61272700	-0.56777600
C	-1.46314700	-2.62719700	3.11302800
H	-0.98946500	-2.91834800	4.04620400
C	-2.63811600	-3.26463400	2.72016500
H	-3.07145100	-4.05161400	3.32580000
O	4.28312600	-3.61315600	-1.61522600
O	4.38019500	3.82386600	1.20212600
C	5.76154900	3.57764600	0.95414900
H	5.93632100	3.37664500	-0.10580900
H	6.27721900	4.48966600	1.24247200
H	6.12285200	2.74404200	1.56163400
C	3.95625200	-4.91316100	-2.08702500

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 H                  3.30423900   -4.86031700   -2.96365100
 H                  4.90164000   -5.37285500   -2.36449500
 H                  3.47747400   -5.50651700   -1.30278300


GS1-conf4 sym
# freq uwb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3
 N                  0.56408100   -0.02661500    0.18689500
 C                 -1.69074400    1.19945200   -0.31462500
 C                  2.74417200    0.64648100    0.23321800
 C                  2.70087300   -0.70382400   -0.31642400
 F                 -2.47425800   -1.50532300   -1.70994800
 C                  1.38654400    0.98681400    0.51729500
 C                  1.34533400   -1.06516200   -0.32799700
 C                 -1.57626700   -1.25366400    1.06702300
 C                 -1.31685400    1.72795800   -1.57408500
 C                 -2.69179600    1.89722500    0.41044100
 C                  3.76011100    1.53242400    0.48602300
 H                  4.78841100    1.27745700    0.26891200
 C                 -3.25644700    3.05940900   -0.10452400
 H                 -4.01748700    3.57689100    0.47515100
 C                  3.67643400   -1.56819800   -0.78025700
 H                  4.71939800   -1.28203100   -0.76668500
 C                 -1.90468700    2.89542300   -2.05711900
 H                 -1.60828400    3.26910300   -3.03470000
 C                 -2.87442400    3.58424300   -1.33721900
 C                  1.05221600    2.24119600    1.07739100
 H                  0.01958700    2.49134000    1.28206800
 F                 -4.21063300   -2.62065900   -1.11743100
 B                 -0.97507600   -0.03970600    0.31917600
 C                  0.93062900   -2.29971500   -0.81626000
 H                 -0.11733600   -2.56806400   -0.83258700
 C                 -0.99565400   -1.75345800    2.27698300
 C                 -2.74374500   -1.94198400    0.61844100
 C                  3.41700300    2.78621700    1.04015800
 C                  3.26280500   -2.81731200   -1.26715300
 C                  2.06850300    3.11968200    1.33061700
 H                  1.87432000    4.09647300    1.75421100
 C                 -0.30636300    1.03023400   -2.45319800
 H                 -0.41303100    1.34876900   -3.49253300
 H                 -0.43355700   -0.05394500   -2.41429800
 H                  0.72348500    1.25042700   -2.15078500
 F                 -4.12611800   -0.51388000   -0.72567600
 C                 -3.15984900    1.41408000    1.76023700
 H                 -3.78274600    2.16619100    2.25011200
 H                 -2.31268900    1.17966900    2.41214700
 H                 -3.74472800    0.49454700    1.66964200
 C                 -3.47677100    4.86350300   -1.85783200
 H                 -4.53276500    4.94433600   -1.58789800
 H                 -3.39735100    4.92571300   -2.94568800
 H                 -2.96548900    5.73747000   -1.43992900
 C                  0.21198400   -1.09546400    2.89674200
 H                  0.34981100   -1.43533600    3.92495700
 H                  0.09920200   -0.00630700    2.90933500
 H                  1.13422200   -1.32006100    2.35185800
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C	1.90263000	-3.16581400	-1.28319100
H	1.63351000	-4.13904000	-1.67394100
C	-3.31825700	-2.98661800	1.34010900
H	-4.20628300	-3.47641900	0.96228600
C	-3.37567000	-1.63531600	-0.71174700
C	-1.57857400	-2.80573700	2.96635500
H	-1.12548500	-3.13751900	3.89620500
C	-2.74483400	-3.42383400	2.52051400
H	-3.19187600	-4.23523600	3.08240900
O	4.10494800	-3.75275900	-1.74545400
O	4.30337300	3.73360500	1.32692400
C	5.68801000	3.50841700	1.06708900
H	5.85879600	3.34065700	0.00110000
H	6.19410400	4.41731400	1.38028200
H	6.05805100	2.66155900	1.64966800
C	5.49555600	-3.47127800	-1.76752200
H	5.88015900	-3.29835800	-0.75773200
H	5.97020900	-4.35480000	-2.18764800
H	5.71398900	-2.60627100	-2.40122900

GS2-conf1 sym

freq uwb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	-0.31231400	0.16721500	-0.13485400
C	2.18682700	-0.30174900	-0.75547700
C	-1.49924400	2.11703300	0.05109400
C	-2.34822100	1.11712600	-0.59102300
F	-1.79925700	-0.74518000	2.11525300
C	-0.26440000	1.46317200	0.30272200
C	-1.55701200	-0.05437700	-0.67661100
C	0.58857900	-2.23130300	0.48928400
C	3.41803900	-0.49353000	-0.07919300
C	2.22169700	0.42836500	-1.97012000
C	-1.67539000	3.42868800	0.39898900
H	-2.60038000	3.96322500	0.22189700
C	3.42115000	0.93776100	-2.45812300
H	3.41908500	1.48035200	-3.40078700
C	-3.63053500	1.12850600	-1.07172400
H	-4.26641800	2.00373300	-1.02376600
C	4.60008300	0.02979600	-0.60085100
H	5.52935400	-0.12818100	-0.05848000
C	4.62728100	0.75560900	-1.78687000
C	0.79819600	2.13664600	0.90918300
H	1.73678300	1.63056600	1.09190400
F	-0.94987900	-1.77578900	3.79534700
B	0.85179200	-0.84734700	-0.13913200
C	-2.05613600	-1.22193400	-1.24867600
H	-1.44650200	-2.11507100	-1.29780000
C	1.11136400	-3.40424600	-0.15209500
C	-0.19855300	-2.47563300	1.65775100
C	-0.60100000	4.11062200	1.01461600
C	-4.13971100	-0.05373200	-1.65299400
C	0.62096500	3.46229700	1.26355900
H	1.43721400	3.99229600	1.73360200
C	3.49331600	-1.24503900	1.22845400

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 H                  3.36127900   -2.32226800    1.08459700
 H                  2.70349800   -0.92876300    1.91386500
 H                  4.46140700   -1.08804800    1.70976300
 F                  0.25063600   -0.37614500    2.69240000
 C                  0.97676800    0.63391700   -2.79877200
 H                  1.23320800    0.91682700   -3.82183900
 H                  0.33934500    1.42620700   -2.39192800
 H                  0.37339400   -0.27805300   -2.83718800
 C                  5.90894600    1.34512500   -2.31596600
 H                  6.77966600    0.79440500   -1.95277100
 H                  6.02213700    2.38707400   -1.99797300
 H                  5.92938700    1.33429100   -3.40864200
 C                  1.94927800   -3.30687700   -1.40228800
 H                  2.08133000   -4.29297400   -1.85281800
 H                  2.94026700   -2.88914500   -1.20496300
 H                  1.47936300   -2.64485400   -2.13633000
 C                 -3.35302500   -1.21265300   -1.73894600
 H                 -3.75129700   -2.11417400   -2.18267200
 C                 -0.50987100   -3.76128400    2.09587600
 H                 -1.11352400   -3.89509900    2.98458300
 C                 -0.66598700   -1.35749000    2.54366600
 C                  0.79803300   -4.67054200    0.31646700
 H                  1.18922300   -5.53466600   -0.21287000
 C                 -0.02520700   -4.86889000    1.42452200
 H                 -0.26908800   -5.86898600    1.76245500
 O                 -0.85057500    5.38800200    1.32316100
 O                 -5.40126800    0.03496600   -2.09603400
 C                  0.16687500    6.16232900    1.94820000
 H                  1.04688900    6.24263400    1.30459600
 H                 -0.26582300    7.14796000    2.09907700
 H                  0.44663700    5.73278700    2.91373600
 C                 -6.00386700   -1.10578300   -2.69432900
 H                 -6.05746800   -1.93700000   -1.98585900
 H                 -7.00907100   -0.79694300   -2.96989100
 H                 -5.45683900   -1.41321400   -3.58983700


GS2-conf2 asym
# freq uwb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3
 N                 -0.31687200   -0.01259500   -0.15591400
 C                  2.19609200    0.44512700   -0.71697200
 C                 -2.08878800    1.42896400    0.09550900
 C                 -2.54022800    0.23820600   -0.61438800
 F                  0.31510700   -0.52536900    2.62781400
 C                 -0.71815500    1.22376800    0.35209700
 C                 -1.38978800   -0.59520400   -0.73083400
 C                  1.34702200   -1.99446000    0.35408900
 C                  3.39657000    0.66056800    0.00416300
 C                  1.99885800    1.20999600   -1.89266300
 C                 -2.71360100    2.58410400    0.49998800
 H                 -3.76435700    2.77440700    0.31921100
 C                  2.95316300    2.13460800   -2.30632400
 H                  2.77861700    2.70121800   -3.21816800
 C                 -3.75107400   -0.15045500   -1.13162300
 H                 -4.62216900    0.48403900   -1.04134500
```

C	4.33093500	1.59400200	-0.44214800
H	5.23918500	1.74732300	0.13602300
C	4.13139400	2.34545400	-1.59533700
C	0.03806400	2.17457000	1.01526800
H	1.09106000	2.01394000	1.20493700
F	-1.45799000	-1.56826000	1.96306700
B	1.12273000	-0.56805900	-0.18183700
C	-1.46244900	-1.84475000	-1.38434600
H	-0.58575500	-2.47480600	-1.45769900
C	2.26562100	-2.86650700	-0.32397600
C	0.66469600	-2.57818000	1.46847300
C	-1.94988600	3.55533200	1.17627100
C	-3.81572600	-1.39974500	-1.78281800
C	-0.58962800	3.34691600	1.42778700
H	-0.00546900	4.09442300	1.94590400
C	3.69391400	-0.08557000	1.28302400
H	3.94824800	-1.13282700	1.09013900
H	2.82533500	-0.09909200	1.94569600
H	4.53373500	0.37128600	1.81170000
F	-0.31474300	-2.32772800	3.61305400
C	0.77371600	1.02248800	-2.75444600
H	0.92982400	1.44332500	-3.74991700
H	-0.10565100	1.51511400	-2.32575600
H	0.52917000	-0.03830700	-2.86619800
C	5.16592200	3.32904400	-2.07782800
H	5.82769000	2.86909900	-2.81940900
H	5.79126300	3.68323800	-1.25503000
H	4.69962500	4.19690200	-2.55081400
C	3.05058400	-2.39883700	-1.52388500
H	3.54117700	-3.24312100	-2.01306600
H	3.81863500	-1.66776700	-1.25771900
H	2.39685400	-1.90442700	-2.24930000
C	-2.66904700	-2.22690800	-1.90178800
H	-2.78636300	-3.17495100	-2.41065500
C	0.80997300	-3.91979300	1.81689900
H	0.26800600	-4.31562000	2.66656400
C	-0.18389700	-1.75829300	2.39574600
C	2.40055400	-4.19191200	0.05632400
H	3.08310300	-4.82756100	-0.50049300
C	1.66787100	-4.74121000	1.10916500
H	1.77901400	-5.78503000	1.37730700
O	-2.62858200	4.65934200	1.53997200
O	-4.92486500	-1.89680300	-2.32451900
C	-1.93642100	5.68616800	2.23455300
H	-1.12325200	6.09416900	1.62693000
H	-2.67266200	6.46365800	2.42403200
H	-1.53966700	5.31969700	3.18601900
C	-6.13810800	-1.15126900	-2.25102600
H	-6.03672500	-0.19394100	-2.76792400
H	-6.88525100	-1.76037200	-2.75237300
H	-6.43146700	-0.99097900	-1.21079600

GS2-conf3 asym

freq uwb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	-0.28388900	0.08791000	-0.10595500
C	2.23231800	0.49409600	-0.69712600
C	-2.04948700	1.51340800	0.15099400
C	-2.52125700	0.33350900	-0.56514000
F	0.41374500	-0.38566000	2.70823300
C	-0.66510000	1.28377400	0.39557700
C	-1.39661800	-0.50608900	-0.69691800
C	1.35259800	-1.91257400	0.42387100
C	3.45174900	0.68927200	-0.00081800
C	2.03001500	1.25509000	-1.87566000
C	-2.65855000	2.67356500	0.56357000
H	-3.70915900	2.84568200	0.37372400
C	2.99465500	2.15791000	-2.31233300
H	2.81525000	2.72103700	-3.22543800
C	-3.73921300	-0.04303500	-1.07504200
H	-4.62487100	0.57487800	-0.99189300
C	4.39578200	1.60100700	-0.47085200
H	5.31758000	1.73939300	0.08936600
C	4.18983300	2.34997700	-1.62450000
C	0.12086700	2.24188600	1.07052600
H	1.17237700	2.06099200	1.24794000
F	-1.39453000	-1.37578200	2.05951700
B	1.14708800	-0.48931400	-0.13501400
C	-1.48213800	-1.72875700	-1.33966100
H	-0.61491900	-2.37129200	-1.42479000
C	2.23808000	-2.81266800	-0.25871600
C	0.69000000	-2.45988200	1.56650400
C	-1.86713400	3.62524400	1.23815300
C	-3.83404300	-1.28690700	-1.73201000
C	-0.48889800	3.39511000	1.48128700
H	0.06321700	4.16585300	2.00337900
C	3.75982900	-0.05428500	1.27685400
H	3.99631800	-1.10609500	1.08592500
H	2.90258300	-0.05186000	1.95422100
H	4.61493700	0.39334800	1.78863100
F	-0.27154800	-2.15648800	3.71340900
C	0.78970200	1.08171700	-2.71863700
H	0.94426000	1.47865200	-3.72415100
H	-0.07383400	1.60285200	-2.29169900
H	0.51723300	0.02565200	-2.80551600
C	5.23413600	3.31023200	-2.13220000
H	5.86568400	2.83677700	-2.89145000
H	5.88845500	3.64826000	-1.32531300
H	4.77607700	4.18971000	-2.59165800
C	2.99699200	-2.38338900	-1.48939100
H	3.45333000	-3.24676900	-1.97847700
H	3.78964300	-1.66666100	-1.25829500
H	2.33331300	-1.88532900	-2.20307000
C	-2.71425500	-2.11510900	-1.86147600
H	-2.79117200	-3.06924100	-2.36375900
C	0.82659600	-3.79423700	1.94408800
H	0.30074900	-4.16304100	2.81556400
C	-0.12790400	-1.60462000	2.48994400
C	2.36623100	-4.13101200	0.14989800
H	3.02498400	-4.78918500	-0.40940100
C	1.65583900	-4.64378300	1.23476700
H	1.76060800	-5.68214800	1.52578200

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 O                 -2.33021400    4.78948800    1.68892900
 O                 -5.05851600   -1.58699700   -2.20155300
 C                 -3.70374200    5.11923500    1.49837700
 H                 -4.34961400    4.39425700    1.99955900
 H                 -3.83406400    6.09879900    1.95022600
 H                 -3.94645600    5.17026500    0.43405900
 C                 -5.24612000   -2.82287300   -2.87520900
 H                 -5.02384600   -3.66773700   -2.21675400
 H                 -6.29577500   -2.84962100   -3.15781300
 H                 -4.62484100   -2.87963700   -3.77392300


GS2-conf4 sym
# freq uwb97xd /6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3
 N                 -0.24802000   -0.01977300   -0.13052300
 C                  2.17687700    0.82112100   -0.62930000
 C                 -2.20041000    1.15224500    0.18235900
 C                 -2.48156700   -0.04842300   -0.59317800
 F                  0.41425600   -0.61102500    2.60848200
 C                 -0.82439200    1.12446500    0.44124200
 C                 -1.22257700   -0.70979600   -0.74417300
 C                  1.67371900   -1.77646600    0.27646000
 C                  3.33169900    1.15842400    0.11810200
 C                  1.88222200    1.61686000   -1.76355100
 C                 -2.99792900    2.18835900    0.64011100
 H                 -4.05945200    2.19923200    0.43256500
 C                  2.70100500    2.68644100   -2.11219800
 H                  2.45870100    3.27038300   -2.99724400
 C                 -3.62330400   -0.57441900   -1.13939100
 H                 -4.57550100   -0.07517300   -1.02382800
 C                  4.12991700    2.23641200   -0.26261700
 H                  5.00856000    2.47621900    0.33162900
 C                  3.83204600    3.02025400   -1.37182700
 C                 -0.20850800    2.13445700    1.16949700
 H                  0.85515800    2.11178900    1.36580200
 F                 -1.18074400   -1.86724900    1.86542800
 B                  1.25449800   -0.36454400   -0.17164800
 C                 -1.12007800   -1.92215300   -1.46761200
 H                 -0.16310900   -2.41726600   -1.56723100
 C                  2.71036900   -2.46727900   -0.43961500
 C                  1.07065000   -2.52003100    1.34063100
 C                 -2.38017300    3.20927300    1.37382700
 C                 -3.51189300   -1.78613100   -1.85738300
 C                 -1.00026500    3.17140300    1.62958800
 H                 -0.56863100    3.98267100    2.20230600
 C                  3.72775600    0.38270000    1.35178000
 H                  4.14345400   -0.59755900    1.09638400
 H                  2.86496700    0.19169700    1.99416100
 H                  4.48159400    0.92635200    1.92596800
 F                  0.05775400   -2.54047900    3.48387500
 C                  0.70323500    1.30712600   -2.65417800
 H                  0.80455900    1.80468300   -3.62094800
 H                 -0.24062900    1.64305300   -2.21138500
 H                  0.61429700    0.23081600   -2.83126400
 C                  4.68519100    4.20395300   -1.74760500
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H	4.75342800	4.31548000	-2.83274700
H	5.69794900	4.10632600	-1.35010400
H	4.26298900	5.13307700	-1.35023800
C	3.42967500	-1.81859200	-1.59563900
H	4.02679000	-2.55527300	-2.13744400
H	4.09580600	-1.01480200	-1.27072500
H	2.71790600	-1.36232300	-2.29075000
C	-2.25907100	-2.43930700	-2.01373500
H	-2.24452500	-3.36488800	-2.57443700
C	1.39925900	-3.84816000	1.60661300
H	0.91105100	-4.36935300	2.42053800
C	0.10666100	-1.88907300	2.30205000
C	3.02613400	-3.78257400	-0.14090300
H	3.79475700	-4.28033100	-0.72526400
C	2.36922500	-4.49501300	0.86349100
H	2.62319100	-5.52829700	1.06755700
O	-3.03356600	4.27601300	1.87753600
O	-4.53855200	-2.40246900	-2.43026300
C	-4.43224600	4.37659100	1.66581700
H	-4.96295700	3.53260800	2.11746300
H	-4.74113400	5.29851800	2.15298700
H	-4.66851600	4.43394000	0.59863800
C	-5.84795100	-1.84333500	-2.32888200
H	-5.88427600	-0.85748700	-2.79803500
H	-6.49829500	-2.52856000	-2.86528100
H	-6.16058400	-1.77998000	-1.28411800

C3

GS1-*E*-Singlet
freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1

N	1.01868000	-0.33353300	-0.07618100
C	-0.95879100	1.37229800	0.07780200
C	3.31010900	-0.09520400	-0.11832400
C	2.98566300	-1.43839100	-0.54728500
F	-1.87146600	-0.76938600	-2.01407000
C	2.09592700	0.55403500	0.15234000
C	1.58744200	-1.55111000	-0.50584300
C	-1.26246500	-1.29627000	0.69841900
C	-0.73275000	2.12712600	-1.09604900
C	-1.76684800	1.93217700	1.09204500
C	4.52943800	0.55530300	0.05888000
H	5.47675000	0.07244500	-0.14617300
C	-2.29789600	3.20784000	0.93270300
H	-2.89966600	3.63234200	1.73138000
C	3.77540500	-2.50819700	-0.96265800
H	4.85524500	-2.41591400	-0.99199900
C	-1.30872800	3.38839200	-1.22746600
H	-1.13626400	3.95115900	-2.14076000
C	-2.08872600	3.95087000	-0.22471800
C	2.08600500	1.85715000	0.64660600
H	1.16351700	2.36553300	0.88750700
F	-3.73586200	-1.84414700	-1.90532300
B	-0.37315600	-0.07980200	0.19682800
C	0.95917500	-2.72509300	-0.91891300
H	-0.11645100	-2.82041100	-0.93422800
C	-0.87908000	-1.95749700	1.88315300
C	-2.45575000	-1.70039800	0.08150000
C	4.48786400	1.85211400	0.52007300
C	3.15350100	-3.68587300	-1.34193500
H	3.74694800	-4.53207600	-1.66730300
C	3.29812300	2.50723800	0.81991300
H	3.33263600	3.52322700	1.19249000
C	0.13330600	1.64741000	-2.23870400
H	-0.16424200	2.13800800	-3.16722000
H	0.07699900	0.57180200	-2.39396400
H	1.18291900	1.89785800	-2.05535400
F	-3.57171000	0.09806700	-0.99536800
C	-2.07530600	1.20129500	2.37760000
H	-2.55265500	1.87297700	3.09290700
H	-1.17714900	0.79996200	2.85138400
H	-2.75390400	0.36286300	2.20095400
C	-2.71642800	5.30791400	-0.39748100
H	-3.71993100	5.21309300	-0.82435400
H	-2.12900600	5.93473000	-1.07149500
H	-2.81379200	5.82469800	0.55965700
C	0.40037100	-1.62523400	2.61497700
H	0.35980700	-1.99415700	3.64081100
H	0.60116600	-0.55253100	2.65311700
H	1.25869000	-2.09409100	2.12417100
C	1.75815800	-3.78428600	-1.32311500
H	1.28435500	-4.70619500	-1.64010400

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 C                 -3.25469700   -2.70870800    0.60740400
 H                 -4.16209600   -3.00636100    0.09858300
 C                 -2.91037200   -1.05391000   -1.19860000
 C                 -1.69643800   -2.95688600    2.40898400
 H                 -1.39922500   -3.45048500    3.32831300
 C                 -2.87460300   -3.33383400    1.78384100
 H                 -3.49240300   -4.11653100    2.20744000
 F                  5.64827400    2.51770600    0.70170300
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GS2-*E*-Singlet

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# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                 -0.78466700    0.01814400   -0.27993500
 C                  1.62799100    1.02788000   -0.21296500
 C                 -2.84356900    1.04048000   -0.14383900
 C                 -2.99979400   -0.20037000   -0.87164300
 F                 -0.00631000   -0.86375600    2.33898100
 C                 -1.48812600    1.14371400    0.19921000
 C                 -1.73424700   -0.80615200   -0.92267600
 C                  1.18081400   -1.68212600   -0.14135100
 C                  2.71629800    1.14369700    0.68081000
 C                  1.48884400    1.99978400   -1.23107000
 C                 -3.75650500    2.02151300    0.23826400
 H                 -4.80795200    1.96311800   -0.01392800
 C                  2.39586900    3.05365100   -1.31129300
 H                  2.27959100    3.78723100   -2.10428400
 C                 -4.10440400   -0.80403500   -1.46835900
 H                 -5.07938500   -0.33183200   -1.42326800
 C                  3.58456300    2.22677000    0.58009700
 H                  4.40216100    2.31389600    1.29015700
 C                  3.44288200    3.19476900   -0.40885100
 C                 -1.02741100    2.20906800    0.96921300
 H                  0.00792400    2.28512600    1.26993800
 F                 -1.38663900   -2.38704500    1.68243600
 B                  0.63748700   -0.19350100   -0.18264300
 C                 -1.55529400   -2.01161900   -1.59955800
 H                 -0.58877100   -2.48950000   -1.66762500
 C                  2.05126000   -2.14506100   -1.14678100
 C                  0.84408100   -2.56703900    0.89610700
 C                 -3.26828100    3.08107300    0.97008700
 C                 -3.93116700   -2.01229600   -2.12201900
 H                 -4.77617500   -2.50123000   -2.59214700
 C                 -1.93255600    3.18914600    1.34483500
 H                 -1.61643400    4.03875300    1.93685800
 C                  2.98000800    0.13342600    1.77207200
 H                  3.20906400   -0.85000700    1.35388500
 H                  2.12023700    0.01247500    2.43145000
 H                  3.82983900    0.44393500    2.38180500
 F                  0.13095800   -2.85915700    3.13359800
 C                  0.39513700    1.95805300   -2.27590000
 H                  0.69803300    2.52306600   -3.15905100
 H                 -0.52754800    2.40757500   -1.89687200
 H                  0.14855300    0.94518000   -2.59730200
 C                  4.41985400    4.33428000   -0.52221700
 H                  5.29479300    4.03274300   -1.10682400
```

H	4.77515700	4.65028500	0.46095600
H	3.96981200	5.19519500	-1.02053200
C	2.45774300	-1.26331400	-2.30203400
H	2.98867300	-1.84129300	-3.05962200
H	3.11041100	-0.45276700	-1.96927200
H	1.59020500	-0.80426900	-2.78332600
C	-2.66458800	-2.60241300	-2.18575300
H	-2.54106800	-3.54456400	-2.70746000
C	1.34071700	-3.86516800	0.94050600
H	1.07247900	-4.52243000	1.75726600
C	-0.09921200	-2.16866600	2.00398600
C	2.53171900	-3.45242000	-1.09676500
H	3.19130900	-3.80308300	-1.88356500
C	2.18508800	-4.30950200	-0.06353100
H	2.57339900	-5.32057300	-0.03804300
F	-4.12082400	4.05448300	1.35632700

GS1-*Z*-Singlet

```
# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)
```

0 1

N	0.89736000	0.59909800	0.06407800
C	-1.71808200	0.69632200	0.05099300
C	2.54672900	2.20457300	0.17770200
C	3.15392900	0.95797100	-0.23488900
F	-0.95428000	-1.51311400	-2.03457300
C	1.17523200	1.95628100	0.34279800
C	2.12777200	0.00277800	-0.28985000
C	-0.32975500	-1.58790500	0.72467900
C	-1.93596000	1.44962400	-1.12504200
C	-2.76391200	0.60823200	0.99659200
C	3.07894600	3.46833000	0.42483100
H	4.13914200	3.65296100	0.29277700
C	-3.96280900	1.27596600	0.77096200
H	-4.74910700	1.21576600	1.51821700
C	4.46623700	0.62349200	-0.56072700
H	5.27257800	1.34535800	-0.52480900
C	-3.16301100	2.07777300	-1.32541500
H	-3.31969500	2.64289900	-2.24007600
C	-4.18718700	2.01047300	-0.38932000
C	0.32462200	2.96418000	0.79625000
H	-0.72940300	2.78571700	0.95436300
F	-1.74726200	-3.51666200	-2.00844400
B	-0.36400300	-0.07382400	0.24526800
C	2.39276200	-1.29729900	-0.71507400
H	1.61353300	-2.03902800	-0.80642500
C	0.30403200	-1.88462200	1.94875500
C	-0.96582700	-2.63857400	0.04690100
C	2.22996800	4.47673400	0.84767400
C	4.70496400	-0.67757900	-0.94469700
C	0.86780800	4.21775700	1.03459300
H	0.21639600	5.01313000	1.37823200
C	-0.88677600	1.63747500	-2.19722000
H	-1.36253800	1.86480900	-3.15290600
H	-0.25765300	0.76020600	-2.33534500
H	-0.22995500	2.47666300	-1.94759300

F	-2.88623600	-1.90926400	-1.14457900
C	-2.63323400	-0.18144200	2.27778600
H	-3.47334700	0.02776400	2.94194200
H	-1.71654200	0.05858900	2.82025600
H	-2.62277400	-1.25615100	2.07877700
C	-5.51153000	2.68237000	-0.63450100
H	-6.22347000	1.97575300	-1.07267200
H	-5.41004800	3.52130300	-1.32582400
H	-5.94679100	3.05155600	0.29673900
C	1.04177500	-0.83770400	2.75044800
H	1.17769300	-1.17212000	3.77987200
H	0.52047700	0.12147400	2.77734400
H	2.03289600	-0.65176700	2.32557500
C	3.69960400	-1.63461000	-1.03252300
H	3.94888000	-2.63590200	-1.36020900
C	-0.99248200	-3.93383900	0.55010100
H	-1.48029600	-4.72417100	-0.00519600
C	-1.64064500	-2.39562100	-1.27551200
C	0.25804300	-3.18458500	2.45018300
H	0.73747000	-3.39975900	3.39942300
C	-0.38272300	-4.20437700	1.76431500
H	-0.40235200	-5.20853100	2.17050200
F	5.96466600	-1.04232600	-1.26428500
H	2.62046900	5.46817000	1.04430500

GS2-*Z*-Singlet

```
# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)
```

0 1

N	0.52977400	-0.60859200	-0.02548600
C	-2.04513200	-0.21794500	-0.27917200
C	1.72522400	-2.51793600	0.45409700
C	2.58216200	-1.61931600	-0.28862600
F	0.05622600	0.82582600	2.41880500
C	0.48762500	-1.87373500	0.59495400
C	1.83374600	-0.46107500	-0.55116000
C	-0.25336400	1.86395700	-0.23861800
C	-3.12214200	0.34175000	0.44364000
C	-2.32630800	-1.22651200	-1.23022600
C	1.93720700	-3.77950700	1.00692700
H	2.89501400	-4.27525000	0.89587000
C	-3.63634800	-1.66297200	-1.40996900
H	-3.83649800	-2.43275300	-2.15020500
C	3.89669300	-1.74277700	-0.73270600
H	4.49079400	-2.62710200	-0.53867000
C	-4.41305500	-0.14181800	0.25066000
H	-5.22661200	0.28259900	0.83219400
C	-4.69330300	-1.14482900	-0.67137600
C	-0.54244400	-2.46250700	1.32633300
H	-1.49029100	-1.96290900	1.46983200
F	2.09131600	1.33672500	1.91333000
B	-0.57142600	0.31354500	-0.14489700
C	2.38379000	0.58164700	-1.29338600
H	1.82500000	1.47623300	-1.52605200
C	-0.63798300	2.59743400	-1.37762200
C	0.38536800	2.55520300	0.80406700

C	0.90434000	-4.38060000	1.70610300
C	4.42129300	-0.68681300	-1.44430600
C	-0.31936200	-3.71999400	1.86574100
H	-1.11218900	-4.19664000	2.43079000
C	-2.93311100	1.45522800	1.44636200
H	-2.57752500	2.36789900	0.96123500
H	-2.20595200	1.19238700	2.21483100
H	-3.87714400	1.68632800	1.94220100
F	0.90692600	2.67833100	3.10907700
C	-1.26598400	-1.86858600	-2.09793600
H	-1.71958200	-2.28614900	-2.99840200
H	-0.76873800	-2.68659500	-1.56803100
H	-0.48789200	-1.17011900	-2.40914700
C	-6.10366400	-1.62225900	-0.89228800
H	-6.60339800	-1.00625900	-1.64665700
H	-6.69156400	-1.55910600	0.02579900
H	-6.12233300	-2.65548800	-1.24487100
C	-1.31991000	1.93180000	-2.54782400
H	-1.40516100	2.62203800	-3.38815000
H	-2.32271700	1.59195600	-2.27892900
H	-0.76292700	1.05669700	-2.89336400
C	3.69318300	0.46191500	-1.73335500
H	4.15928400	1.25436700	-2.30519900
C	0.64290900	3.91966000	0.72768400
H	1.12780800	4.42872200	1.55031900
C	0.85580800	1.85026800	2.05214800
C	-0.36266400	3.96202300	-1.44622100
H	-0.65206500	4.51513300	-2.33352400
C	0.26997900	4.62393600	-0.40510200
H	0.46987700	5.68647800	-0.47381000
F	5.69340900	-0.76779200	-1.89034100
H	1.04531500	-5.36171000	2.14402700

GS1-*E*-triplet

freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	1.00701600	-0.43647200	-0.04696100
C	-0.84649800	1.40933400	-0.09226200
C	3.29131400	-0.38795900	-0.09974200
C	2.84793300	-1.54195300	-0.87396100
F	-2.43137500	-0.67969800	-1.81875200
C	2.09754900	0.23890500	0.37431200
C	1.44146900	-1.52255300	-0.81583400
C	-1.33252500	-1.20701700	0.84708500
C	-0.42203100	2.04900300	-1.28175900
C	-1.56442500	2.19369100	0.84835900
C	4.51823100	0.13559600	0.21731800
H	5.45298200	-0.29798400	-0.11354300
C	-1.81579900	3.53828000	0.59845200
H	-2.35717000	4.11978300	1.34113100
C	3.49874500	-2.53122200	-1.58051600
H	4.58003800	-2.56472500	-1.63745200
C	-0.69247100	3.39918300	-1.49629500
H	-0.36172000	3.86178600	-2.42330900
C	-1.38793400	4.16671300	-0.56931700

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 C                  2.13593100    1.39837800    1.17622400
 H                  1.21886800    1.86199400    1.51444100
 F                 -4.37015100   -1.39072200   -1.23142800
 B                 -0.46787200   -0.07009200    0.24735800
 C                  0.66222100   -2.47041100   -1.45936400
 H                 -0.41766800   -2.43053900   -1.40875900
 C                 -0.84038900   -2.05767900    1.88668600
 C                 -2.66677300   -1.47171800    0.41724400
 C                  4.52375700    1.28758800    1.01322600
 C                  2.72149600   -3.49921200   -2.23123400
 H                  3.21313500   -4.28577800   -2.79058900
 C                  3.37182300    1.91752800    1.49215300
 H                  3.47439600    2.80658000    2.09984100
 C                  0.30083400    1.29032100   -2.36854200
 H                  0.22769000    1.81648400   -3.32271200
 H                 -0.12281400    0.29179200   -2.49770600
 H                  1.36763400    1.17017300   -2.14864800
 F                 -3.67435600    0.50100600   -0.49841400
 C                 -2.05275700    1.60504600    2.14808400
 H                 -2.40757000    2.38780200    2.82242200
 H                 -1.26092700    1.04067900    2.65031100
 H                 -2.87454900    0.90373500    1.97956300
 C                 -1.70096500    5.61752400   -0.82853600
 H                 -2.71664800    5.73462500   -1.22087600
 H                 -1.01363900    6.04852100   -1.56004100
 H                 -1.63724400    6.20764800    0.08937100
 C                  0.53378300   -1.86094400    2.47590000
 H                  0.63341100   -2.41143800    3.41309600
 H                  0.72235900   -0.80210100    2.68160200
 H                  1.32798400   -2.21111100    1.80881100
 C                  1.33263300   -3.46502100   -2.17333800
 H                  0.75752700   -4.22339500   -2.69004600
 C                 -3.45983800   -2.45275500    1.00822800
 H                 -4.46819900   -2.61642800    0.65130900
 C                 -3.27031900   -0.75819700   -0.76220300
 C                 -1.64546300   -3.03926900    2.44608000
 H                 -1.24598500   -3.64800300    3.25195500
 C                 -2.95789000   -3.24100500    2.02858000
 H                 -3.57466500   -4.00371200    2.48866000
 F                  5.70290000    1.81478200    1.33114400


GS2-E-triplet
# freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3
 N                 -0.67199800   -0.23314300    0.35908400
 C                  1.93332700   -0.46481600    0.30978300
 C                 -2.36473100   -1.75529000    0.17516300
 C                 -2.73212500   -0.80031300    1.21329300
 F                 -2.31291000    1.46253100   -1.17898400
 C                 -1.08259600   -1.33477500   -0.29989400
 C                 -1.66387300    0.10983800    1.28943900
 C                  0.66471700    2.00235000   -0.07458000
 C                  2.98504300   -0.37245600   -0.63806100
 C                  2.04789100   -1.46359000    1.30992700
 C                 -2.96616500   -2.86807800   -0.35405400
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H	-3.93340000	-3.23035600	-0.03056500
C	3.14400200	-2.32043300	1.33531600
H	3.21180200	-3.06656100	2.12367500
C	-3.82456200	-0.65914200	2.04361200
H	-4.65713900	-1.35094700	1.99998200
C	4.06868700	-1.24647200	-0.57672900
H	4.85800400	-1.15715400	-1.31933600
C	4.16853300	-2.23522000	0.39669900
C	-0.40045700	-2.03998600	-1.31423800
H	0.57039500	-1.70661500	-1.65423000
F	-1.67230100	2.66993800	-2.83453800
B	0.68967400	0.48206900	0.20668000
C	-1.65807100	1.16852700	2.18018400
H	-0.82944700	1.86433600	2.21221300
C	1.61034600	2.84655700	0.59437900
C	-0.25958200	2.67584600	-0.92880100
C	-2.26483300	-3.54377100	-1.35911300
C	-3.83084100	0.40761600	2.95164800
H	-4.67965700	0.53821200	3.61177800
C	-1.01041900	-3.15440100	-1.84115800
H	-0.54364000	-3.74088300	-2.62113600
C	2.96168000	0.64881400	-1.74987700
H	3.15665500	1.65912000	-1.37595600
H	1.98355000	0.68505800	-2.23539800
H	3.71934800	0.41862900	-2.50227800
F	-0.64041900	0.83697200	-2.39604200
C	1.02177100	-1.59552500	2.40921600
H	1.42616400	-2.15899900	3.25249300
H	0.12048200	-2.11973800	2.07350700
H	0.70768100	-0.61336000	2.77498800
C	5.33029400	-3.19396300	0.42253400
H	6.21922300	-2.75388800	-0.03516700
H	5.09488900	-4.10979100	-0.13007700
H	5.58122900	-3.48575100	1.44531000
C	2.63511000	2.27912000	1.54429000
H	3.12535400	3.07987000	2.10193600
H	3.40747000	1.70516000	1.02515500
H	2.16861400	1.59054200	2.25572700
C	-2.76749100	1.30114600	3.01735200
H	-2.79947900	2.11808400	3.72779200
C	-0.29195800	4.06314500	-1.05180200
H	-1.01382900	4.52873500	-1.71037200
C	-1.20543400	1.92030100	-1.81665600
C	1.56543700	4.22450300	0.44049700
H	2.28247500	4.83411800	0.98256000
C	0.61358600	4.84899700	-0.36235200
H	0.58864000	5.92812500	-0.45516000
F	-2.82698000	-4.62782800	-1.88605000

GS1-*Z*-triplet
freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	1.00980600	0.41163900	0.23626700
C	-1.54141500	0.87709300	-0.13431000
C	2.83299000	1.79779400	0.45737400

C	3.22102000	0.61626600	-0.30487800
F	-1.41506900	-1.71924200	-1.92107400
C	1.47046600	1.62358300	0.76390900
C	2.04033600	-0.18391900	-0.40162900
C	-0.57145600	-1.56899800	0.88579500
C	-1.41230300	1.66628000	-1.30152200
C	-2.69125200	1.08816500	0.67031000
C	3.49976300	2.92799400	0.88135000
H	4.54822900	3.08143000	0.65620600
C	-3.63673900	2.04275900	0.31195300
H	-4.50351500	2.19187500	0.95171800
C	4.38976200	0.19496100	-0.88479600
H	5.31204200	0.75959500	-0.84175700
C	-2.38062100	2.61402800	-1.62799500
H	-2.25939200	3.19984800	-2.53618300
C	-3.50381000	2.82108000	-0.83597900
C	0.75111700	2.55862700	1.49068300
H	-0.29931800	2.41022400	1.70466300
F	-2.68178800	-3.40560000	-1.51677700
B	-0.43741100	-0.13039900	0.33048500
C	2.03053000	-1.41038800	-1.09766600
H	1.12218900	-1.99298600	-1.16805200
C	0.18091500	-2.00677700	2.02180200
C	-1.44404600	-2.54336500	0.31438200
C	2.78283800	3.88143400	1.61696400
C	4.34982800	-1.02920600	-1.56330200
C	1.43710600	3.69783900	1.91501300
H	0.90818400	4.45254200	2.48382300
C	-0.24824600	1.49076300	-2.24649900
H	-0.47094400	1.92861900	-3.22177600
H	-0.01893000	0.43261500	-2.39358200
H	0.65955000	1.97867200	-1.87384900
F	-3.25857700	-1.46168900	-0.81795700
C	-2.91294400	0.30617500	1.94082300
H	-3.73727700	0.72854900	2.51999200
H	-2.01379700	0.29918900	2.56448500
H	-3.15017000	-0.73925800	1.72538900
C	-4.55882600	3.82704900	-1.21681000
H	-5.40608300	3.33830600	-1.70925400
H	-4.16381400	4.57618900	-1.90670700
H	-4.94935200	4.34509100	-0.33697500
C	1.09244800	-1.06450300	2.76756000
H	1.34197700	-1.46764500	3.75072200
H	0.61384800	-0.09041000	2.91091700
H	2.03609200	-0.88783500	2.24173400
C	3.20670100	-1.82470300	-1.68177500
H	3.26915900	-2.75470300	-2.23078100
C	-1.59244500	-3.81886100	0.85370800
H	-2.26721100	-4.52497300	0.38790300
C	-2.19237700	-2.27329300	-0.96257800
C	0.02623200	-3.28894900	2.52845400
H	0.59421900	-3.57637400	3.40849700
C	-0.86148400	-4.20117800	1.96497700
H	-0.97766100	-5.19306500	2.38500200
F	5.47304700	-1.45889500	-2.13174300
H	3.28734600	4.77737500	1.95761600

GS2-*Z*-triplet
freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	0.50275200	-0.54804800	-0.00807000
C	-2.05135300	-0.15604500	-0.41439400
C	1.65089700	-2.42075600	0.67709400
C	2.42084400	-1.73894200	-0.35562600
F	2.35665900	0.98549400	1.53553600
C	0.48646200	-1.65270100	0.85634500
C	1.64130500	-0.59914400	-0.72717600
C	-0.26156400	1.97590000	-0.11876500
C	-3.16275600	0.31775200	0.32636600
C	-2.27586400	-1.23284800	-1.30650500
C	1.84854200	-3.56720400	1.41894200
H	2.73877700	-4.17167100	1.29424900
C	-3.54146300	-1.79776300	-1.43218300
H	-3.68764200	-2.61376900	-2.13606500
C	3.62370700	-1.98146000	-0.96690400
H	4.25373200	-2.82767400	-0.72519900
C	-4.41618400	-0.27156200	0.17136700
H	-5.25143700	0.10810900	0.75499100
C	-4.63010900	-1.33608500	-0.69796400
C	-0.49499700	-2.00553700	1.76686700
H	-1.38653000	-1.40466000	1.88611600
F	1.76369600	2.53891700	2.89369300
B	-0.63365100	0.48228400	-0.20308800
C	2.07428000	0.30270900	-1.72241900
H	1.47170300	1.16417500	-1.97797100
C	-0.86948700	2.90003800	-1.03411000
C	0.69847300	2.54490100	0.77525300
C	0.86289800	-3.93399300	2.34369100
C	4.02486800	-1.06912000	-1.94974900
C	-0.28432300	-3.16624900	2.51247600
H	-1.03071200	-3.47273500	3.23498100
C	-3.02923500	1.45222000	1.31386600
H	-2.90521500	2.41543700	0.80857700
H	-2.15008000	1.32354700	1.94963400
H	-3.91556600	1.51886200	1.94880500
F	0.41811200	0.91336000	2.48889700
C	-1.16983900	-1.77184500	-2.18090500
H	-1.57736200	-2.36033400	-3.00533000
H	-0.48876800	-2.42420200	-1.62345100
H	-0.57097500	-0.96012800	-2.60537500
C	-5.98445200	-1.98412400	-0.82255900
H	-6.78513600	-1.28205000	-0.57889000
H	-6.07470600	-2.83584700	-0.14003100
H	-6.15381100	-2.35815100	-1.83522900
C	-1.88626100	2.44448400	-2.05052600
H	-2.08244600	3.23600500	-2.77679700
H	-2.83682400	2.16367300	-1.58927800
H	-1.53247700	1.55727600	-2.58508500
C	3.28038200	0.05110700	-2.33431900
H	3.67344300	0.70274500	-3.10317100
C	1.07986900	3.88364200	0.71117900
H	1.81407500	4.26752700	1.40801900

C	1.29648900	1.75403100	1.90202400
C	-0.48094000	4.23015000	-1.06308900
H	-0.94336900	4.89317200	-1.78847600
C	0.50249900	4.73476100	-0.21297800
H	0.79978100	5.77523100	-0.26507600
F	5.19007700	-1.28184600	-2.55433100
H	0.99750300	-4.83083200	2.93603400

C4

GS1-*E*-Singlet

```
# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                  1.10301000   -1.18259700   -0.25386300
 C                  0.04758800    1.16660100    0.26596000
 C                  2.26030800   -2.93711600   -1.11030000
 C                  3.20966800   -1.98253400   -0.59263500
 F                 -1.50193100   -0.00042800   -2.22306300
 C                  1.02877900   -2.43615400   -0.87399500
 C                  2.46715400   -0.90834500   -0.06816700
 C                 -1.39330100   -1.19923700    0.34817000
 C                  0.63054400    1.96112600   -0.74508800
 C                 -0.50201800    1.81552000    1.39648200
 C                 -0.42859700    3.19848800    1.50845700
 H                 -0.83639500    3.67896800    2.39348300
 C                  4.60540900   -1.97080300   -0.51525100
 H                  5.18454700   -2.79330000   -0.91999100
 C                  0.65660200    3.34864200   -0.60636000
 H                  1.09912400    3.94499100   -1.39968800
 C                  0.14250300    3.98727900    0.51278300
 F                 -3.64608100   -0.18899500   -2.32442900
 B                 -0.04755500   -0.39113500    0.09597500
 C                  3.09243200    0.16148500    0.57081200
 H                  2.52161500    0.97550900    0.99703100
 C                 -1.41895400   -2.15552700    1.38405400
 C                 -2.58626500   -0.96610200   -0.35336800
 C                  5.22898500   -0.89637200    0.09399300
 H                  6.31049400   -0.86850800    0.16340800
 C                  1.25901900    1.39851800   -1.99991500
 H                  1.07569000    2.06875000   -2.84232800
 H                  0.88273800    0.41396800   -2.26728100
 H                  2.34292100    1.31405100   -1.87422000
 F                 -2.76586300    1.29756500   -1.04214300
 C                 -1.17258100    1.05660400    2.51732400
 H                 -1.38312800    1.72190600    3.35618500
 H                 -0.55327700    0.23965800    2.89302800
 H                 -2.12032200    0.62338400    2.18746600
 C                  0.16853100    5.48691700    0.63987600
 H                 -0.81234400    5.90941300    0.40053100
 H                  0.89775300    5.93154200   -0.03995100
 H                  0.41559500    5.79216300    1.65943200
 C                 -0.18985000   -2.50863800    2.18989000
 H                 -0.47506000   -2.91944900    3.15964000
 H                  0.46383200   -1.65270800    2.36593800
 H                  0.40994200   -3.26158600    1.66957900
 C                  4.47635400    0.15503800    0.63636300
 H                  4.98524100    0.98021400    1.12136500
 C                 -3.76674000   -1.63171700   -0.04588600
 H                 -4.66623000   -1.43634300   -0.61469000
 C                 -2.62658900    0.03311700   -1.47761300
 C                 -2.61326600   -2.80617400    1.69323800
 H                 -2.62483000   -3.52794900    2.50339800
 C                 -3.77997400   -2.55093900    0.99096300
 H                 -4.69636600   -3.06986900    1.24543900
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H	2.48412400	-3.87456300	-1.59568100
H	0.06147400	-2.84770300	-1.11693700

GS2-*E*-Singlet

```
# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)
```

0 1

N	-0.03251900	1.25051600	0.56085200
C	-1.00810000	-1.12245900	-0.01514200
C	0.27241900	3.28462600	1.51949600
C	-0.92485400	3.34049300	0.71718400
F	1.34411800	0.78492200	-1.87582600
C	0.78154100	2.04162100	1.38263100
C	-1.08578800	2.07105000	0.13286500
C	1.66073300	-0.69271500	0.54054000
C	-0.93280600	-2.07149500	-1.06129900
C	-2.15233700	-1.13153100	0.81436500
C	-3.18191000	-2.03815000	0.56748200
H	-4.04680400	-2.03969500	1.22529300
C	-1.84226900	4.35751200	0.43677400
H	-1.72795400	5.33896800	0.88332900
C	-1.99410300	-2.94172000	-1.28755100
H	-1.92599300	-3.65358200	-2.10537800
C	-3.13289000	-2.93918200	-0.48735700
F	2.87847200	1.97453500	-0.93406800
B	0.18369100	-0.15110900	0.31743800
C	-2.12320700	1.80639900	-0.75943300
H	-2.22895200	0.83739800	-1.22888000
C	1.91469400	-1.62931200	1.56235400
C	2.74137900	-0.29077500	-0.26058600
C	-2.88974700	4.08898700	-0.42655500
H	-3.61138300	4.86474400	-0.65640100
C	0.26807700	-2.18043400	-1.97035400
H	1.17513100	-2.41021300	-1.40610700
H	0.44965900	-1.25242300	-2.51357700
H	0.12045000	-2.97426500	-2.70406200
F	3.41119500	0.48239800	-2.39304000
C	-2.33944000	-0.20892100	1.99885600
H	-2.90184200	-0.71792000	2.78423700
H	-2.90819000	0.67897900	1.70718100
H	-1.40221200	0.14009100	2.43071000
C	-4.27566700	-3.87815900	-0.76642200
H	-3.91631300	-4.83952600	-1.14022800
H	-4.93974800	-3.45728900	-1.52800100
H	-4.87190800	-4.05656700	0.13059700
C	0.81604200	-2.11224800	2.47724200
H	1.22479500	-2.72918900	3.27857600
H	0.07861800	-2.70493400	1.93087800
H	0.28386800	-1.27752200	2.94051100
C	-3.02296900	2.82628400	-1.02246700
H	-3.84282800	2.64401900	-1.70783000
C	4.02510400	-0.79344800	-0.07029600
H	4.83482900	-0.47405200	-0.71388800
C	2.58797300	0.73045400	-1.35931900
C	3.20710800	-2.11572000	1.75014300
H	3.39127600	-2.83000100	2.54574400

C	4.25751100	-1.70926400	0.94117300
H	5.25360600	-2.10566800	1.09733500
H	1.66546800	1.61002200	1.82512100
H	0.69256600	4.08250100	2.11214700

GS1-*Z*-Singlet

```
# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)
```

0 1

N	-0.98073100	-1.27620400	0.23220100
C	1.54557400	-0.68031800	0.31275500
C	-1.95086300	-3.28668600	0.64144000
C	-2.96029600	-2.39988300	0.11637300
F	0.32177100	0.80640500	-2.20078600
C	-0.79471900	-2.59049400	0.67946900
C	-2.33236400	-1.16400300	-0.12800500
C	-0.44218500	1.24851800	0.48824600
C	2.03889500	-1.56641100	-0.67074900
C	2.46149400	-0.14463100	1.25074100
C	3.79787100	-0.52025600	1.21063300
H	4.48295100	-0.11296600	1.94910700
C	-4.31803000	-2.56219300	-0.17211300
H	-4.80941300	-3.51058700	0.01425800
C	3.39496600	-1.89685300	-0.69003600
H	3.75862000	-2.56755200	-1.46364300
C	4.28876500	-1.39448200	0.24324300
F	0.54964400	2.91510300	-2.58647400
B	0.03166700	-0.25544900	0.30950400
C	-3.02838100	-0.09579200	-0.69213600
H	-2.54301800	0.84444200	-0.91445200
C	-1.19906100	1.58766200	1.62781900
C	-0.09785600	2.27904900	-0.39833500
C	-5.01743600	-1.49355000	-0.70532600
H	-6.07147300	-1.59967900	-0.93550900
C	1.17891900	-2.19106500	-1.74813300
H	1.77082900	-2.34653400	-2.65227700
H	0.31589400	-1.58409800	-2.01195400
H	0.80413100	-3.16843900	-1.42898600
F	2.01715500	1.88289800	-1.39838700
C	2.04498700	0.83616200	2.32168500
H	2.86702400	1.01175300	3.01740700
H	1.19287800	0.47786900	2.90264200
H	1.76207200	1.79806500	1.88699100
C	5.74919000	-1.75742500	0.20937200
H	6.35804800	-0.88589700	-0.04875100
H	5.94890100	-2.53833700	-0.52646800
H	6.08709900	-2.11217600	1.18664900
C	-1.65455900	0.55424600	2.63079900
H	-1.88179400	1.02524200	3.58834000
H	-0.90914600	-0.22316900	2.80808200
H	-2.56153200	0.05296200	2.27923400
C	-4.37486300	-0.27542200	-0.96647200
H	-4.93857200	0.54300300	-1.39936600
C	-0.47196000	3.59942400	-0.17844600
H	-0.20108700	4.36855000	-0.88973600
C	0.69755600	1.97587200	-1.63794400

C	-1.55552300	2.91746700	1.84596500
H	-2.12745500	3.17022500	2.73272000
C	-1.19957400	3.91912600	0.95641800
H	-1.49199100	4.94549100	1.14310800
H	-2.08752500	-4.31104600	0.95202500
H	0.18093300	-2.89447600	1.02491400

GS2-*Z*-Singlet

```
# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)
```

0 1

N	-0.51210800	-1.23973500	-0.22769200
C	1.90775500	-0.29930700	-0.07106000
C	-1.18467400	-3.13496200	-1.27934600
C	-2.27460500	-2.66644300	-0.45931300
F	-0.70338500	0.80407000	-2.17799200
C	-0.16089500	-2.27328400	-1.10453500
C	-1.83505500	-1.48971500	0.17638600
C	-0.29733700	1.22093100	0.60403800
C	2.72123500	0.66316300	-0.71530300
C	2.54286600	-1.39694400	0.55507300
C	3.93024300	-1.52538300	0.49538100
H	4.40038800	-2.36672200	0.99705800
C	-3.55838300	-3.15922900	-0.21148000
H	-3.90251600	-4.06334800	-0.70124300
C	4.09940400	0.48418100	-0.76918000
H	4.70644200	1.22608800	-1.28042900
C	4.72627600	-0.60711500	-0.17479400
F	-2.76711700	1.05998700	-1.60617300
B	0.34751600	-0.12379800	0.06405100
C	-2.64845100	-0.81489500	1.08595500
H	-2.31446800	0.07655400	1.59820300
C	-0.00707200	1.64622100	1.91596600
C	-1.15216500	2.02081500	-0.16824600
C	-4.37441600	-2.47672000	0.67347100
H	-5.37399500	-2.84274700	0.87871800
C	2.15340200	1.90126100	-1.36780500
H	1.62435900	2.52615700	-0.64456700
H	1.44805400	1.65312900	-2.16150100
H	2.95237000	2.50078100	-1.80650900
F	-1.64201900	2.73179100	-2.36745800
C	1.80029300	-2.45625700	1.34199500
H	2.44486100	-2.86003300	2.12502700
H	1.50174500	-3.28878300	0.69815000
H	0.89222700	-2.08202200	1.81408400
C	6.21824200	-0.78385900	-0.26544600
H	6.73530800	0.17596400	-0.19682500
H	6.49280100	-1.23615400	-1.22363000
H	6.59088200	-1.43488400	0.52772200
C	0.88684800	0.83551800	2.82134200
H	0.95462800	1.29269800	3.80924000
H	1.89596100	0.75059400	2.41199400
H	0.50118600	-0.17938100	2.95356900
C	-3.91814300	-1.31912400	1.31797300
H	-4.56935400	-0.80500900	2.01560800
C	-1.71001000	3.19418200	0.33048800

H	-2.35966900	3.79475800	-0.29375900
C	-1.55903900	1.64993200	-1.57117000
C	-0.57922200	2.81787600	2.40653100
H	-0.35620600	3.12904400	3.42165500
C	-1.42437200	3.59173300	1.62489100
H	-1.85568400	4.50276600	2.02193300
H	0.81835700	-2.26738000	-1.55678300
H	-1.18417500	-4.00303000	-1.92037100

GS1-*E*-triplet

```
# freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)
```

0 3

N	1.10467500	-1.20398700	-0.25733400
C	0.04446400	1.14767500	0.26951400
C	2.44379500	-2.94085100	-1.06504800
C	3.28866400	-1.96746400	-0.61630800
F	-1.56947000	0.01962000	-2.25772700
C	1.06538700	-2.45652700	-0.82506800
C	2.49027600	-0.89268700	-0.07274900
C	-1.39887100	-1.22804900	0.32499300
C	0.60318200	1.96157700	-0.74081800
C	-0.48609200	1.78735000	1.41366000
C	-0.43228800	3.17183600	1.53427800
H	-0.83333900	3.64023100	2.42942200
C	4.71556500	-1.87160500	-0.55036400
H	5.32871100	-2.65420400	-0.98064400
C	0.62626600	3.34776800	-0.59031400
H	1.05505200	3.95411500	-1.38428900
C	0.11780300	3.97516200	0.53900400
F	-3.71653800	-0.10781400	-2.26609200
B	-0.04902300	-0.41641800	0.09981400
C	3.06388700	0.16467700	0.57468500
H	2.46495700	0.94856800	1.01756700
C	-1.44237000	-2.22410500	1.32911600
C	-2.60095100	-0.95892500	-0.35567600
C	5.27783000	-0.78261200	0.07219900
H	6.35608800	-0.69482000	0.13571900
C	1.21399100	1.40031600	-2.00330100
H	1.07411700	2.09413400	-2.83509700
H	0.78205800	0.44232300	-2.28585600
H	2.29161400	1.25217200	-1.87649200
F	-2.74259900	1.32685900	-0.99506600
C	-1.11744300	1.00419300	2.53991900
H	-1.31327700	1.65032600	3.39781700
H	-0.47545500	0.18701200	2.87701400
H	-2.06719800	0.56036900	2.22906400
C	0.12777600	5.47524600	0.67298600
H	-0.84003400	5.89594500	0.38164600
H	0.89022900	5.92671300	0.03470200
H	0.31873600	5.77965600	1.70490200
C	-0.21723500	-2.62159300	2.11606100
H	-0.49987700	-3.08981700	3.06027400
H	0.43022900	-1.77019300	2.33490700
H	0.38814400	-3.34079200	1.55333900
C	4.47324300	0.22062000	0.64207200

H	4.93999000	1.05777400	1.14637500
C	-3.79169300	-1.61238700	-0.05233600
H	-4.69426200	-1.37974700	-0.60190900
C	-2.65267700	0.06620900	-1.45701100
C	-2.64193900	-2.86763100	1.62684200
H	-2.65680600	-3.61589000	2.41307300
C	-3.81395000	-2.56720400	0.94997800
H	-4.73783500	-3.07599300	1.19830100
H	2.69592100	-3.89602600	-1.49918600
H	0.13236300	-2.89577100	-1.13628200

GS2-*E*-triplet

freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	0.07506900	1.20354200	0.66758300
C	-1.13578400	-1.04332000	0.01063300
C	0.55543600	3.33020100	1.49987400
C	-0.58447800	3.44672500	0.75692400
F	1.47045900	0.83479500	-1.81779900
C	0.95818600	1.90963500	1.44438400
C	-0.88814000	2.15032800	0.19818800
C	1.58009400	-0.88649700	0.51698800
C	-1.15394700	-1.94620300	-1.07755800
C	-2.28518500	-0.98332900	0.83348700
C	-3.39875300	-1.76947000	0.54447200
H	-4.26886200	-1.70753200	1.19324800
C	-1.42516600	4.55660200	0.42590600
H	-1.22940100	5.53001600	0.85923400
C	-2.28869200	-2.70971100	-1.33926600
H	-2.28515100	-3.38394000	-2.19190700
C	-3.42641600	-2.63602900	-0.54168200
F	3.01492000	1.80927300	-0.66945300
B	0.15205400	-0.20671900	0.36662000
C	-1.90287400	1.97862000	-0.70171000
H	-2.09925400	1.01586200	-1.15362700
C	1.75246700	-1.96299300	1.41570600
C	2.70170100	-0.50677900	-0.24806200
C	-2.46581200	4.35961000	-0.44941700
H	-3.11136400	5.18842400	-0.71526300
C	0.03644400	-2.11341500	-1.99169600
H	0.87849500	-2.57123600	-1.46464400
H	0.38521700	-1.15512400	-2.37845500
H	-0.21528800	-2.75195300	-2.84065300
F	3.53721700	0.44362200	-2.24891100
C	-2.36690000	-0.08905700	2.04824200
H	-3.10858100	-0.46762600	2.75436100
H	-2.66531500	0.92735100	1.77126800
H	-1.41118700	-0.00907800	2.56876400
C	-4.62924300	-3.49758200	-0.82388200
H	-4.51136200	-4.48806600	-0.37244300
H	-4.76971800	-3.64243500	-1.89760300
H	-5.54006300	-3.05507600	-0.41481500
C	0.61390800	-2.44932200	2.27840800
H	0.97075800	-3.16093400	3.02508400
H	-0.15659700	-2.93904600	1.67767800

H	0.13036200	-1.62232900	2.80405600
C	-2.70214600	3.09521100	-1.02206900
H	-3.51357500	2.97291400	-1.72896700
C	3.93192600	-1.14822200	-0.12420900
H	4.77058200	-0.83572700	-0.73296200
C	2.66727000	0.63325700	-1.23761000
C	2.98901200	-2.59502800	1.52945300
H	3.10042400	-3.41506300	2.23168900
C	4.07730900	-2.19584000	0.76866200
H	5.03184100	-2.69896200	0.86761900
H	1.77730300	1.42097400	1.94386800
H	1.09031200	4.10382500	2.02873900

GS1-*Z*-triplet
freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	-0.98103800	-1.29153900	0.25009600
C	1.54617800	-0.70699300	0.32008100
C	-2.11309500	-3.31541500	0.53268500
C	-3.03741100	-2.40274000	0.11749800
F	0.32061600	0.86892600	-2.26165700
C	-0.81068600	-2.61484400	0.59619000
C	-2.35566900	-1.14948500	-0.12036000
C	-0.43235500	1.24240700	0.48325900
C	2.04992200	-1.58285700	-0.66844600
C	2.46073900	-0.19506600	1.27247800
C	3.79817000	-0.57119000	1.23569400
H	4.47863800	-0.17489700	1.98509500
C	-4.44014200	-2.49183600	-0.16000100
H	-4.97178900	-3.41404500	0.04095900
C	3.40272300	-1.92695800	-0.67922400
H	3.76766200	-2.59373300	-1.45627700
C	4.29424700	-1.43724700	0.26383000
F	0.67557900	2.97363900	-2.53447100
B	0.03138500	-0.26875600	0.31304200
C	-2.99727100	-0.08635400	-0.68905800
H	-2.47875400	0.83181400	-0.92522300
C	-1.20404200	1.60354200	1.61139200
C	-0.05124200	2.27749500	-0.38841800
C	-5.08054100	-1.39651000	-0.68850300
H	-6.14062100	-1.44570500	-0.90821800
C	1.18371200	-2.17664000	-1.75402400
H	1.78440300	-2.41090900	-2.63515700
H	0.38201500	-1.50419900	-2.05606500
H	0.71408700	-3.10815900	-1.41733100
F	2.05899800	1.80355900	-1.37639300
C	2.03405100	0.76823600	2.35474600
H	2.83808800	0.91380600	3.07870300
H	1.15692400	0.41104900	2.89826000
H	1.77799600	1.74529900	1.93625300
C	5.75493100	-1.80273500	0.23182500
H	6.36233100	-0.94867000	-0.08347200
H	5.94482700	-2.62291900	-0.46332200
H	6.10773900	-2.10440700	1.22166500

C	-1.69478400	0.57897400	2.60549100
H	-1.94286400	1.05304800	3.55662600
H	-0.95755500	-0.20305400	2.79566600
H	-2.59840200	0.08318400	2.23585400
C	-4.37744500	-0.21029100	-0.96675900
H	-4.89907800	0.62903600	-1.40981800
C	-0.39512200	3.60692100	-0.16105900
H	-0.08844800	4.37504100	-0.85868400
C	0.74951100	1.98044100	-1.62774400
C	-1.53800600	2.93786500	1.83105100
H	-2.12016700	3.19747800	2.70954800
C	-1.13855700	3.93910700	0.95853800
H	-1.40683500	4.97167200	1.14801100
H	-2.26252200	-4.36012800	0.75821500
H	0.11902700	-2.95811800	1.01855500

GS2-*Z*-triplet

freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	-0.52820300	-1.21395000	-0.26879000
C	1.91619900	-0.33490200	-0.08107000
C	-1.39707700	-3.14777500	-1.24288700
C	-2.37161300	-2.64447300	-0.42927600
F	-0.72347800	0.88273500	-2.26987500
C	-0.23686100	-2.23770600	-1.13195700
C	-1.84930400	-1.46460100	0.21974600
C	-0.26217400	1.24564300	0.56632200
C	2.75703900	0.63292300	-0.68283200
C	2.53688100	-1.46762800	0.50034200
C	3.92066000	-1.62546700	0.43571600
H	4.37204500	-2.49865800	0.89998000
C	-3.69196400	-3.08866200	-0.10285600
H	-4.10801900	-3.95528700	-0.60231200
C	4.13398500	0.43494400	-0.73347700
H	4.75641300	1.18791600	-1.21013100
C	4.73959700	-0.69274100	-0.18739700
F	-2.74216300	0.85995800	-1.51409900
B	0.35974600	-0.12166300	0.05904400
C	-2.55536000	-0.81526300	1.19276400
H	-2.15428900	0.04414600	1.71143900
C	0.10447900	1.74389000	1.83553700
C	-1.14313800	2.02936300	-0.20279000
C	-4.40436500	-2.40100900	0.85043500
H	-5.40530900	-2.72267400	1.11299800
C	2.21323200	1.90909200	-1.28086200
H	1.80823600	2.56825000	-0.50788200
H	1.40777300	1.71331300	-1.98870300
H	3.00115600	2.45305700	-1.80538900
F	-1.91907100	2.66617700	-2.34637900
C	1.75941000	-2.52999600	1.24106600
H	2.40912500	-3.06643900	1.93507200
H	1.33203400	-3.26683700	0.55134900
H	0.92529000	-2.11106200	1.80786800
C	6.22873200	-0.89667900	-0.28100000
H	6.76449900	0.05308900	-0.21348500

H	6.49726200	-1.35676500	-1.23755700
H	6.59073400	-1.55284700	0.51349200
C	1.04318100	0.97063800	2.72831800
H	1.08989500	1.41675700	3.72324500
H	2.05418100	0.94690200	2.31360700
H	0.71963200	-0.06819500	2.83773900
C	-3.84819500	-1.28665500	1.50442000
H	-4.42062000	-0.77612400	2.26912900
C	-1.65796400	3.23494500	0.26751200
H	-2.33194500	3.81542400	-0.34918400
C	-1.61911000	1.60575000	-1.57093000
C	-0.41651100	2.95177000	2.29351400
H	-0.13082600	3.31282800	3.27637800
C	-1.29569800	3.69687100	1.52119800
H	-1.69301500	4.63442900	1.89156400
H	0.67984800	-2.23893100	-1.69778600
H	-1.42736600	-4.03979500	-1.84926300

C5

GS1-*E*-Singlet
freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1

N	0.52314800	-0.45418700	-0.07627600
C	-1.27972100	1.44345100	0.05273600
C	2.35756600	-1.74722900	-0.58717400
C	2.82056700	-0.44473900	-0.14028900
F	-2.42783400	-0.61237000	-1.97169000
C	0.95098600	-1.71479300	-0.52835300
C	1.68609000	0.30289500	0.15130400
C	-1.83607100	-1.16723300	0.73669800
C	-0.96989400	2.15125200	-1.13174300
C	-2.04111100	2.09628100	1.04734700
C	2.99413600	-2.91068400	-1.03227000
H	4.07128000	-2.97857700	-1.08913800
C	-2.44780700	3.41292400	0.85827700
H	-3.01419200	3.90788500	1.64210900
C	4.11994000	0.11899600	0.04630200
C	-1.42280400	3.45818900	-1.29267600
H	-1.18833500	3.98523800	-2.21336100
C	-2.15740900	4.11028700	-0.30988900
C	0.18017900	-2.79825700	-0.94576000
H	-0.89887900	-2.75912600	-0.94320400
F	-4.38229900	-1.50815500	-1.82923900
B	-0.83753700	-0.05439100	0.20301100
C	1.77034900	1.60934900	0.68596800
H	0.88009700	2.16581200	0.94013800
C	-1.50297800	-1.84606800	1.92669100
C	-3.07335200	-1.45728200	0.14288700
C	2.23026400	-4.00025400	-1.41409200
H	2.72023600	-4.90374900	-1.75772500
C	4.19855600	1.44556900	0.55409300
C	0.83460300	-3.94033600	-1.37639800
H	0.25049200	-4.79528900	-1.69652000
C	-0.14440200	1.56746600	-2.25599800
H	-0.35679800	2.09249400	-3.18898500
H	-0.33452500	0.50767900	-2.41689500
H	0.92443400	1.68156000	-2.04994100
F	-4.02934600	0.42239800	-0.94848600
C	-2.42633100	1.42419500	2.34427900
H	-2.83257700	2.15456300	3.04588300
H	-1.57569100	0.93986400	2.82806000
H	-3.18822400	0.65792400	2.17977000
C	-2.65231100	5.51679000	-0.51509200
H	-3.65719100	5.50849900	-0.94910200
H	-2.00328400	6.07111100	-1.19607600
H	-2.70719500	6.06004000	0.43069400
C	-0.18612500	-1.63197400	2.63589100
H	-0.23643000	-2.01484800	3.65611500
H	0.09950000	-0.57907100	2.68910600
H	0.62273900	-2.15782000	2.11993300
C	3.00525000	2.15561400	0.86994700
H	3.09300500	3.15868500	1.27334600
C	-3.96276400	-2.37021400	0.69693800

H	-4.90338000	-2.58164700	0.20548100
C	-3.47962000	-0.78834600	-1.14192500
C	-2.41000500	-2.74808000	2.48073800
H	-2.15035700	-3.25553900	3.40383600
C	-3.63030200	-3.01196500	1.87880600
H	-4.31801800	-3.72064800	2.32435400
C	5.32990600	-0.55735400	-0.24290000
H	5.30595100	-1.56433200	-0.63284400
C	5.46698900	2.04146800	0.75104900
H	5.51001300	3.05393100	1.13912900
C	6.54533800	0.04690400	-0.04232800
H	7.45696100	-0.49210300	-0.27406300
C	6.61986800	1.36062100	0.46013700
H	7.58585300	1.82719500	0.61432100

GS2-*E*-Singlet

freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1

N	-0.25371300	-0.37583800	-0.30644400
C	1.41357300	1.64371900	-0.22950000
C	-2.09316700	-1.57942400	-0.98429500
C	-2.54987400	-0.40941000	-0.25425600
F	0.75785500	-0.73698200	2.35781000
C	-0.68506900	-1.53427000	-0.97950700
C	-1.41130900	0.28404000	0.13335100
C	2.27579400	-0.95661100	-0.06686700
C	2.30983800	2.26787500	0.66762600
C	0.85416600	2.42102400	-1.27039700
C	-2.73958400	-2.63585100	-1.63442200
H	-3.81780500	-2.70752200	-1.65884500
C	1.17037500	3.77374200	-1.37036900
H	0.73892000	4.35519100	-2.18037300
C	-3.84255700	0.07855600	0.10855900
C	2.57766100	3.62795800	0.54635900
H	3.24928100	4.09816900	1.25915300
C	2.01836200	4.40102500	-0.46612600
C	0.07372400	-2.50232500	-1.63428800
H	1.15310600	-2.46279800	-1.64844100
F	0.25316600	-2.72890200	1.69630500
B	1.10335900	0.10414600	-0.17310300
C	-1.47546200	1.44840900	0.93166000
H	-0.57526800	1.94968300	1.25730500
C	3.30119900	-0.97584000	-1.03174700
C	2.35115100	-1.87558100	0.99239200
C	-1.98600600	-3.61008600	-2.26613400
H	-2.48378300	-4.43070500	-2.76937600
C	-3.90515900	1.27265000	0.88013000
C	-0.59055600	-3.53965700	-2.26732400
H	-0.01377700	-4.30565900	-2.77267200
C	2.99533300	1.51555700	1.78367400
H	3.56322100	2.20210400	2.41341900
H	3.69069400	0.77055200	1.38834400
H	2.28302800	0.98865700	2.41875300
F	1.75440200	-2.44302400	3.21162900
C	-0.07695600	1.85676800	-2.32120000

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 H                -0.06962900    2.49211100   -3.20840700
 H                -1.10671600    1.81445700   -1.95417800
 H                 0.19345200    0.84691000   -2.63345300
 C                 2.35619400    5.86170700   -0.59966000
 H                 3.28934700    5.99017100   -1.15724000
 H                 2.49227600    6.32703600    0.37899200
 H                 1.57357000    6.40330200   -1.13453400
 C                 3.28823500   -0.03348800   -2.21042600
 H                 4.06078800   -0.30606600   -2.93070300
 H                 3.46228500    0.99753200   -1.89371400
 H                 2.32714200   -0.05487800   -2.73137300
 C                -2.70328800    1.92468800    1.28065100
 H                -2.77995500    2.81940600    1.88905900
 C                 3.39785800   -2.78458300    1.09931800
 H                 3.43654900   -3.47465400    1.93188600
 C                 1.28396200   -1.94438300    2.05623500
 C                 4.33766400   -1.90072800   -0.91953800
 H                 5.11604400   -1.91592500   -1.67513000
 C                 4.39327000   -2.79770200    0.13628200
 H                 5.21065300   -3.50488600    0.21043000
 C                -5.06004200   -0.54843100   -0.25101500
 H                -5.04707200   -1.45671800   -0.83550500
 C                -5.16683400    1.79178300    1.25591900
 H                -5.19845300    2.70268600    1.84484100
 C                -6.26864200   -0.02047100    0.12758900
 H                -7.18648300   -0.51935800   -0.16221600
 C                -6.32767200    1.16287500    0.88902800
 H                -7.28810800    1.57029400    1.18269400


GS1-Z-Singlet
# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                 0.47647100    0.52549400    0.13233000
 C                -2.12568200    0.78021600   -0.01505900
 C                 2.22108900    2.00936600    0.36076900
 C                 2.75955300    0.72363800   -0.04823400
 F                -1.43714000   -1.50315700   -2.01636700
 C                 0.82426400    1.85249400    0.45073900
 C                 1.67644900   -0.13769600   -0.17123000
 C                -0.92175500   -1.57120000    0.76314500
 C                -2.23262100    1.53093600   -1.20838400
 C                -3.22282500    0.76914000    0.87411200
 C                 2.78936700    3.25096200    0.66578700
 H                 3.85610400    3.41331300    0.60387600
 C                -4.36555600    1.50416600    0.57638600
 H                -5.19222700    1.50306000    1.28123300
 C                 4.08067500    0.25863800   -0.32804400
 C                -3.40712700    2.22695400   -1.48243100
 H                -3.48022900    2.78845900   -2.40968400
 C                -4.48294400    2.23275600   -0.60287000
 C                 0.00264800    2.89479700    0.87762100
 H                -1.06580700    2.76492900    0.97318600
 F                -2.35317300   -3.45345400   -1.99297400
 B                -0.83504600   -0.06868800    0.25800000
 C                 1.82640900   -1.46850300   -0.62281700
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 H                  0.97109000   -2.11171700   -0.76431700
 C                 -0.35666400   -1.88591600    2.01586700
 C                 -1.60550500   -2.58826700    0.08002600
 C                  1.97149400    4.29511800    1.06094700
 H                  2.40820700    5.25872800    1.29587000
 C                  4.23082900   -1.09366200   -0.74483800
 C                  0.59005900    4.11419400    1.17078000
 H                 -0.03613300    4.93773800    1.49392900
 C                 -1.11519400    1.64206600   -2.22051900
 H                 -1.51837000    1.91508800   -3.19733000
 H                 -0.55278000    0.71719400   -2.33589600
 H                 -0.40641500    2.42209500   -1.92557900
 F                 -3.42593100   -1.76404100   -1.20453300
 C                 -3.20554200   -0.00338200    2.17216300
 H                 -4.05958600    0.27393700    2.79213700
 H                 -2.30069100    0.18605600    2.75332100
 H                 -3.25811600   -1.08001900    1.99104900
 C                 -5.74907700    2.97801700   -0.92967100
 H                 -6.45527500    2.32207500   -1.44856300
 H                 -5.55103700    3.83120000   -1.58168900
 H                 -6.24100700    3.34030700   -0.02448400
 C                  0.41972400   -0.87582600    2.82854500
 H                  0.50288600   -1.20491900    3.86522900
 H                 -0.04359400    0.11323000    2.82909800
 H                  1.43310400   -0.75456000    2.43391800
 C                  3.08294500   -1.92369600   -0.89014700
 H                  3.22255600   -2.94241600   -1.23515800
 C                 -1.74310100   -3.86737700    0.60521500
 H                 -2.26394500   -4.63319000    0.04553600
 C                 -2.20852600   -2.32791300   -1.27370200
 C                 -0.51449600   -3.16875700    2.53871600
 H                 -0.08762300   -3.39730900    3.50962500
 C                 -1.20046700   -4.15459200    1.84733700
 H                 -1.30692900   -5.14613800    2.27065900
 C                  5.24582300    1.05548500   -0.21451700
 H                  5.16671800    2.08573700    0.10015700
 C                  5.52407400   -1.59483900   -1.02717700
 H                  5.62241800   -2.62784800   -1.34459900
 C                  6.48649600    0.54087700   -0.49394900
 H                  7.36303100    1.17143200   -0.39724800
 C                  6.63221500   -0.79855000   -0.90498500
 H                  7.61758700   -1.19349500   -1.12319200


GS2-Z-Singlet
# freq wb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 1
 N                  0.23331400   -0.38184500    0.08496300
 C                 -2.33346500   -0.63841600   -0.36630600
 C                  1.81285000   -1.93100300    0.71660900
 C                  2.47495000   -0.87302400   -0.02695600
 F                  1.13035600    1.91950200    2.02965800
 C                  0.44733500   -1.59521700    0.76087800
 C                  1.49200900    0.04698200   -0.37227000
 C                 -1.12690400    1.82134700   -0.26097000
 C                 -3.56779200   -0.34464200    0.25492900
```

C	-2.28553100	-1.70375900	-1.29584700
C	2.24628900	-3.09871600	1.35449200
H	3.28587000	-3.39439300	1.34643200
C	-3.43326000	-2.44844000	-1.55429000
H	-3.38230400	-3.25814000	-2.27696800
C	3.82997200	-0.65925400	-0.42407600
C	-4.68432300	-1.13142800	-0.01322600
H	-5.61971600	-0.90760600	0.49193900
C	-4.63986500	-2.18898600	-0.91535600
C	-0.47460500	-2.37153100	1.45971400
H	-1.51608800	-2.08839500	1.51926400
F	-0.41217800	2.94593600	3.12442900
B	-1.05009100	0.24213400	-0.14473500
C	1.78321800	1.19379500	-1.14523200
H	1.01008600	1.89303300	-1.42685000
C	-1.61535000	2.41964200	-1.43880700
C	-0.75504700	2.66438800	0.79936200
C	1.32669800	-3.89060500	2.02017000
H	1.65872900	-4.79616800	2.51443800
C	4.12147200	0.50975200	-1.18083300
C	-0.02175400	-3.52519200	2.07665700
H	-0.72498900	-4.14739700	2.61803600
C	-3.73462400	0.79996000	1.22626100
H	-4.73092400	0.78065300	1.67059700
H	-3.61018500	1.76360300	0.72530400
H	-3.00549100	0.75895300	2.03536300
F	-0.74439800	0.93200600	2.44256500
C	-1.03601600	-2.08437900	-2.05931900
H	-1.30086600	-2.65027800	-2.95397900
H	-0.37989300	-2.71427100	-1.45167100
H	-0.44871600	-1.22082100	-2.37529400
C	-5.87074200	-2.99967100	-1.22103300
H	-6.44188500	-2.53833700	-2.03296400
H	-6.52846900	-3.06441100	-0.35173000
H	-5.61079800	-4.01273800	-1.53464500
C	-2.02621000	1.59144300	-2.63169000
H	-2.19847800	2.22790100	-3.50070000
H	-2.94326800	1.03366200	-2.42804200
H	-1.25702300	0.86314300	-2.90199100
C	3.07385800	1.40956500	-1.52610000
H	3.31998600	2.28774000	-2.11329100
C	-0.85617000	4.04797800	0.70432100
H	-0.57222100	4.67281600	1.54085200
C	-0.19863200	2.11592100	2.08981000
C	-1.69893800	3.80812600	-1.52511700
H	-2.06398400	4.25895300	-2.44191000
C	-1.32744300	4.62095000	-0.46521500
H	-1.40601800	5.69825200	-0.54837300
C	4.89773400	-1.53666300	-0.11467200
H	4.71038300	-2.43470700	0.45555900
C	5.45278900	0.75963300	-1.59115800
H	5.65883100	1.65609400	-2.16695000
C	6.17845400	-1.26786800	-0.52667400
H	6.97818200	-1.95532300	-0.27532000
C	6.46439900	-0.10748800	-1.27247800
H	7.48035000	0.09424000	-1.59150200

GS1-*E*-triplet
freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	0.49244100	-0.47900900	0.01962300
C	-1.25923100	1.45870200	0.08457400
C	2.36317100	-1.78700600	-0.44364300
C	2.83159300	-0.51026400	-0.08008300
F	-2.33145400	-0.57771400	-2.06488900
C	0.93750700	-1.75718100	-0.40046400
C	1.64883900	0.28938300	0.28112700
C	-1.93078300	-1.14675400	0.67790600
C	-0.88617100	2.17621700	-1.07528600
C	-2.03845600	2.11897300	1.05944300
C	3.00935500	-2.98656100	-0.81009900
H	4.08745300	-3.06276600	-0.79881100
C	-2.40187700	3.44971100	0.87676400
H	-2.98419200	3.94791000	1.64694400
C	4.15786400	0.07438200	0.00420600
C	-1.29503800	3.49820300	-1.23180200
H	-1.01016200	4.03207900	-2.13434500
C	-2.04791000	4.15690200	-0.26724100
C	0.18684000	-2.84566700	-0.79353600
H	-0.89200900	-2.81274100	-0.81295100
F	-4.32483900	-1.39533100	-2.04280100
B	-0.86635100	-0.05754600	0.22490900
C	1.76457000	1.49415900	0.87823400
H	0.90267700	2.06276100	1.19611300
C	-1.69807900	-1.84040800	1.88351800
C	-3.13584500	-1.39623700	0.00489600
C	2.24821100	-4.08744600	-1.16352800
H	2.73995300	-5.01171000	-1.44292600
C	4.26083200	1.36282300	0.63082000
C	0.85508000	-4.01561800	-1.17123600
H	0.27292400	-4.87838400	-1.47239600
C	-0.03160100	1.58780200	-2.17423000
H	-0.19607800	2.12605100	-3.10946600
H	-0.23609700	0.53358100	-2.35233000
H	1.02968300	1.67861700	-1.92172600
F	-3.94941900	0.51995800	-1.13849400
C	-2.49118000	1.43850400	2.33008600
H	-2.91219600	2.16774500	3.02429800
H	-1.67056500	0.93181900	2.84227800
H	-3.26008500	0.68919400	2.12475900
C	-2.49446200	5.58043600	-0.46797100
H	-3.47815800	5.60951100	-0.94737500
H	-1.79963600	6.12839100	-1.10785200
H	-2.57734900	6.10839600	0.48450400
C	-0.42024000	-1.67607100	2.67256500
H	-0.55759600	-2.02233400	3.69796800
H	-0.07442300	-0.64101300	2.71132100
H	0.38614900	-2.26623100	2.22611100
C	3.08394700	2.03340300	1.07554200
H	3.18745700	3.00335200	1.54699900
C	-4.08818400	-2.28178500	0.49651600
H	-5.00190700	-2.46066900	-0.05500900

C	-3.43685800	-0.71172300	-1.30036700
C	-2.66612800	-2.71490000	2.37384500
H	-2.48243800	-3.23265600	3.30956500
C	-3.85354400	-2.93756200	1.69380800
H	-4.59118200	-3.62441000	2.09119200
C	5.30267900	-0.52423700	-0.48811800
H	5.24117000	-1.46654800	-1.01444300
C	5.52461400	1.94015400	0.77261100
H	5.60978100	2.90545300	1.26013200
C	6.57284800	0.08306900	-0.34116400
H	7.45111100	-0.41877900	-0.72893000
C	6.67856900	1.29705300	0.29118500
H	7.64621400	1.76921900	0.41682800

GS2-*E*-triplet

```
# freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)
```

0 3

N	-0.23218400	-0.40503500	-0.23454100
C	1.32276100	1.69831700	-0.21398000
C	-2.08282200	-1.68256100	-0.83719700
C	-2.56933800	-0.52885300	-0.19369300
F	0.96628500	-0.75202800	2.36576900
C	-0.65752800	-1.60426700	-0.86217100
C	-1.39131700	0.22941900	0.25663000
C	2.33303200	-0.85444900	-0.16113100
C	2.22824300	2.35835700	0.64531800
C	0.68433800	2.45788400	-1.22332700
C	-2.71488800	-2.80914500	-1.40472300
H	-3.78821400	-2.92675200	-1.35463100
C	0.93543400	3.82306900	-1.32818300
H	0.44207100	4.38890000	-2.11386100
C	-3.90215800	-0.02827500	0.08802000
C	2.43294700	3.73059200	0.52031700
H	3.11628000	4.22500300	1.20517800
C	1.79677900	4.48362000	-0.45959700
C	0.09918100	-2.57140800	-1.49013900
H	1.17620200	-2.50826100	-1.53646800
F	0.56144000	-2.77203100	1.72574500
B	1.09665500	0.13902700	-0.17275800
C	-1.49589300	1.27847100	1.09776100
H	-0.62635400	1.79609200	1.47718800
C	3.28681600	-0.81038000	-1.19618000
C	2.53965700	-1.77114900	0.88326400
C	-1.94551500	-3.78802400	-2.00889800
H	-2.42626200	-4.65649200	-2.44337700
C	-3.99733300	1.10330200	0.96821700
C	-0.55688800	-3.66612300	-2.06312800
H	0.03211400	-4.43388400	-2.55075400
C	2.99417400	1.63352800	1.72679600
H	3.57805200	2.33954200	2.31949800
H	3.68563400	0.90218600	1.30051500
H	2.33109900	1.09488000	2.40405300
F	2.14133700	-2.38244100	3.13476300
C	-0.27211200	1.85948800	-2.23051800
H	-0.34414200	2.50150200	-3.11005100

H	-1.27654600	1.76559300	-1.80646200
H	0.02806500	0.86568400	-2.56621200
C	2.06386100	5.95817000	-0.60411900
H	2.88303300	6.13342700	-1.30883800
H	2.34885400	6.40521300	0.35049100
H	1.18556600	6.48473300	-0.98371600
C	3.13424300	0.13533300	-2.36188200
H	3.87260700	-0.08181100	-3.13498200
H	3.26127800	1.17376800	-2.04686000
H	2.14351400	0.05365200	-2.81684800
C	-2.81190000	1.71610500	1.47491400
H	-2.91266300	2.56332100	2.14263000
C	3.64259100	-2.61807900	0.90688200
H	3.78056600	-3.30829600	1.72887700
C	1.55676400	-1.91486900	2.01837100
C	4.38208800	-1.67171200	-1.16573600
H	5.10450400	-1.63643300	-1.97450900
C	4.56577000	-2.56877200	-0.12451700
H	5.42646600	-3.22669100	-0.11456700
C	-5.06137000	-0.56236700	-0.44406100
H	-5.00959100	-1.37907500	-1.15062100
C	-5.26347200	1.59042700	1.29797800
H	-5.34181900	2.43439800	1.97499800
C	-6.33434400	-0.04769000	-0.10135100
H	-7.22306200	-0.49705100	-0.52781200
C	-6.42976800	1.01122500	0.76717500
H	-7.39900300	1.41034300	1.04355000

GS1-*Z*-triplet
freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	0.45243400	0.54375200	0.03340500
C	-2.15901100	0.77000800	0.04924600
C	2.24091300	2.02530300	0.21637800
C	2.78071500	0.76401500	-0.09946500
F	-1.55010700	-1.49163500	-2.03613600
C	0.82267800	1.88774900	0.30268700
C	1.63865000	-0.14293800	-0.29819000
C	-0.87788700	-1.57579500	0.71374700
C	-2.36985200	1.50378400	-1.14030800
C	-3.18845900	0.74791300	1.01522900
C	2.81856000	3.29338700	0.43892700
H	3.88266100	3.44594800	0.32539400
C	-4.36707800	1.45291600	0.79296700
H	-5.14057500	1.44161700	1.55589300
C	4.13541800	0.26994500	-0.26457300
C	-3.57584200	2.17234600	-1.33621000
H	-3.72699400	2.72201000	-2.26127600
C	-4.58621100	2.16435900	-0.38224800
C	0.02329800	2.94946400	0.67321500
H	-1.04695600	2.83984000	0.77168700
F	-2.45227800	-3.44671700	-1.97268100
B	-0.83672600	-0.06049700	0.22958100
C	1.79206600	-1.37435700	-0.82776600
H	0.95171200	-2.01394100	-1.05180400

C	-0.24721000	-1.90405100	1.93283600
C	-1.59598400	-2.58939700	0.06144500
C	2.00579500	4.35983700	0.78084900
H	2.44455900	5.33611800	0.94966200
C	4.28237700	-1.05257200	-0.80575200
C	0.62714200	4.18882500	0.91098100
H	0.00483500	5.02948200	1.19403100
C	-1.32644700	1.63217100	-2.22614700
H	-1.80067700	1.87163600	-3.17966800
H	-0.73883900	0.72588300	-2.36000500
H	-0.62911500	2.44295900	-1.99151200
F	-3.48916200	-1.76799700	-1.11698000
C	-3.05833300	-0.01121900	2.31453000
H	-3.86687600	0.25661400	2.99677600
H	-2.11445800	0.19915000	2.82173400
H	-3.10468000	-1.09044700	2.14652300
C	-5.88978100	2.87714800	-0.62449000
H	-6.61775600	2.19910800	-1.08119400
H	-5.75973800	3.72507200	-1.30016600
H	-6.32181000	3.24219800	0.30979400
C	0.57837200	-0.90557500	2.70933100
H	0.70919900	-1.23799600	3.74012800
H	0.13046800	0.08998600	2.73246000
H	1.57289400	-0.79955800	2.26468700
C	3.12627200	-1.83547000	-1.10077300
H	3.26388200	-2.82623000	-1.51671900
C	-1.70722900	-3.87329100	0.58417900
H	-2.25893700	-4.63364200	0.04699500
C	-2.27341200	-2.32386800	-1.25502600
C	-0.37700500	-3.19022700	2.45300200
H	0.10118300	-3.42609200	3.39805100
C	-1.10035500	-4.17146300	1.79245800
H	-1.18595800	-5.16587300	2.21390600
C	5.26941800	0.98312900	0.07808100
H	5.18088100	1.95732900	0.53849500
C	5.56925100	-1.55022800	-1.01855500
H	5.68586500	-2.54179000	-1.44277200
C	6.56442400	0.45584100	-0.13939200
H	7.43191700	1.04596600	0.13036300
C	6.70799200	-0.79365700	-0.68996900
H	7.69438500	-1.20617000	-0.86836000

GS2-*Z*-triplet
freq uwb97xd/6-311g(d,p) scrf=(solvent=tetrahydrofuran)

0 3

N	0.17141900	-0.44520200	-0.06040300
C	-2.43754400	-0.54266300	-0.30732300
C	1.78266200	-2.02213800	0.51746900
C	2.45230800	-0.96196400	-0.12405200
F	1.35118000	1.69567000	1.91891800
C	0.39644000	-1.69445400	0.56873600
C	1.41854000	-0.00220500	-0.54819300
C	-1.06483800	1.83380700	-0.21384900
C	-3.59737000	-0.20773900	0.42512900
C	-2.53401200	-1.55749400	-1.28855400

C	2.21273300	-3.24552000	1.07361000
H	3.24619200	-3.55459700	1.00555400
C	-3.74448200	-2.21439900	-1.49052100
H	-3.80306400	-2.98602800	-2.25337100
C	3.85002600	-0.69925000	-0.41292000
C	-4.78249900	-0.90638700	0.20810400
H	-5.65915200	-0.65108400	0.79677800
C	-4.87915500	-1.91354000	-0.74546800
C	-0.51056500	-2.50331100	1.22072700
H	-1.55407600	-2.23177100	1.29372000
F	-0.04717700	2.76988600	3.15202200
B	-1.08485700	0.24771600	-0.16028600
C	1.70441900	1.03016800	-1.36888100
H	0.94695500	1.70968500	-1.73071800
C	-1.59724200	2.51329800	-1.32636300
C	-0.56365100	2.60539700	0.84806900
C	1.29076900	-4.07096500	1.69377100
H	1.61627000	-5.01247300	2.12019100
C	4.13723200	0.41384500	-1.27455800
C	-0.05168000	-3.69973100	1.78110200
H	-0.75719600	-4.34754900	2.28775600
C	-3.61001700	0.88879100	1.46344800
H	-4.57821100	0.92874300	1.96512200
H	-3.42757500	1.86587500	1.00858800
H	-2.84334100	0.73802700	2.22361200
F	-0.54969900	0.80852100	2.42420400
C	-1.37061600	-1.97682600	-2.15962100
H	-1.73418500	-2.47623400	-3.05927700
H	-0.72003500	-2.68056700	-1.63141100
H	-0.74727300	-1.13756300	-2.47192900
C	-6.18116000	-2.62725700	-0.99360700
H	-6.74732000	-2.12841100	-1.78664500
H	-6.80574500	-2.63634100	-0.09804100
H	-6.01361500	-3.65934500	-1.30893000
C	-2.14499900	1.76235900	-2.51558200
H	-2.34801000	2.44453200	-3.34237800
H	-3.07276600	1.24356800	-2.26288000
H	-1.43981000	1.00757700	-2.87434900
C	3.07483800	1.23509400	-1.75394200
H	3.31706800	2.06595100	-2.40574500
C	-0.57902000	3.99564800	0.81330200
H	-0.19408100	4.56469400	1.64936000
C	0.04330100	1.97045500	2.07497000
C	-1.59755600	3.90662600	-1.35254500
H	-1.99944000	4.41844800	-2.22075800
C	-1.09581400	4.64800300	-0.29387900
H	-1.10898800	5.73075700	-0.32896100
C	4.90052600	-1.43986400	0.09667300
H	4.71123400	-2.24695400	0.79051000
C	5.46709800	0.67537300	-1.61084200
H	5.68825600	1.50553300	-2.27322200
C	6.24213500	-1.15225900	-0.25155000
H	7.04052100	-1.75935000	0.15782500
C	6.51653100	-0.11088800	-1.10282300
H	7.53896600	0.11596300	-1.38266100

10.2 Fluorescence Cycle calculations for C1-C5 (TD-DFT)

Catalyst C1

C1-GS1 – S_0 optimized Geometry

0 1

N	1.19405500	0.33676300	0.01088800
C	-1.35253000	0.94280500	0.11694800
C	3.12163700	1.60646300	0.02141000
C	3.45550000	0.27833900	-0.44847600
F	-1.11037600	-1.31242400	-2.05126800
C	1.74321500	1.61652300	0.28110800
C	2.26890400	-0.46940400	-0.43841400
C	-0.41692700	-1.59153700	0.67957300
C	-1.48181500	1.73443500	-1.04665900
C	-2.35115900	1.05432000	1.11010700
C	3.89536900	2.74150300	0.24488400
H	4.95950400	2.72932800	0.04077500
C	-3.41027700	1.93682900	0.93926700
H	-4.15440700	2.02171700	1.72478800
C	4.64958500	-0.29067200	-0.88032400
H	5.56444500	0.28993600	-0.88596000
C	-2.57516900	2.58400700	-1.18942700
H	-2.66330000	3.17303900	-2.09681900
C	-3.54841700	2.70628300	-0.20921500
C	1.13344000	2.75407400	0.80284500
H	0.07914600	2.77384200	1.03331500
F	-2.27791100	-3.12570600	-2.03940800
B	-0.16557600	-0.08250700	0.23854000
C	2.25883400	-1.78176700	-0.90182700
H	1.35040700	-2.36193000	-0.94449000
C	0.18535700	-2.05729700	1.86589200
C	-1.26868500	-2.47608700	-0.00017500
C	3.28453800	3.88005600	0.73846500
H	3.86830600	4.77435300	0.91855700
C	4.64587100	-1.60572300	-1.31008400
H	5.56453200	-2.06768900	-1.65013200
C	1.91638100	3.87751700	1.01769800
H	1.45148700	4.77150700	1.41566900
C	-0.47607900	1.73014600	-2.17469700
H	-0.94849900	2.07139400	-3.09656100
H	-0.05063600	0.74772300	-2.36171200
H	0.35100900	2.41164800	-1.95971900
F	-3.05137000	-1.35374200	-1.09624900
C	-2.31493700	0.25785900	2.39232000
H	-3.07108400	0.62448600	3.08688300
H	-1.34935800	0.32417000	2.89506500
H	-2.51603700	-0.79937300	2.21025500
C	-4.73008500	3.61863600	-0.39267300
H	-5.58894600	3.06456000	-0.78225600
H	-4.50790800	4.41988600	-1.09867200
H	-5.03489300	4.06803800	0.55393100
C	1.14571400	-1.21761000	2.67377500
H	1.23893800	-1.61636700	3.68403300
H	0.83644600	-0.17556500	2.75480600

H	2.14107300	-1.22204600	2.22279800
C	3.45667900	-2.33707000	-1.32408000
H	3.46315700	-3.35988400	-1.68098600
C	-1.52911100	-3.75909100	0.46153500
H	-2.17774700	-4.41575800	-0.10170800
C	-1.92840900	-2.06903600	-1.28502900
C	-0.09790000	-3.34075200	2.32754500
H	0.36267000	-3.67875800	3.24896100
C	-0.94549100	-4.19039800	1.63916200
H	-1.14609000	-5.18630500	2.01386900

C1-GS1 – S_1 optimized Geometry

0 1

N	1.24764100	0.08465700	0.04740400
C	-1.15535400	1.13866000	-0.05636300
C	3.38406000	0.91759900	0.18051800
C	3.38969700	-0.23055900	-0.72217900
F	-1.72482600	-1.32686000	-1.91529100
C	2.04636800	1.05457300	0.62108700
C	2.05259600	-0.68872800	-0.77268800
C	-0.68334200	-1.49306300	0.82911600
C	-0.93777500	1.95918300	-1.19324600
C	-2.18958400	1.53949500	0.83720000
C	4.34173300	1.79820900	0.62242000
H	5.37197100	1.71910600	0.29878000
C	-2.90406300	2.70554000	0.60696900
H	-3.67216100	2.99511900	1.31842100
C	4.36052600	-0.87045800	-1.45558300
H	5.39200700	-0.54195500	-1.43131800
C	-1.68304200	3.11851000	-1.38779000
H	-1.49660600	3.71720500	-2.27453800
C	-2.66861900	3.51971200	-0.49860000
C	1.65662200	2.06684700	1.49521100
H	0.62634800	2.16536100	1.80532500
F	-3.28877500	-2.72989700	-1.46732900
B	-0.25823200	-0.09476900	0.28164900
C	1.67618500	-1.77695100	-1.55458300
H	0.64931600	-2.11025800	-1.58556000
C	0.02076800	-2.13710700	1.88967900
C	-1.78135900	-2.22530500	0.29072400
C	3.95731500	2.81618400	1.50908000
H	4.70301200	3.51654500	1.86320700
C	3.98812000	-1.96774200	-2.24598600
H	4.74355400	-2.48076100	-2.82745800
C	2.64239400	2.94584100	1.93509700
H	2.37718700	3.74436400	2.61570600
C	0.05932700	1.58323500	-2.25736500
H	-0.09577600	2.17918500	-3.15784500
H	-0.03164400	0.52943600	-2.52708300
H	1.09114900	1.74977100	-1.93584000
F	-3.39645100	-0.74099900	-0.67193500
C	-2.52907800	0.74736600	2.07318900
H	-3.19198200	1.31866200	2.72479100
H	-1.63255200	0.48093000	2.63758300
H	-3.03083100	-0.18889400	1.82141300

C	-3.45047200	4.78811700	-0.70740500
H	-4.51858900	4.62928100	-0.54202600
H	-3.31774200	5.17352100	-1.71943800
H	-3.12979300	5.56934300	-0.01140200
C	1.17693800	-1.47056700	2.58464400
H	1.42872400	-1.99972100	3.50418500
H	0.93946100	-0.43526800	2.84220500
H	2.07733500	-1.45051500	1.96584500
C	2.67196400	-2.40679700	-2.29611500
H	2.41404200	-3.25404700	-2.91815500
C	-2.17267900	-3.45992400	0.79637200
H	-3.00890400	-3.97948300	0.35003500
C	-2.53688000	-1.74998100	-0.91813500
C	-0.38531600	-3.37455900	2.36852500
H	0.16204800	-3.81856200	3.19319100
C	-1.48241700	-4.04160000	1.84331200
H	-1.78926300	-5.00168800	2.23828100

C1-GS2 – S_0 optimized Geometry

0 1

N	-0.62236200	0.71703800	-0.20185200
C	1.89753500	0.00349300	-0.19119100
C	-1.62603500	2.76392800	0.15352100
C	-2.52550800	1.94774300	-0.63437900
F	-0.52832600	-0.66168800	2.31931900
C	-0.48057600	1.99306300	0.39594000
C	-1.89835100	0.70680700	-0.82036100
C	-0.14006100	-1.84619400	-0.26205300
C	2.82340800	-0.61369200	0.67871000
C	2.39745200	0.90422200	-1.16084500
C	-1.73613700	4.05176000	0.66983100
H	-2.62257600	4.64568600	0.48104900
C	3.76039500	1.17288500	-1.22448800
H	4.12301200	1.85921300	-1.98323300
C	-3.78017100	2.19904200	-1.18094000
H	-4.26128800	3.15857600	-1.03228400
C	4.17554700	-0.29666400	0.59546300
H	4.86632800	-0.76624700	1.28826600
C	4.66821200	0.59273800	-0.34952800
C	0.54909900	2.48688500	1.19117000
H	1.42348000	1.89421000	1.41420400
F	-2.56554800	-0.94029100	1.66142800
B	0.35903400	-0.33852800	-0.19039600
C	-2.51130400	-0.28299100	-1.58261700
H	-2.04279500	-1.23944400	-1.75635000
C	0.24005200	-2.68335600	-1.32904300
C	-0.94042000	-2.40698700	0.74773200
C	-0.69981400	4.55496100	1.43550500
H	-0.76559200	5.55470200	1.84695300
C	-4.39851200	1.20709900	-1.92074600
H	-5.37556200	1.38214100	-2.35401600
C	0.42732600	3.77200400	1.69526800
H	1.22426900	4.17202800	2.31057600
C	2.41154800	-1.60396000	1.74099400
H	1.91340800	-2.47340600	1.30967800

H	1.72372200	-1.16348100	2.46241200
H	3.28612300	-1.95790700	2.28691100
F	-1.66165900	-2.36268800	2.99993700
C	1.51933900	1.60534100	-2.17267100
H	2.12052200	1.94749400	-3.01555100
H	1.03575500	2.48271100	-1.73691300
H	0.72939600	0.96701900	-2.56689300
C	6.13981100	0.88812900	-0.44820400
H	6.62363500	0.21144700	-1.15852000
H	6.63564700	0.76107600	0.51512900
H	6.31747900	1.90716600	-0.79530600
C	1.08484700	-2.17906300	-2.47224400
H	1.19527100	-2.94963700	-3.23497000
H	2.08056700	-1.88790800	-2.13560400
H	0.63575300	-1.30616900	-2.95099200
C	-3.76192900	-0.01935400	-2.11901200
H	-4.25167400	-0.78589900	-2.70750100
C	-1.35337500	-3.73266300	0.70972400
H	-1.95773200	-4.13359100	1.51178600
C	-1.41930600	-1.59643700	1.92163900
C	-0.19228400	-4.00679400	-1.36027200
H	0.09990600	-4.63452100	-2.19437500
C	-0.98021700	-4.53537400	-0.35253900
H	-1.29933600	-5.56932200	-0.39186200

C1-GS2 – S_1 optimized Geometry

0 1

N	-0.60212400	0.65340000	-0.23374400
C	1.95173700	0.04480600	-0.28301400
C	-1.79757200	2.54413800	0.28273700
C	-2.39715000	1.92308900	-0.89446500
F	-0.83460000	-0.74323900	2.42891000
C	-0.71020800	1.71590700	0.64507600
C	-1.61515700	0.77706900	-1.16630200
C	-0.03445500	-1.91308000	-0.10180400
C	2.93245500	-0.52812000	0.57441200
C	2.38218000	1.09330600	-1.13859200
C	-2.06156800	3.68290600	1.00582600
H	-2.88277200	4.33781100	0.74256500
C	3.69823500	1.54005600	-1.11057600
H	3.99529500	2.33467100	-1.78878900
C	-3.46985300	2.22603000	-1.69759900
H	-4.08706500	3.09493800	-1.50622800
C	4.23664300	-0.04809500	0.57010700
H	4.95761600	-0.49412200	1.24912100
C	4.64761700	0.98942000	-0.25990000
C	0.11608000	2.01641500	1.72421000
H	0.94570700	1.37461800	1.98155300
F	-2.63372500	-0.60081200	1.23824800
B	0.46808300	-0.44298000	-0.21312300
C	-1.90086800	-0.07256300	-2.23095000
H	-1.30906000	-0.95905400	-2.40812400
C	0.56024700	-2.90985300	-0.93959400
C	-1.10717000	-2.36826800	0.71755200
C	-1.23661200	3.98746400	2.09819900

H	-1.43406800	4.88097200	2.67670500
C	-3.75676700	1.37987400	-2.77975900
H	-4.60034400	1.60710200	-3.41906500
C	-0.17010200	3.16902600	2.44828700
H	0.44930900	3.43146800	3.29602400
C	2.60536700	-1.63400200	1.54795000
H	2.46353400	-2.59491300	1.04702500
H	1.68093200	-1.42965000	2.09044600
H	3.41346400	-1.75453300	2.27102900
F	-2.41849000	-2.17653900	2.68204900
C	1.45474400	1.71880200	-2.14705300
H	2.01513100	2.31305100	-2.86990400
H	0.72421700	2.38401700	-1.67941900
H	0.89209400	0.95924000	-2.69576300
C	6.05918900	1.50882400	-0.21871500
H	6.77174400	0.70936400	-0.00672000
H	6.17830900	2.26542500	0.56319900
H	6.33928700	1.97279600	-1.16604800
C	1.69237200	-2.59169500	-1.88254400
H	1.86186700	-3.42590800	-2.56443100
H	2.62768600	-2.39165200	-1.35682500
H	1.47597900	-1.69831400	-2.47320400
C	-2.98525800	0.25575900	-3.04024000
H	-3.23382100	-0.38105000	-3.87927300
C	-1.58978300	-3.67233000	0.66848800
H	-2.40626900	-3.96467100	1.31423000
C	-1.73737000	-1.48395400	1.74780500
C	0.06223000	-4.20382100	-0.96264200
H	0.52180300	-4.92413300	-1.63099300
C	-1.01503300	-4.59843700	-0.17801800
H	-1.38980700	-5.61309200	-0.22144900

Catalyst C2

C2-GS1-conf1-sym – S_0 optimized Geometry

0 1

N	0.61736200	0.13215800	0.06943900
C	-1.87360800	0.92544600	-0.05136500
C	2.63723500	1.26188200	0.01283000
C	2.89737100	-0.14427400	-0.22269900
F	-1.69121600	-1.61411300	-1.90343000
C	1.25013500	1.40182200	0.17336600
C	1.65851800	-0.80191500	-0.17780100
C	-1.16407100	-1.57538900	0.87988600
C	-1.89703300	1.55401100	-1.31689200
C	-2.89709000	1.24732900	0.86712600
C	3.48643600	2.35264800	0.10958500
H	4.55793500	2.25525600	-0.01258300
C	-3.87680000	2.17222600	0.52692400
H	-4.64111400	2.41963600	1.25673000
C	4.06967000	-0.83671100	-0.47856000
H	5.03089500	-0.33965600	-0.51662100
C	-2.91404700	2.45245300	-1.62718500
H	-2.92066800	2.91380700	-2.60982100
C	-3.91115600	2.78122500	-0.72112900
C	0.71661800	2.64649400	0.47233900
H	-0.34253400	2.78410900	0.62883500
F	-2.98533500	-3.33037100	-1.73083000
B	-0.77307900	-0.15655700	0.26732200
C	1.59330900	-2.16200800	-0.43943200
H	0.65399600	-2.69244600	-0.45940900
C	-0.66551000	-1.91987200	2.15308500
C	-2.04156200	-2.48332700	0.26698700
C	2.94558300	3.60279700	0.38057200
C	4.00512200	-2.20623900	-0.70308600
C	1.56676500	3.74165200	0.56606500
H	1.13825600	4.70778400	0.79084800
C	-0.85076700	1.32352200	-2.38277100
H	-1.27001300	1.53018500	-3.36832200
H	-0.46525800	0.30780400	-2.38927200
H	-0.00080900	1.99627600	-2.24113200
F	-3.67770900	-1.40295200	-1.07252900
C	-2.97246900	0.63504000	2.24511700
H	-3.72638300	1.14452800	2.84572800
H	-2.02533900	0.70359200	2.78148400
H	-3.24404200	-0.42105400	2.19704600
C	-5.01050500	3.74093900	-1.08620100
H	-5.87230900	3.20434300	-1.49349500
H	-4.68083900	4.45389000	-1.84329400
H	-5.35604000	4.29907800	-0.21455000
C	0.31254000	-1.05010300	2.90578300
H	0.31136800	-1.30836500	3.96492600
H	0.09016400	0.01327100	2.82093500
H	1.32854500	-1.19440800	2.53009600
C	2.76903700	-2.85926800	-0.68981900
H	2.70668200	-3.92010000	-0.88536900
C	-2.42365000	-3.67307200	0.87252300

H	-3.08890100	-4.35276900	0.35804200
C	-2.60016300	-2.20763400	-1.09810400
C	-1.06990300	-3.10825300	2.75700300
H	-0.68757400	-3.35073400	3.74215600
C	-1.94020000	-3.98281600	2.13078100
H	-2.23623700	-4.90395000	2.61699100
O	5.19235500	-2.82714000	-0.94072300
O	3.83255800	4.63217100	0.45759800
C	3.33875500	5.92943600	0.74198900
H	2.84816600	5.96554800	1.71900100
H	4.20659100	6.58461500	0.75278600
H	2.64033400	6.26933800	-0.02812800
C	5.18713300	-4.22140000	-1.19324200
H	4.60942400	-4.46333500	-2.08995700
H	6.22611200	-4.50120900	-1.35040900
H	4.78834100	-4.78052200	-0.34188000

C2-GS1-conf1-sym – S_1 optimized Geometry

0 1

N	0.66716200	-0.02160400	0.12830400
C	-1.57592900	1.20540800	-0.46873600
C	2.89428800	0.54036500	0.11010000
C	2.75785800	-0.83051800	-0.37574000
F	-2.46205900	-1.65060800	-1.39802600
C	1.57652200	0.97585400	0.40088000
C	1.36831500	-1.11003600	-0.34860000
C	-1.46307000	-0.99320000	1.28746100
C	-1.23944900	1.55120100	-1.80232800
C	-2.55117400	2.01805800	0.17614700
C	3.95821200	1.37773400	0.30280500
H	4.97921400	1.08783000	0.09090900
C	-3.10633200	3.10817200	-0.47835500
H	-3.83582300	3.71680200	0.04854000
C	3.64758500	-1.77773000	-0.80378100
H	4.71592000	-1.60701800	-0.83478200
C	-1.82678200	2.64961100	-2.42424400
H	-1.55560600	2.87514400	-3.45159100
C	-2.75878600	3.45112400	-1.78235700
C	1.33258900	2.26052100	0.87637800
H	0.32341500	2.59420900	1.07224900
F	-4.20026600	-2.61265900	-0.58066200
B	-0.85697700	0.06603800	0.32163200
C	0.87739300	-2.34526100	-0.75759200
H	-0.18257200	-2.55344300	-0.73733400
C	-0.85318300	-1.32612900	2.53587500
C	-2.64863800	-1.72481800	0.97639100
C	3.71392500	2.67733600	0.79674600
C	3.15096900	-3.03014100	-1.22213900
C	2.41456600	3.10738300	1.07704600
H	2.23663000	4.10681200	1.44516200
C	-0.28430300	0.71945200	-2.61898800
H	-0.36424500	0.97189500	-3.67744700
H	-0.49466100	-0.34569300	-2.50745600
H	0.75721400	0.87821800	-2.32693200
F	-4.04874200	-0.47452800	-0.51298800

C	-3.00199700	1.75367300	1.59011200
H	-3.58956500	2.59173900	1.96847500
H	-2.15336500	1.59401500	2.25920400
H	-3.62055800	0.85607700	1.64970100
C	-3.36411700	4.65245200	-2.45713500
H	-4.44177600	4.70479600	-2.28607700
H	-3.19295000	4.62983600	-3.53455000
H	-2.93182600	5.58201100	-2.07402400
C	0.38156500	-0.61776600	3.02480900
H	0.55320200	-0.83307500	4.07998200
H	0.28832700	0.46519400	2.90977900
H	1.27823000	-0.92238800	2.48036400
C	1.78095900	-3.30212200	-1.20050700
H	1.40883300	-4.26320700	-1.52264100
C	-3.20384700	-2.65387300	1.84909100
H	-4.10079300	-3.18541500	1.56362000
C	-3.32763900	-1.60361000	-0.35770600
C	-1.42504000	-2.26309900	3.38355900
H	-0.94450700	-2.46463700	4.33514500
C	-2.60189400	-2.92607700	3.06318800
H	-3.03611800	-3.64721200	3.74385000
O	4.08958800	-3.90327500	-1.62440000
O	4.81212500	3.43342300	0.95678300
C	4.67364500	4.75980900	1.45409900
H	4.23430500	4.75844500	2.45415100
H	5.68082600	5.16438900	1.49944400
H	4.06487400	5.36806000	0.78151500
C	3.68775700	-5.19270500	-2.07307100
H	3.03776600	-5.11748700	-2.94773300
H	4.60406000	-5.70975600	-2.34378200
H	3.17838200	-5.74255000	-1.27844400

C2-GS1-conf2-asym – S_0 optimized Geometry

0 1

N	0.58332800	0.00062700	0.07556800
C	-1.80090300	1.07125300	-0.04295000
C	2.71438600	0.89849500	0.03510400
C	2.81418900	-0.52241100	-0.22557500
F	-1.90567300	-1.43100400	-1.94229900
C	1.35137500	1.18989500	0.20234300
C	1.51586400	-1.03630000	-0.18859600
C	-1.38559100	-1.51058100	0.84326300
C	-1.74387700	1.72213200	-1.29574900
C	-2.78680000	1.49071900	0.87747900
C	3.67941000	1.88769300	0.14737400
H	4.73371600	1.67599000	0.02011800
C	-3.65136700	2.52833700	0.55154700
H	-4.38727400	2.84751300	1.28273900
C	3.91602400	-1.33365300	-0.49875800
H	4.90905000	-0.90744600	-0.52107100
C	-2.64867900	2.73778300	-1.59233500
H	-2.59620500	3.21518800	-2.56585400
C	-3.60734900	3.16124800	-0.68444000
C	0.95958800	2.48050300	0.52556100
H	-0.07748000	2.73178300	0.68847400

F	-3.39133200	-2.98793100	-1.80534100
B	-0.83290000	-0.13417200	0.26068500
C	1.29782500	-2.38349800	-0.47510000
H	0.30596600	-2.80726900	-0.50022700
C	-0.93451900	-1.93664000	2.10939300
C	-2.35886700	-2.29916800	0.20958100
C	3.28053600	3.18482000	0.44090200
C	3.69415300	-2.67796800	-0.74673300
C	1.92573800	3.47284100	0.63447800
H	1.60756100	4.47649500	0.87727100
C	-0.72509600	1.39265100	-2.36223500
H	-1.11496600	1.65848700	-3.34568500
H	-0.45432500	0.34073300	-2.38286900
H	0.19339700	1.96522000	-2.20849300
F	-3.85552000	-1.00738800	-1.10573700
C	-2.94108000	0.86482200	2.24281900
H	-3.63362500	1.44749000	2.85076000
H	-1.99560400	0.81138600	2.78382900
H	-3.33428900	-0.15103700	2.17285100
C	-4.58683500	4.24799300	-1.03437200
H	-5.51373800	3.82074900	-1.42781900
H	-4.18389200	4.91606600	-1.79685300
H	-4.84886100	4.84344900	-0.15822600
C	0.13114600	-1.19886900	2.88411700
H	0.08926700	-1.47166200	3.93882600
H	0.03523200	-0.11565700	2.81522600
H	1.12719700	-1.45508000	2.51456600
C	2.38723200	-3.18786300	-0.73919200
H	2.25203300	-4.23912600	-0.95972100
C	-2.87497700	-3.45100100	0.78809100
H	-3.61107900	-4.03949600	0.25801600
C	-2.87896400	-1.93157200	-1.14920000
C	-1.47261100	-3.08493100	2.68606600
H	-1.12359100	-3.39104100	3.66583300
C	-2.43361500	-3.84147700	2.03942100
H	-2.83306500	-4.73413100	2.50431200
O	4.67087100	-3.58298300	-1.02160600
O	4.27612300	4.10872400	0.53143500
C	3.92845500	5.44854800	0.83436600
H	3.44567100	5.52530000	1.81290500
H	4.86315800	6.00401700	0.85186300
H	3.27103000	5.87362300	0.07046700
C	6.01172000	-3.12689900	-1.05885400
H	6.31933200	-2.71501900	-0.09320500
H	6.62007400	-3.99851000	-1.28798200
H	6.15423800	-2.37195200	-1.83759800

C2-GS1-conf2-asym – S_1 optimized Geometry

0 1

N	0.60979500	-0.05904100	0.11633200
C	-1.65405300	1.14264700	-0.45143700
C	2.82276900	0.54947100	0.14286900
C	2.71887100	-0.80451700	-0.39522600
F	-2.46396200	-1.69658100	-1.49742700
C	1.49410000	0.94731000	0.43688700
C	1.34101000	-1.11190100	-0.39478300

C	-1.50783500	-1.11893600	1.22108900
C	-1.31325300	1.54766700	-1.76742300
C	-2.65276200	1.90826800	0.21486300
C	3.86643500	1.40105900	0.37665300
H	4.89554500	1.14219300	0.16362300
C	-3.22427400	3.01210300	-0.40149300
H	-3.97154200	3.58384100	0.14155400
C	3.64839700	-1.71341700	-0.84913900
H	4.70253700	-1.47599000	-0.84211700
C	-1.91727000	2.65782700	-2.35098300
H	-1.64180600	2.92932100	-3.36601300
C	-2.87149100	3.41422000	-1.68701500
C	1.21893600	2.20672800	0.95788200
H	0.20131200	2.51154500	1.15691900
F	-4.18552600	-2.73151500	-0.73580300
B	-0.91676400	-0.01042400	0.30085100
C	0.87956700	-2.34582700	-0.86093100
H	-0.17562900	-2.57796000	-0.86390900
C	-0.90429300	-1.48116700	2.46394200
C	-2.67219100	-1.86561700	0.87037800
C	3.59046500	2.67724300	0.91712200
C	3.18203900	-2.95264100	-1.31876700
C	2.28127700	3.06910500	1.20122100
H	2.07848900	4.04945100	1.60580900
C	-0.33460500	0.76762200	-2.60690800
H	-0.41086800	1.05922500	-3.65553100
H	-0.52443500	-0.30496800	-2.53868500
H	0.70101600	0.93581400	-2.29947700
F	-4.08820800	-0.59441700	-0.58544700
C	-3.11223200	1.57761400	1.61192000
H	-3.72294000	2.38634900	2.01654200
H	-2.26735200	1.41037700	2.28398000
H	-3.71049900	0.66457800	1.62851500
C	-3.49420600	4.62976900	-2.31909900
H	-4.57209400	4.66169900	-2.14481000
H	-3.32463000	4.64679500	-3.39688200
H	-3.07362000	5.55137100	-1.90483400
C	0.30751000	-0.76108300	2.99148700
H	0.47464900	-1.01093600	4.03975300
H	0.18767000	0.32271700	2.91502100
H	1.21657100	-1.02293400	2.44531200
C	1.81067500	-3.25043100	-1.32314400
H	1.50710900	-4.21914400	-1.69712700
C	-3.21443600	-2.83855600	1.70258300
H	-4.09527800	-3.38033300	1.38772700
C	-3.34060800	-1.71068800	-0.46562500
C	-1.46236500	-2.46146600	3.27087100
H	-0.98744100	-2.68581700	4.22015400
C	-2.61909900	-3.14030000	2.91288000
H	-3.04294700	-3.89601600	3.56183100
O	3.98491500	-3.92397500	-1.78459200
O	4.67206700	3.44785100	1.11469400
C	4.50202300	4.75295900	1.65690700
H	4.05363400	4.70713900	2.65185400
H	5.50017300	5.17603600	1.72618200
H	3.88666100	5.37161600	0.99999600
C	5.39151000	-3.70993100	-1.81377200

H	5.78370600	-3.54140100	-0.80824300
H	5.81974700	-4.62131400	-2.22145600
H	5.64726900	-2.86703700	-2.45984900

C2-GS1-conf3-asym – S_0 optimized Geometry

0 1

N	0.57315100	0.13168900	0.10766700
C	-1.85745000	1.09709000	-0.01917400
C	2.65902400	1.12556900	0.06839400
C	2.82743200	-0.28838200	-0.19475600
F	-1.82668300	-1.40322700	-1.92926600
C	1.29090700	1.35136600	0.23559700
C	1.54803500	-0.86533200	-0.15877600
C	-1.33210600	-1.46451800	0.86168100
C	-1.82386700	1.75273100	-1.27011200
C	-2.87290600	1.46189100	0.89292800
C	3.59205300	2.15737600	0.18157900
H	4.64435100	1.95165200	0.04474600
C	-3.78939000	2.45121200	0.56024100
H	-4.54761900	2.72952800	1.28531100
C	3.95155600	-1.05225000	-0.46695800
H	4.94390200	-0.62008100	-0.49874400
C	-2.78020100	2.71819200	-1.57402600
H	-2.74438700	3.19956100	-2.54629500
C	-3.76867200	3.08742900	-0.67492100
C	0.83709100	2.62827300	0.56511500
H	-0.21031300	2.83137800	0.72919900
F	-3.25053300	-3.01828100	-1.80808200
B	-0.83667300	-0.06301200	0.28708300
C	1.39362100	-2.21351000	-0.44450600
H	0.42187100	-2.68150600	-0.47032300
C	-0.87326900	-1.87432600	2.13033200
C	-2.26382700	-2.29302300	0.21703400
C	3.13015700	3.42817900	0.47904600
C	3.79667900	-2.40969400	-0.71680500
C	1.75840700	3.64929400	0.67430000
H	1.43726400	4.65347000	0.92068600
C	-0.78036900	1.48017500	-2.32886700
H	-1.17672300	1.72535000	-3.31507900
H	-0.45247100	0.44455500	-2.34799200
H	0.10431600	2.10202000	-2.16840000
F	-3.79888100	-1.05895800	-1.10926600
C	-3.00530200	0.82681300	2.25629700
H	-3.72624600	1.37646300	2.86196000
H	-2.06103400	0.81474700	2.80175100
H	-3.35227800	-0.20552100	2.18243300
C	-4.80244700	4.12047000	-1.03117400
H	-5.71807800	3.64285200	-1.39163700
H	-4.44566300	4.78484800	-1.81927700
H	-5.07157900	4.72734700	-0.16493400
C	0.15327700	-1.09254200	2.91442000
H	0.12308600	-1.37675800	3.96648200
H	0.00386400	-0.01471000	2.85537200
H	1.16125700	-1.29564800	2.54434600
C	2.52048600	-2.98122200	-0.71134300

H	2.38880600	-4.03198500	-0.92567700
C	-2.73426500	-3.46811300	0.78797500
H	-3.43956500	-4.08644000	0.25002000
C	-2.78637000	-1.94360800	-1.14558100
C	-1.36571800	-3.04654900	2.69934900
H	-1.01241000	-3.33990500	3.68149200
C	-2.28735400	-3.84237800	2.04225100
H	-2.65196200	-4.75264600	2.50162600
O	4.94020500	-3.10276400	-0.97027600
O	3.92210900	4.52530700	0.61443200
C	5.31816100	4.36638400	0.43319400
H	5.55102700	4.01242400	-0.57538000
H	5.75490300	5.35156200	0.57813000
H	5.73895300	3.67311100	1.16737000
C	4.84261400	-4.48908800	-1.24719200
H	4.24771000	-4.67657000	-2.14567300
H	5.86050500	-4.83371200	-1.41336300
H	4.41025800	-5.03574600	-0.40418500

C2-GS1-conf3-asym – S_1 optimized Geometry

0 1

N	0.61721000	0.04482600	0.16443000
C	-1.65960400	1.21521000	-0.41811800
C	2.81957000	0.68556600	0.19532500
C	2.73872100	-0.66778600	-0.34822900
F	-2.43898400	-1.62935200	-1.46713500
C	1.48964300	1.05976400	0.48833600
C	1.36060800	-0.99886100	-0.34898300
C	-1.49232000	-1.04511600	1.25401100
C	-1.32166300	1.62118400	-1.73412300
C	-2.66643100	1.97094500	0.24611600
C	3.86595700	1.54766300	0.43183400
H	4.88217500	1.26022200	0.20368600
C	-3.24960800	3.06744400	-0.37287700
H	-4.00287900	3.63256100	0.16874200
C	3.66615300	-1.56337300	-0.80527700
H	4.72810100	-1.35430500	-0.81736200
C	-1.93745400	2.72325900	-2.32066400
H	-1.66341700	2.99636300	-3.33564100
C	-2.90046200	3.47040800	-1.65887700
C	1.19589400	2.31981600	1.01809800
H	0.17475100	2.61130500	1.21918900
F	-4.15144200	-2.68205500	-0.70940200
B	-0.91137500	0.07056400	0.33815800
C	0.91904900	-2.23166400	-0.81411800
H	-0.13281600	-2.47853300	-0.81443900
C	-0.88650000	-1.40495000	2.49707300
C	-2.64869000	-1.80372100	0.89999700
C	3.56950700	2.80951000	0.97566300
C	3.21941800	-2.81530500	-1.28219600
C	2.24559300	3.17907000	1.25952400
H	2.07518700	4.16622800	1.66800700
C	-0.33156400	0.85169700	-2.56987900
H	-0.40673800	1.14263600	-3.61876300
H	-0.51019600	-0.22284800	-2.50200900

H	0.70095600	1.03077000	-2.25823300
F	-4.07533200	-0.54435000	-0.55597000
C	-3.12355800	1.63794800	1.64350600
H	-3.74348000	2.44075200	2.04586900
H	-2.27790200	1.48142200	2.31711000
H	-3.71186800	0.71846400	1.66105000
C	-3.53716400	4.67666600	-2.29484100
H	-4.61850600	4.68466600	-2.13980000
H	-3.34909800	4.70402000	-3.36935400
H	-3.14356200	5.60393500	-1.86731800
C	0.31581300	-0.67254000	3.02947500
H	0.48149600	-0.92120200	4.07825400
H	0.18500000	0.41001000	2.95384000
H	1.22965700	-0.92470400	2.48673700
C	1.86144000	-3.13714500	-1.28728300
H	1.52722000	-4.09617800	-1.65378500
C	-3.18111700	-2.78482300	1.72891400
H	-4.05600400	-3.33482000	1.41167500
C	-3.31693900	-1.65320700	-0.43634400
C	-1.43486100	-2.39354200	3.30020200
H	-0.95904100	-2.61497400	4.24973700
C	-2.58395600	-3.08398000	2.93897300
H	-3.00066500	-3.84571300	3.58549500
O	4.19452100	-3.63434300	-1.71026000
O	4.49954500	3.73765800	1.25243200
C	5.86971700	3.44884800	0.99641600
H	6.03928500	3.26128800	-0.06626500
H	6.41905600	4.33556000	1.29985300
H	6.20652500	2.59238500	1.58487400
C	3.84595200	-4.91784600	-2.21703600
H	3.20160000	-4.82991000	-3.09467800
H	4.78359600	-5.38835600	-2.49926400
H	3.35037900	-5.51918400	-1.45152600

C2-GS1-conf4-sym – S_0 optimized Geometry

0 1

N	0.52973200	0.04008500	0.09840400
C	-1.84258200	1.13843800	-0.01485500
C	2.66465600	0.91845900	0.08409700
C	2.75444400	-0.49601600	-0.20726900
F	-1.95320300	-1.32531500	-1.96433500
C	1.30990800	1.21627900	0.25322000
C	1.45117400	-1.00010000	-0.18506000
C	-1.45993200	-1.46472100	0.82296100
C	-1.76679000	1.81578300	-1.25235400
C	-2.83290800	1.54839700	0.90564900
C	3.65182000	1.89678000	0.22069300
H	4.69239600	1.63915100	0.08225200
C	-3.68238400	2.60268200	0.59499200
H	-4.42138200	2.91421500	1.32635800
C	3.84962300	-1.31283400	-0.49432100
H	4.84749000	-0.89757900	-0.50483800
C	-2.65757600	2.84801800	-1.53459000
H	-2.59062700	3.34616700	-2.49672400
C	-3.61920100	3.26275100	-0.62614000

C	0.92501600	2.50898100	0.60864600
H	-0.11024300	2.76536600	0.77501500
F	-3.45493800	-2.87018100	-1.87205100
B	-0.89000200	-0.08277400	0.27179100
C	1.22147000	-2.33902900	-0.50031700
H	0.22579400	-2.75292100	-0.53666400
C	-1.02290700	-1.92019700	2.08368400
C	-2.43481100	-2.23136700	0.16545000
C	3.25825200	3.18396900	0.54356900
C	3.61556700	-2.64915500	-0.77116500
C	1.89980100	3.47580000	0.74083600
H	1.63321800	4.49067600	1.00747100
C	-0.74289800	1.49789400	-2.31758200
H	-1.12377600	1.78511100	-3.29853600
H	-0.48028400	0.44440600	-2.35604000
H	0.17888500	2.06042500	-2.14727800
F	-3.90671100	-0.89938800	-1.13768000
C	-3.00701300	0.89462500	2.25545900
H	-3.70108900	1.47015600	2.86839500
H	-2.06785800	0.82185100	2.80517100
H	-3.40784300	-0.11611300	2.15972000
C	-4.58207000	4.36943500	-0.95908500
H	-5.52381200	3.96167600	-1.33763200
H	-4.17776100	5.03064500	-1.72667000
H	-4.81781400	4.96853500	-0.07787600
C	0.04334500	-1.20774000	2.88095000
H	-0.00478900	-1.50611500	3.92840700
H	-0.04670800	-0.12258700	2.83855600
H	1.03963700	-1.46002800	2.50944000
C	2.30394300	-3.14766200	-0.77809100
H	2.16018900	-4.19288900	-1.02069800
C	-2.96622900	-3.38970400	0.71644200
H	-3.70303200	-3.96079000	0.16860100
C	-2.93880800	-1.83199800	-1.19041700
C	-1.57641500	-3.07459900	2.63286700
H	-1.23849500	-3.40345900	3.60914200
C	-2.53901800	-3.80899000	1.96336500
H	-2.95056700	-4.70693200	2.40702600
O	4.58460600	-3.55769900	-1.06219100
O	4.10799600	4.23377400	0.70359100
C	5.49365000	4.00394600	0.52089600
H	5.70958700	3.65916000	-0.49465200
H	5.98251900	4.96087300	0.68711500
H	5.87501100	3.27377000	1.24083100
C	5.92973600	-3.11428500	-1.08564700
H	6.23801900	-2.72544100	-0.11066700
H	6.53046400	-3.98685800	-1.33070700
H	6.08243700	-2.34487300	-1.84820700

C2-GS1-conf4-sym – S_1 optimized Geometry

0 1

N	0.56218000	-0.00527100	0.15050000
C	-1.71733300	1.17997200	-0.39120500
C	2.76053400	0.63974100	0.22733000
C	2.68645200	-0.68818600	-0.37855600

F	-2.46945500	-1.61588400	-1.57045400
C	1.42788300	0.99705300	0.52846700
C	1.31507100	-1.02033500	-0.40593800
C	-1.54782300	-1.15129700	1.18092900
C	-1.37233200	1.64758000	-1.68500200
C	-2.73542000	1.89754300	0.29808500
C	3.80104400	1.49405000	0.51012600
H	4.82061100	1.22385200	0.27584800
C	-3.32118800	3.01722100	-0.27523300
H	-4.08324400	3.55156600	0.28502400
C	3.63455500	-1.55735200	-0.86896600
H	4.68485900	-1.30507700	-0.84113700
C	-1.99064800	2.77141500	-2.22546200
H	-1.71086900	3.09202700	-3.22486900
C	-2.96399100	3.48139700	-1.53817800
C	1.12564500	2.22888100	1.11415300
H	0.10192200	2.50599100	1.32245400
F	-4.17512700	-2.72144500	-0.87579100
B	-0.96657500	0.00744700	0.31829200
C	0.87901900	-2.23625500	-0.93574400
H	-0.17197200	-2.48590800	-0.95889900
C	-0.95131000	-1.55898500	2.41330100
C	-2.69611800	-1.90044400	0.78484900
C	3.49613000	2.72999000	1.11048000
C	3.19372300	-2.78078300	-1.40491300
C	2.17044500	3.08112500	1.40286100
H	1.99309100	4.04713700	1.85629000
C	-0.37198600	0.92231600	-2.54761300
H	-0.44122800	1.26048700	-3.58264600
H	-0.54542100	-0.15502700	-2.53064700
H	0.65731000	1.09231400	-2.22058500
F	-4.12525900	-0.59221200	-0.62398200
C	-3.20162500	1.49809700	1.67479300
H	-3.82955200	2.27802100	2.10852300
H	-2.36024500	1.31565400	2.34719000
H	-3.78441800	0.57539800	1.64542800
C	-3.60125700	4.71327600	-2.12228400
H	-4.67848300	4.72841500	-1.94210900
H	-3.43678600	4.77176800	-3.19943600
H	-3.18711200	5.62284100	-1.67615700
C	0.24240300	-0.84309200	2.98584400
H	0.40334400	-1.13712000	4.02356500
H	0.10424800	0.24080500	2.95748000
H	1.16130800	-1.06461500	2.43829800
C	1.82950100	-3.10191700	-1.43535000
H	1.54517500	-4.05547800	-1.85982000
C	-3.23062700	-2.91796600	1.56740300
H	-4.09947100	-3.45887600	1.21943800
C	-3.35476600	-1.69681500	-0.54933100
C	-1.50096200	-2.58316100	3.16961300
H	-1.03218800	-2.84162000	4.11326200
C	-2.64277800	-3.26394600	2.76939200
H	-3.06087000	-4.05425600	3.37970900
O	4.01895100	-3.71165100	-1.91248400
O	4.42203400	3.64642400	1.43496800
C	5.79489700	3.37558700	1.17365700
H	5.97137000	3.23902300	0.10436000

H	6.33832300	4.24959400	1.52132100
H	6.13271000	2.49431300	1.72361600
C	5.42095600	-3.46838300	-1.92492500
H	5.80689900	-3.34354300	-0.91068100
H	5.86859600	-4.34925900	-2.37643400
H	5.66182600	-2.58903600	-2.52668200

C2-GS2-conf1-sym – S_0 optimized Geometry

0 1

N	-0.29374300	0.24734600	-0.16430000
C	2.24037700	-0.32279700	-0.49376800
C	-1.38122200	2.28337000	0.00565500
C	-2.34624600	1.28742900	-0.41477100
F	0.34033000	-0.69070000	2.47768500
C	-0.15072200	1.62577500	0.14722300
C	-1.66591300	0.06225000	-0.49167200
C	0.37214100	-2.26076400	0.07889600
C	3.34486400	-0.72401900	0.29093800
C	2.50088200	0.40790800	-1.67601700
C	-1.50898300	3.63532500	0.28221300
H	-2.45377500	4.15407200	0.17819700
C	3.80951800	0.72659400	-2.02620700
H	3.98477200	1.27908400	-2.94404100
C	-3.69316200	1.38348200	-0.72466700
H	-4.22690700	2.32391500	-0.66791700
C	4.63461100	-0.36286200	-0.08388600
H	5.46571600	-0.66487800	0.54547600
C	4.89257000	0.36136000	-1.24038200
C	0.95242700	2.32267400	0.61560200
H	1.90417900	1.83664200	0.76904800
F	-1.73788900	-1.25248100	2.32482900
B	0.75086700	-0.73425600	-0.16536900
C	-2.34324900	-1.07102600	-0.91470200
H	-1.85225200	-2.02754300	-1.00623100
C	0.60631100	-3.23094100	-0.91542300
C	-0.16858400	-2.70296900	1.29812800
C	-0.39346100	4.33934200	0.71710700
C	-4.37362800	0.24107000	-1.12562400
C	0.82742500	3.67921900	0.88883000
H	1.69522800	4.21491200	1.24603000
C	3.19646900	-1.51949100	1.56510100
H	2.67025900	-2.45960300	1.39548700
H	2.63830800	-0.96987700	2.32308800
H	4.17679100	-1.75646900	1.97890000
F	-0.41765300	-2.34970500	3.62315200
C	1.41605800	0.87625700	-2.61950900
H	1.83225700	1.04815800	-3.61280100
H	0.97934400	1.81823500	-2.27889400
H	0.59874500	0.16382000	-2.71978600
C	6.30087100	0.70181000	-1.64503400
H	6.75349800	-0.12238400	-2.20396000
H	6.92999100	0.88802100	-0.77304800
H	6.32806700	1.58565400	-2.28386700
C	1.16147800	-2.86200500	-2.26838400
H	1.21729700	-3.73991000	-2.91184700
H	2.16135100	-2.43416900	-2.18828500

H	0.53193800	-2.12542000	-2.77304100
C	-3.69527900	-0.97704200	-1.22260700
H	-4.21324300	-1.86973800	-1.54267500
C	-0.46826400	-4.03979800	1.53048700
H	-0.87166600	-4.34438600	2.48655900
C	-0.49112000	-1.75233800	2.41934900
C	0.29126000	-4.56539400	-0.67229100
H	0.46988500	-5.29680900	-1.45229500
C	-0.23950300	-4.97539200	0.53869600
H	-0.47057700	-6.01917100	0.71079600
O	-0.58476000	5.66425900	0.96428000
O	-5.69467200	0.40381700	-1.41159200
C	0.51484000	6.43160500	1.42194800
H	1.33079200	6.43532000	0.69342400
H	0.14151700	7.44534500	1.54669900
H	0.88689500	6.06413300	2.38269800
C	-6.43973800	-0.72747000	-1.82639700
H	-6.45076900	-1.50349600	-1.05558800
H	-7.45443900	-0.37350300	-1.99278800
H	-6.04715100	-1.14570500	-2.75788700

C2-GS2-conf1-sym – S_1 optimized Geometry

0 1

N	-0.32753100	0.10988700	-0.17239600
C	2.22103500	0.02993900	-0.79743400
C	-1.89266400	1.78212300	-0.00150600
C	-2.50723300	0.63596200	-0.66428700
F	0.37961900	-0.10311300	2.72880000
C	-0.55929700	1.39438800	0.27752500
C	-1.49190200	-0.35074900	-0.74249400
C	0.98577600	-2.01943000	0.64350500
C	3.47888100	0.07594300	-0.13440800
C	2.13472100	0.69108000	-2.05014600
C	-2.33760800	3.03246700	0.33390700
H	-3.34600300	3.36890300	0.13043100
C	3.23591200	1.34970500	-2.58580800
H	3.13547500	1.83487100	-3.55244400
C	-3.75491400	0.38788700	-1.16529500
H	-4.55822700	1.11202400	-1.12172100
C	4.55276000	0.74992200	-0.70456800
H	5.49365900	0.78396700	-0.16271600
C	4.46043900	1.39533800	-1.93262600
C	0.32698100	2.27179500	0.89099300
H	1.34666000	1.97640500	1.09122000
F	-1.58451200	-0.81712800	2.17203700
B	0.99942900	-0.66177600	-0.10924400
C	-1.74335700	-1.59264600	-1.31708900
H	-0.97533100	-2.35225900	-1.34816400
C	1.67449000	-3.13822500	0.06941800
C	0.26461500	-2.30372600	1.84164900
C	-1.44280800	3.91913200	0.96615900
C	-4.00700600	-0.86657000	-1.76122300
C	-0.12616400	3.53678400	1.23763400
H	0.55520200	4.22345400	1.71740900
C	3.69801600	-0.55353900	1.22029600
H	3.75234200	-1.64370200	1.16319900

H	2.88244000	-0.32207700	1.90724300
H	4.63283800	-0.19873200	1.65727600
F	-0.61320700	-1.59047500	3.92380700
C	0.87390400	0.66122700	-2.87494900
H	1.07490900	0.98488800	-3.89712300
H	0.10107100	1.32027000	-2.47148200
H	0.44861900	-0.34473600	-2.91517400
C	5.64935000	2.08977300	-2.54043300
H	6.27584800	1.38593100	-3.09721600
H	6.27876000	2.54541400	-1.77335100
H	5.34048300	2.87200100	-3.23600200
C	2.46492300	-3.02063500	-1.20911000
H	2.74861400	-4.01033100	-1.56949900
H	3.37654000	-2.43406500	-1.08331200
H	1.88429100	-2.52029300	-1.98799500
C	-3.00801800	-1.84038900	-1.83377300
H	-3.21171900	-2.80145100	-2.28195500
C	0.17879000	-3.58281500	2.38318000
H	-0.37950800	-3.73961400	3.29590500
C	-0.37838600	-1.21954100	2.64786600
C	1.57551300	-4.39901000	0.63538900
H	2.08866200	-5.22477900	0.15400900
C	0.82411500	-4.64311900	1.78062600
H	0.75583200	-5.63997400	2.19710900
O	-1.95711700	5.12490700	1.26373600
O	-5.25687400	-1.02805300	-2.22564100
C	-1.13139600	6.08975400	1.90537100
H	-0.27309000	6.34816400	1.28091500
H	-1.75665300	6.96718000	2.04516000
H	-0.78767900	5.72714700	2.87678400
C	-5.61138700	-2.25836200	-2.84689100
H	-5.51067700	-3.09236400	-2.14876400
H	-6.65232400	-2.15214200	-3.13904600
H	-4.99912300	-2.43961600	-3.73314100

C2-GS2-conf2-asym – S_0 optimized Geometry

0 1

N	-0.33087700	0.06243100	-0.19234600
C	2.24127900	0.44822300	-0.48315700
C	-2.08143000	1.55835600	0.01370800
C	-2.61410400	0.29603600	-0.45472700
F	0.56581000	-0.63858300	2.44873800
C	-0.69651700	1.38772300	0.15941200
C	-1.53994100	-0.59115000	-0.55310800
C	1.18730100	-2.04525100	0.02527600
C	3.40588500	0.45495400	0.31652700
C	2.23305000	1.25327200	-1.64591100
C	-2.69212700	2.76285700	0.32794400
H	-3.75997800	2.90848800	0.22305200
C	3.34015500	2.03473800	-1.96152800
H	3.31460800	2.63675700	-2.86436400
C	-3.91413400	-0.08566100	-0.78894000
H	-4.72475300	0.62386700	-0.70050100
C	4.48086200	1.26955200	-0.02403400
H	5.35698600	1.27384900	0.61650500

C	4.47183100	2.06803300	-1.15976800
C	0.07625900	2.42103100	0.66681700
H	1.13861300	2.30776600	0.82267800
F	-1.18643000	-1.87651900	2.21339300
B	0.99731200	-0.47998300	-0.19135400
C	-1.75578100	-1.88431000	-1.02746800
H	-0.95007300	-2.59368600	-1.13775100
C	1.77537500	-2.84896000	-0.97112000
C	0.81691700	-2.67336700	1.22660800
C	-1.91059900	3.80721700	0.80386900
C	-4.12293600	-1.37897400	-1.23658600
C	-0.53389800	3.62959400	0.97742100
H	0.07778100	4.43153300	1.36508600
C	3.54090100	-0.37375100	1.57092100
H	3.39586700	-1.43604200	1.37078000
H	2.81087100	-0.08592800	2.32736800
H	4.53447900	-0.24817000	2.00146300
F	0.39111300	-2.48398500	3.54545500
C	1.06479300	1.31403600	-2.60376500
H	1.39542400	1.68577500	-3.57415000
H	0.28941400	1.99153900	-2.23864800
H	0.59354800	0.34499600	-2.76263800
C	5.66406400	2.90842300	-1.52775300
H	6.38669300	2.32432700	-2.10496600
H	6.17872100	3.27707700	-0.63899500
H	5.37321200	3.76520000	-2.13717400
C	2.18352600	-2.28288700	-2.30788000
H	2.59288200	-3.06542900	-2.94649600
H	2.93625300	-1.50139500	-2.20048100
H	1.33136200	-1.84476500	-2.83296200
C	-3.04091400	-2.26349400	-1.35587400
H	-3.24157500	-3.26326700	-1.71969600
C	1.01490000	-4.03190800	1.44017000
H	0.72912100	-4.47772100	2.38299700
C	0.15249500	-1.91994400	2.34737500
C	1.95784200	-4.21121500	-0.74701600
H	2.40366500	-4.81607800	-1.52836500
C	1.58626800	-4.80514200	0.44671200
H	1.74369800	-5.86480500	0.60415500
O	-2.57055900	4.96365800	1.08789200
O	-5.33331900	-1.88683500	-1.59353100
C	-1.82710400	6.05968900	1.59057400
H	-1.06414800	6.38626500	0.87793900
H	-2.54345300	6.86384900	1.74165700
H	-1.35183100	5.81699800	2.54544700
C	-6.46569000	-1.04183500	-1.49509300
H	-6.36954300	-0.16840100	-2.14690800
H	-7.31598400	-1.63815300	-1.81738100
H	-6.62684000	-0.70966800	-0.46524900

C2-GS2-conf2-asym – S_1 optimized Geometry

0 1

N	-0.30641300	-0.00696800	-0.20274800
C	2.20532300	0.50476500	-0.77234100
C	-2.19681600	1.26826200	0.05875100

C	-2.54378500	0.06839700	-0.69686900
F	0.42045100	-0.26842300	2.69821000
C	-0.81225700	1.16041500	0.33560400
C	-1.34189100	-0.66183300	-0.82808400
C	1.42746200	-1.85924400	0.49578200
C	3.42330600	0.76222400	-0.08324600
C	1.98711100	1.22722800	-1.97469300
C	-2.90356300	2.36415000	0.47429500
H	-3.96012000	2.49104500	0.27633200
C	2.92755000	2.14026900	-2.43822300
H	2.73124200	2.66609900	-3.36818300
C	-3.71960600	-0.39988700	-1.23672700
H	-4.63807700	0.15906900	-1.13010900
C	4.33404900	1.68708400	-0.58113100
H	5.24477800	1.87556800	-0.01977800
C	4.11311900	2.39062500	-1.75975100
C	-0.14044600	2.15932600	1.02773400
H	0.91829100	2.07729700	1.22646900
F	-1.34341700	-1.33939200	2.05012500
B	1.15461000	-0.47836600	-0.16182900
C	-1.31524600	-1.88557500	-1.50343100
H	-0.40004500	-2.45521100	-1.58061900
C	2.34099900	-2.76196000	-0.14067100
C	0.78091200	-2.37377300	1.65883800
C	-2.22479100	3.37485800	1.18736600
C	-3.68721500	-1.62474100	-1.92541600
C	-0.85906200	3.26814500	1.45656300
H	-0.34506600	4.04790700	1.99843500
C	3.76475800	0.09229400	1.22594300
H	4.04944800	-0.95426200	1.09051800
H	2.91541000	0.09356700	1.91092000
H	4.60102600	0.60233500	1.70684100
F	-0.24236000	-2.01402800	3.76569200
C	0.76390200	0.99892200	-2.82479600
H	0.89571200	1.43883100	-3.81428600
H	-0.13205000	1.44617100	-2.38716200
H	0.56076500	-0.06714000	-2.95294200
C	5.13226100	3.36175000	-2.29206200
H	5.88652300	2.85017800	-2.89814500
H	5.65903200	3.86946400	-1.48160300
H	4.66695000	4.12065300	-2.92353000
C	3.09261800	-2.38910900	-1.39336800
H	3.57848900	-3.26876600	-1.81756700
H	3.86081200	-1.63595200	-1.20992200
H	2.42256200	-1.96553000	-2.14531800
C	-2.49125500	-2.34831800	-2.05166600
H	-2.52578700	-3.28921800	-2.58446500
C	0.96937300	-3.67626300	2.11104000
H	0.45477400	-4.01215200	3.00077500
C	-0.08281600	-1.51102800	2.52385500
C	2.51278900	-4.05149800	0.33677500
H	3.19175100	-4.71304300	-0.19073300
C	1.82830800	-4.52967200	1.44933700
H	1.97367400	-5.54485900	1.79590000
O	-2.99181700	4.41395700	1.56006500
O	-4.76542400	-2.18832900	-2.49411700
C	-2.39922900	5.48301200	2.28844300

H	-1.61416100	5.96771300	1.70350600
H	-3.20099500	6.19108500	2.47852200
H	-1.98991500	5.13007600	3.23778700
C	-6.02435100	-1.53002000	-2.40514500
H	-5.99127100	-0.55236500	-2.89124400
H	-6.72900000	-2.17064800	-2.92785500
H	-6.33610900	-1.41856700	-1.36424100

C2-GS2-conf3-asym – S_0 optimized Geometry

0 1

N	-0.29013200	0.16209900	-0.14898400
C	2.29047400	0.47436400	-0.45696000
C	-1.98818800	1.71363600	0.06313500
C	-2.56710400	0.47113000	-0.40340800
F	0.60530400	-0.57064300	2.48385100
C	-0.61639300	1.49712400	0.20303700
C	-1.51858100	-0.45685400	-0.50623400
C	1.16839800	-1.98792600	0.05431600
C	3.46247200	0.44191300	0.33159500
C	2.29643400	1.28331700	-1.61693700
C	-2.57159700	2.94147200	0.37997200
H	-3.63717900	3.08001100	0.26315500
C	3.42492300	2.03008300	-1.94118600
H	3.40955900	2.63590200	-2.84169800
C	-3.86822000	0.12413900	-0.73253300
H	-4.68541100	0.83056200	-0.65648100
C	4.55938600	1.22278000	-0.01718800
H	5.44113400	1.19778500	0.61508700
C	4.56479100	2.02463100	-1.15072200
C	0.19677100	2.50850600	0.71277700
H	1.25518500	2.36018200	0.86567300
F	-1.17940500	-1.76555200	2.27022700
B	1.02233300	-0.41718300	-0.15708700
C	-1.77829500	-1.73560900	-0.97495800
H	-0.99659300	-2.47115600	-1.08675500
C	1.72309900	-2.80463800	-0.95053500
C	0.79091400	-2.60936800	1.25664900
C	-1.75240700	3.95213400	0.85373200
C	-4.12773000	-1.16473000	-1.17896300
C	-0.37790800	3.72360800	1.02210200
H	0.22555700	4.53254800	1.41409600
C	3.58263600	-0.39366700	1.58294200
H	3.40552700	-1.45083400	1.38137400
H	2.86691700	-0.08670000	2.34552100
H	4.58254600	-0.29797200	2.00642000
F	0.40027800	-2.41285100	3.58083800
C	1.12169100	1.38595000	-2.56337800
H	1.45732400	1.73827500	-3.53928400
H	0.37885800	2.09738800	-2.19495200
H	0.60870700	0.43664200	-2.71121500
C	5.77938300	2.82816500	-1.52764800
H	6.47922000	2.22253400	-2.11074600
H	6.31192900	3.18018200	-0.64269900
H	5.51016100	3.69397900	-2.13419100
C	2.13791900	-2.24424300	-2.28765300

H	2.49684100	-3.03886700	-2.94153300
H	2.93145500	-1.50358300	-2.18353000
H	1.30168700	-1.75614700	-2.79360200
C	-3.08260700	-2.08518500	-1.30202700
H	-3.27314000	-3.08760500	-1.65761400
C	0.95029800	-3.97410400	1.46329000
H	0.66058600	-4.41485200	2.40734400
C	0.15978800	-1.84128200	2.38660000
C	1.86682000	-4.17261600	-0.73352700
H	2.28729900	-4.78727000	-1.52128700
C	1.48883200	-4.76006000	0.46151800
H	1.61622900	-5.82455100	0.61355000
O	-2.18173600	5.19607900	1.19738300
O	-5.42633900	-1.44082700	-1.48128900
C	-3.56142100	5.48632300	1.06212000
H	-4.16998400	4.83521700	1.69658500
H	-3.68541900	6.51789900	1.38294000
H	-3.88910400	5.38932400	0.02280400
C	-5.75034900	-2.74002700	-1.94325500
H	-5.50677100	-3.50237200	-1.19754900
H	-6.82411300	-2.73808100	-2.11548100
H	-5.23610700	-2.97161800	-2.88063000

C2-GS2-conf3-asym – S_1 optimized Geometry

0 1

N	-0.28156600	0.07698500	-0.13810600
C	2.22673300	0.58182000	-0.72874700
C	-2.16292100	1.36401800	0.11722800
C	-2.52020300	0.16266300	-0.63132200
F	0.44202800	-0.17906700	2.74358500
C	-0.78419500	1.24829600	0.39242000
C	-1.31943000	-0.58039000	-0.75853700
C	1.45300700	-1.77684800	0.55179700
C	3.44308700	0.84857300	-0.04165900
C	2.00667700	1.29122500	-1.93776700
C	-2.87838400	2.46859600	0.52511900
H	-3.93257400	2.55647700	0.30503600
C	2.94548500	2.20117600	-2.41083300
H	2.74799000	2.71770800	-3.34571800
C	-3.68488800	-0.30919300	-1.16908000
H	-4.62505100	0.22152700	-1.09203700
C	4.35239900	1.77007600	-0.54869900
H	5.26240700	1.96643100	0.01107500
C	4.13029700	2.46067600	-1.73458900
C	-0.10367700	2.25315900	1.08389500
H	0.95430100	2.16770000	1.28508900
F	-1.32174200	-1.26068800	2.11368800
B	1.17837200	-0.39948000	-0.10814900
C	-1.29974900	-1.80384200	-1.41846000
H	-0.38775300	-2.37953400	-1.48706900
C	2.36824900	-2.68143800	-0.08117000
C	0.80451700	-2.28952300	1.71537300
C	-2.19362800	3.47229700	1.22792700
C	-3.66368800	-1.54581800	-1.85269800
C	-0.82076100	3.35389100	1.49680300

H	-0.34249600	4.15924000	2.03819100
C	3.78534400	0.19143300	1.27388600
H	4.07340300	-0.85538100	1.14760800
H	2.93565800	0.19604700	1.95835600
H	4.61957700	0.70827000	1.75100000
F	-0.20703900	-1.92087700	3.82598100
C	0.78256300	1.05306800	-2.78385900
H	0.91084500	1.48640900	-3.77669900
H	-0.11388300	1.50051100	-2.34743600
H	0.58246300	-0.01460000	-2.90353300
C	5.14731400	3.42893800	-2.27618100
H	5.90468700	2.91271600	-2.87435800
H	5.67032300	3.94807700	-1.47057600
H	4.68072200	4.17865300	-2.91755300
C	3.12248900	-2.31093200	-1.33291100
H	3.61247100	-3.19065800	-1.75223900
H	3.88760800	-1.55451500	-1.15032800
H	2.45317500	-1.89248500	-2.08852100
C	-2.48209700	-2.27848200	-1.97334500
H	-2.47539600	-3.22725500	-2.48869000
C	0.99115300	-3.59183700	2.16922300
H	0.47554700	-3.92580400	3.05916600
C	-0.05708300	-1.42468500	2.58015900
C	2.53756000	-3.97023900	0.39798500
H	3.21739500	-4.63288300	-0.12705600
C	1.84999400	-4.44697000	1.50991400
H	1.99415100	-5.46178400	1.85804800
O	-2.77506400	4.59657200	1.68018700
O	-4.85039400	-1.93331700	-2.34751000
C	-4.16562500	4.79760800	1.45585700
H	-4.75778000	4.01379300	1.93374500
H	-4.40176400	5.75667500	1.90835000
H	-4.38990800	4.83429200	0.38727100
C	-4.93644600	-3.16586100	-3.05409300
H	-4.66414000	-4.00506900	-2.41021600
H	-5.97564200	-3.26085400	-3.35608000
H	-4.29733100	-3.15428400	-3.93986800

C2-GS2-conf4-sym – S_0 optimized Geometry

0 1

N	-0.27789400	0.05337200	-0.16098000
C	2.20879200	0.82609600	-0.42972500
C	-2.22340100	1.27039200	0.08252100
C	-2.56756600	-0.03571200	-0.43581300
F	0.72113300	-0.61092400	2.45331800
C	-0.83533100	1.29540800	0.23409900
C	-1.37586000	-0.75590800	-0.55572900
C	1.53589800	-1.81280100	-0.01977400
C	3.36482000	0.97054400	0.36982500
C	2.07738600	1.66586100	-1.55984100
C	-3.01657800	2.36452600	0.43461900
H	-4.08919500	2.31891400	0.30891400
C	3.05828300	2.61072900	-1.84499500
H	2.94055500	3.23738400	-2.72344200
C	-3.79735200	-0.58935400	-0.79673600

H	-4.70315000	-0.00900500	-0.69161900
C	4.30872300	1.94430900	0.06111600
H	5.17850500	2.05087700	0.70145800
C	4.17790200	2.77616000	-1.04299600
C	-0.21744800	2.41454200	0.79068000
H	0.84939600	2.44941100	0.95293900
F	-0.82643800	-2.08980500	2.17645600
B	1.11714000	-0.28557100	-0.17576200
C	-1.40068900	-2.04902400	-1.07650400
H	-0.50068400	-2.63092500	-1.20262900
C	2.23012600	-2.48062500	-1.04777500
C	1.26495900	-2.53731100	1.15328100
C	-2.39202100	3.48511200	0.95477900
C	-3.81459900	-1.88171100	-1.29230600
C	-0.99985600	3.49697600	1.13443900
H	-0.55202700	4.38464200	1.56299300
C	3.62479900	0.12206900	1.59087800
H	3.64295500	-0.94100300	1.34739900
H	2.85988400	0.26475800	2.35400400
H	4.58786200	0.37968000	2.03178100
F	0.83696700	-2.50135300	3.47883400
C	0.90730900	1.59500800	-2.51493300
H	1.18245900	2.02972800	-3.47642500
H	0.05182600	2.15705600	-2.13288400
H	0.56528200	0.57702500	-2.69602700
C	5.23415800	3.79355000	-1.37794300
H	6.03475500	3.34052700	-1.96984600
H	5.68902500	4.20449600	-0.47521900
H	4.82097000	4.61781300	-1.96088400
C	2.55039900	-1.80453000	-2.35716200
H	3.05018700	-2.49738400	-3.03385500
H	3.19892300	-0.93967000	-2.21420300
H	1.64517000	-1.45337600	-2.85799700
C	-2.61592600	-2.59713300	-1.43106400
H	-2.66851900	-3.60186000	-1.83095500
C	1.65601200	-3.86148100	1.30933700
H	1.44055900	-4.38314200	2.23179500
C	0.50498500	-1.93519900	2.30415000
C	2.60622500	-3.81099800	-0.88150300
H	3.13099000	-4.31218700	-1.68685900
C	2.32764000	-4.50230400	0.28492100
H	2.63514600	-5.53443300	0.39714200
O	-3.03697200	4.62060800	1.33591900
O	-4.93724900	-2.54510200	-1.68045100
C	-4.44472100	4.66948800	1.18835000
H	-4.93580900	3.89859100	1.78952300
H	-4.75118400	5.65062100	1.54314100
H	-4.73971100	4.55550800	0.14098300
C	-6.18047400	-1.87698500	-1.56252500
H	-6.20846100	-0.97432000	-2.18013000
H	-6.93376400	-2.57700600	-1.91602500
H	-6.39313100	-1.61193600	-0.52263700

C2-GS2-conf4-sym – S_1 optimized Geometry

0 1

N	-0.24410200	0.00944800	-0.16989400
C	2.20890800	0.79190300	-0.68147700
C	-2.23632100	1.08870300	0.17691700
C	-2.47738800	-0.07487900	-0.67195700
F	0.48856900	-0.42019100	2.69363500
C	-0.85396300	1.08067700	0.45475900
C	-1.21608300	-0.68411900	-0.85312200
C	1.65105200	-1.72842200	0.38668900
C	3.39309100	1.10948300	0.03973700
C	1.92809300	1.57964700	-1.82779300
C	-3.05189400	2.08470700	0.66625800
H	-4.10904300	2.09439300	0.44278900
C	2.77860300	2.61110100	-2.20948100
H	2.53685600	3.18604200	-3.09877000
C	-3.60701500	-0.60339100	-1.25113900
H	-4.57250600	-0.14104000	-1.10435000
C	4.21329100	2.15255900	-0.37526500
H	5.09902800	2.38330400	0.20976600
C	3.93117800	2.92049700	-1.49931800
C	-0.27180500	2.08146600	1.23346200
H	0.78906900	2.07769800	1.43767500
F	-1.16428600	-1.60156100	1.95210600
B	1.25295900	-0.33094800	-0.15977900
C	-1.08129000	-1.84350800	-1.62083400
H	-0.11893700	-2.32128500	-1.73718300
C	2.64795500	-2.48837000	-0.30939900
C	1.04963600	-2.39390300	1.49666800
C	-2.46510800	3.08720800	1.45727100
C	-3.46683700	-1.76439500	-2.03439400
C	-1.08953700	3.07418900	1.72987900
H	-0.68891800	3.87160400	2.34141200
C	3.79149000	0.37487200	1.29709800
H	4.17463100	-0.62641600	1.08407100
H	2.94346900	0.24270100	1.97082000
H	4.57373000	0.92243300	1.82526700
F	-0.00245300	-2.29963300	3.61748700
C	0.73534200	1.30118400	-2.70568800
H	0.82797400	1.82449200	-3.65836900
H	-0.20053200	1.62762300	-2.24524500
H	0.63521600	0.23318100	-2.91434200
C	4.85444200	4.02324200	-1.94274900
H	5.66336200	3.63341400	-2.56851600
H	5.31785800	4.52113600	-1.08866600
H	4.32309400	4.77567700	-2.52808400
C	3.36827700	-1.94621600	-1.51775700
H	3.93871500	-2.73874600	-2.00385100
H	4.05949000	-1.14062900	-1.26437600
H	2.66527900	-1.52925500	-2.24290300
C	-2.21252700	-2.36588000	-2.21079800
H	-2.16320400	-3.26111700	-2.81605800
C	1.35436000	-3.70704200	1.84250700
H	0.86877100	-4.16071700	2.69559900
C	0.10765800	-1.68804200	2.41984100
C	2.93454200	-3.79179200	0.06278900
H	3.67415200	-4.34283500	-0.50839000
C	2.29077300	-4.42112900	1.12364100
H	2.52691500	-5.44410600	1.38738000

O	-3.15178800	4.11095100	1.99341000
O	-4.49238800	-2.37400500	-2.65023600
C	-4.55398100	4.20085100	1.76997200
H	-5.07327700	3.32894100	2.17446000
H	-4.87989800	5.09284000	2.29767400
H	-4.77650000	4.30656900	0.70556500
C	-5.80489800	-1.83913800	-2.51757800
H	-5.85921800	-0.82662300	-2.92381100
H	-6.44970400	-2.49569100	-3.09487900
H	-6.12527200	-1.84045600	-1.47338700

Catalyst C3

C3-GS1-*E* – S_0 optimized geometry

0 1

N	1.01735000	-0.35328000	-0.03628900
C	-0.93604000	1.38485500	0.09125600
C	3.31359800	-0.13152700	-0.11273100
C	2.97351800	-1.47042300	-0.54126300
F	-1.84871000	-0.74906600	-2.01332200
C	2.10943000	0.52703600	0.17645400
C	1.57625500	-1.57650600	-0.47817700
C	-1.29392800	-1.28108500	0.71168500
C	-0.70870200	2.12268100	-1.09287200
C	-1.73055900	1.97496100	1.09921600
C	4.53931800	0.50779700	0.05007600
H	5.48080800	0.02065900	-0.16800100
C	-2.24521100	3.25352300	0.92336500
H	-2.83462900	3.69598900	1.71999700
C	3.75051100	-2.53951300	-0.97730700
H	4.82951900	-2.45239500	-1.02346900
C	-1.26936400	3.38791000	-1.23952300
H	-1.09482500	3.93213800	-2.16229800
C	-2.03549900	3.97630100	-0.24423600
C	2.12079500	1.82740200	0.67274900
H	1.20813100	2.34367500	0.92769400
F	-3.72923700	-1.80224900	-1.93508800
B	-0.37317300	-0.07800100	0.22385000
C	0.94044700	-2.74402100	-0.89195500
H	-0.13431400	-2.83571100	-0.89278200
C	-0.95106700	-1.95535700	1.90118800
C	-2.47999700	-1.67040000	0.06986400
C	4.51642800	1.80076100	0.51540000
C	3.11994800	-3.70980500	-1.35784300
H	3.70471600	-4.55448400	-1.70029800
C	3.33992000	2.46526200	0.83261900
H	3.39153700	3.47892300	1.20786400
C	0.13762500	1.62080100	-2.24011100
H	-0.16141400	2.11245900	-3.16657000
H	0.05784300	0.54774300	-2.39138900
H	1.19297400	1.85255100	-2.07421300
F	-3.55654900	0.13986400	-1.02621700
C	-2.04196900	1.27743800	2.40156200
H	-2.50672600	1.97236900	3.10127600
H	-1.14898100	0.87691500	2.88266800
H	-2.73264100	0.44558400	2.25178900
C	-2.64519700	5.33817100	-0.43353800
H	-3.65406700	5.25477600	-0.84791000
H	-2.05671600	5.94491800	-1.12318200
H	-2.72486200	5.87271800	0.51432800
C	0.31286500	-1.65482500	2.67082100
H	0.23349500	-2.03227100	3.69037600
H	0.53404700	-0.58903300	2.72752400
H	1.17614900	-2.13713100	2.20580200
C	1.72686300	-3.80204800	-1.31863600
H	1.24414100	-4.71804200	-1.63712000

C	-3.30190400	-2.67057900	0.57089900
H	-4.19829500	-2.95289100	0.03613000
C	-2.90532400	-1.02154300	-1.21463000
C	-1.79361400	-2.94496800	2.40261700
H	-1.52273600	-3.44413800	3.32606200
C	-2.95938900	-3.30596000	1.75091200
H	-3.59570800	-4.08277000	2.15599700
F	5.68765300	2.45504900	0.68433200

C3-GS1-*E* – S_1 optimized geometry

0 1

N	1.01136700	-0.38509100	-0.08320100
C	-0.91869900	1.39144700	-0.10966100
C	3.30340700	-0.30492900	-0.10700100
C	2.87718700	-1.42591700	-0.93738200
F	-2.38749400	-0.82776700	-1.78433800
C	2.11037400	0.28521000	0.38795700
C	1.46653400	-1.41939500	-0.89766900
C	-1.26262500	-1.21609200	0.90304300
C	-0.52586700	2.05121800	-1.30334200
C	-1.69656400	2.14579400	0.81530700
C	4.52438700	0.22113400	0.23375600
H	5.46458400	-0.18445600	-0.11541700
C	-1.99834900	3.47481400	0.55953500
H	-2.57459400	4.02915400	1.29477000
C	3.54118100	-2.37949300	-1.67430600
H	4.62291900	-2.40612100	-1.71508300
C	-0.85596500	3.38575200	-1.52097700
H	-0.54703600	3.85593400	-2.44994400
C	-1.58531900	4.12456100	-0.60162900
C	2.13343300	1.40722000	1.22215600
H	1.21494900	1.85334500	1.57420900
F	-4.28747600	-1.61641100	-1.16502400
B	-0.45037100	-0.05377000	0.25000700
C	0.70871100	-2.35217800	-1.59175500
H	-0.37068900	-2.33134900	-1.55611600
C	-0.73051300	-2.01494800	1.95815300
C	-2.57504100	-1.56707100	0.47282700
C	4.51952500	1.33702700	1.07255000
C	2.78399200	-3.32541300	-2.37895500
H	3.29196600	-4.08244900	-2.96249400
C	3.36885000	1.93071400	1.56554900
H	3.45713300	2.79767400	2.20567800
C	0.20509800	1.32458400	-2.40172200
H	0.18463000	1.90388300	-3.32588100
H	-0.24968500	0.35239200	-2.60003400
H	1.25618600	1.14886200	-2.15664800
F	-3.68117200	0.32677100	-0.48938200
C	-2.19194200	1.55563500	2.11014600
H	-2.58242500	2.33732300	2.76348200
H	-1.39722800	1.02530900	2.63974300
H	-2.99084500	0.83179700	1.93818200
C	-1.91493200	5.57335600	-0.83790900
H	-2.95981700	5.78750100	-0.60175400
H	-1.73728900	5.85605500	-1.87660400

H	-1.30242400	6.22594600	-0.20822700
C	0.63064500	-1.74633500	2.54087900
H	0.76332200	-2.29490800	3.47378600
H	0.76925500	-0.68250400	2.75007700
H	1.43621300	-2.05178500	1.86870400
C	1.39735600	-3.30641900	-2.34006500
H	0.83680600	-4.04613100	-2.89694700
C	-3.31042800	-2.58169300	1.07516700
H	-4.30071500	-2.81368400	0.70921100
C	-3.21926800	-0.91845700	-0.71972500
C	-1.48265400	-3.02825300	2.53543400
H	-1.05074300	-3.59557400	3.35296500
C	-2.77331700	-3.31552700	2.11614200
H	-3.34709000	-4.10358900	2.58693700
F	5.70166600	1.86338400	1.41216100

C3-GS2-*E* – S_0 optimized geometry

0 1

N	-0.77351300	0.09048200	-0.31387000
C	1.72051200	0.88159600	-0.22323800
C	-2.74644700	1.27604200	-0.15493400
C	-3.01263500	0.04728700	-0.86989300
F	-0.07376200	-0.82435100	2.31948700
C	-1.38158000	1.27658800	0.16487800
C	-1.80251400	-0.65944500	-0.93537100
C	1.03241900	-1.78397800	-0.14442200
C	2.78313900	0.94037700	0.70708000
C	1.69942700	1.83588000	-1.26636000
C	-3.57464000	2.32429000	0.23674500
H	-4.63130900	2.34755100	0.00391200
C	2.69444600	2.80567000	-1.34359200
H	2.66475600	3.52109400	-2.15919000
C	-4.17064800	-0.46609400	-1.44635300
H	-5.10233400	0.08431600	-1.39096600
C	3.74204600	1.94196600	0.60596100
H	4.53718400	1.98101400	1.34360900
C	3.71959900	2.88580000	-0.41286500
C	-0.83342000	2.30818500	0.92068600
H	0.20769700	2.30953100	1.20532200
F	-1.59087600	-2.22025900	1.67962500
B	0.62331500	-0.24952000	-0.20335300
C	-1.73758500	-1.87776200	-1.60592200
H	-0.81681600	-2.43457600	-1.68636300
C	1.86305200	-2.34936900	-1.13139300
C	0.61647800	-2.61766200	0.90761800
C	-2.99833200	3.34450000	0.95518200
C	-4.10913700	-1.68556400	-2.09485400
H	-4.99821400	-2.10404800	-2.54998900
C	-1.65543000	3.35358300	1.30728000
H	-1.26900900	4.17930500	1.89023800
C	2.92139100	-0.03418200	1.85146400
H	2.99191800	-1.06366400	1.49784300
H	2.07153400	0.01525800	2.53194600
H	3.82175400	0.18338700	2.42601300
F	-0.12939500	-2.81426700	3.14350800

C	0.64076900	1.86374900	-2.34578400
H	1.00478600	2.41770500	-3.21147800
H	-0.26778700	2.36066100	-1.99764500
H	0.35207400	0.87018100	-2.68663000
C	4.79274900	3.93418200	-0.52085000
H	5.68846100	3.52411100	-0.99609800
H	5.08697900	4.30221800	0.46355300
H	4.46036600	4.78270600	-1.12004400
C	2.35348500	-1.54825300	-2.31136800
H	2.91329700	-2.18293200	-2.99805000
H	3.00287900	-0.73018500	-1.99751100
H	1.52557000	-1.10914200	-2.87232900
C	-2.89867100	-2.37770800	-2.17283100
H	-2.86088300	-3.32859000	-2.69059600
C	0.99690900	-3.95122900	0.98561000
H	0.66880400	-4.55897500	1.81762600
C	-0.28790000	-2.12057900	2.00274400
C	2.22556700	-3.69131400	-1.04692100
H	2.85630400	-4.11374100	-1.82072100
C	1.80263500	-4.49149000	0.00023100
H	2.10248800	-5.53066500	0.05130300
F	-3.77114400	4.38124400	1.35170500

C3-GS2-*E* – S_1 optimized geometry

0 1

N	-0.66372700	0.19827200	-0.41820100
C	1.92268700	0.62940900	-0.29370100
C	-2.54197100	1.49622700	-0.20977100
C	-2.75207800	0.56174300	-1.30926400
F	-0.57755800	-0.83856800	2.42447300
C	-1.24605600	1.21504400	0.29612000
C	-1.56816100	-0.19975400	-1.39721700
C	0.82242000	-1.90832600	0.11546000
C	2.97202400	0.59507200	0.66837600
C	1.98827200	1.65248700	-1.27624000
C	-3.29385700	2.50449400	0.34144700
H	-4.28344700	2.76636900	-0.00844800
C	3.02490400	2.57933000	-1.27126900
H	3.04648800	3.34345100	-2.04274800
C	-3.78997500	0.32337600	-2.17971900
H	-4.70980200	0.89243900	-2.12771300
C	3.98719600	1.54275600	0.63554400
H	4.75983200	1.50446800	1.39808800
C	4.03975300	2.54815800	-0.32475100
C	-0.69590300	1.94320500	1.35419000
H	0.29486900	1.72086200	1.72115200
F	-2.18083800	-1.54900400	1.15949300
B	0.73725400	-0.38361200	-0.19703500
C	-1.41064500	-1.20385100	-2.34156400
H	-0.50725400	-1.79566800	-2.37984300
C	1.82083200	-2.69106000	-0.54663700
C	-0.06002500	-2.63841800	0.96213500
C	-2.72337200	3.21027200	1.40022700
C	-3.63554200	-0.68208800	-3.14477800

H	-4.44453900	-0.88191000	-3.83562700
C	-1.45950500	2.95464800	1.90960300
H	-1.09272400	3.55340000	2.73184000
C	3.00943600	-0.42096200	1.78369200
H	3.28747700	-1.41522100	1.42512600
H	2.03455400	-0.52764200	2.26215300
H	3.73815300	-0.12715400	2.54065700
F	-1.51934000	-2.72977800	2.82733000
C	0.98004800	1.74164700	-2.39181200
H	1.33126100	2.41354800	-3.17593900
H	0.01462500	2.12280700	-2.04910900
H	0.79695000	0.76269800	-2.84171900
C	5.16919100	3.54212300	-0.34925200
H	6.05904800	3.11688500	-0.82358900
H	5.45539900	3.84363900	0.66058600
H	4.89705600	4.43906900	-0.90783600
C	2.82081100	-2.07923100	-1.49436900
H	3.35315700	-2.86087700	-2.03772600
H	3.56082200	-1.46506700	-0.97823700
H	2.33090300	-1.42466300	-2.21907700
C	-2.46827400	-1.42696000	-3.22305700
H	-2.37648900	-2.19995500	-3.97511700
C	-0.00020700	-4.02191500	1.09672800
H	-0.69427300	-4.52546500	1.75526700
C	-1.06806600	-1.94823900	1.82700200
C	1.86075800	-4.06839800	-0.38834900
H	2.61586100	-4.63029500	-0.92758400
C	0.95524700	-4.74909800	0.41630100
H	1.00297300	-5.82597300	0.51590200
F	-3.44123400	4.19738000	1.94889100

C3-GS1-*Z* – S_0 optimized geometry

0 1

N	0.90467200	0.58909600	0.10983900
C	-1.71128300	0.70787700	0.06405300
C	2.55644300	2.20006000	0.18452900
C	3.15990800	0.95085900	-0.22395200
F	-0.92825700	-1.49044800	-2.03044500
C	1.18802600	1.95349200	0.36927100
C	2.13704400	-0.00844100	-0.25388300
C	-0.35234300	-1.59764500	0.73913800
C	-1.92082200	1.44320000	-1.12483000
C	-2.76524600	0.64834000	1.00256300
C	3.09117400	3.46468200	0.41330900
H	4.14890000	3.64841100	0.26659000
C	-3.95756900	1.31798900	0.75675600
H	-4.74577400	1.27671000	1.50163700
C	4.46619800	0.61873500	-0.57006700
H	5.27172600	1.34133900	-0.55502700
C	-3.14211000	2.07331800	-1.34387000
H	-3.28795600	2.62094200	-2.26962800
C	-4.17258600	2.02996600	-0.41650300
C	0.34710500	2.96670400	0.82278400
H	-0.70369600	2.79223800	0.99648200
F	-1.72561500	-3.49442100	-2.04004800

B	-0.36373000	-0.07503900	0.27467300
C	2.40310700	-1.30772700	-0.67537500
H	1.62707700	-2.05298500	-0.74902700
C	0.25584500	-1.92393200	1.96823200
C	-0.98047100	-2.63728900	0.03547100
C	2.25058100	4.47670700	0.83777700
C	4.70396100	-0.68085500	-0.95011100
C	0.89283600	4.22087200	1.04387600
H	0.24676800	5.01910200	1.38895600
C	-0.87193600	1.60753300	-2.20045800
H	-1.34942700	1.82739400	-3.15602900
H	-0.25440400	0.72311200	-2.33220900
H	-0.20627300	2.44296700	-1.96844900
F	-2.87796600	-1.89288000	-1.18300800
C	-2.65320700	-0.10788700	2.30461400
H	-3.50090100	0.12283200	2.95014700
H	-1.74550700	0.14406100	2.85424600
H	-2.64588300	-1.18676300	2.13933000
C	-5.49016500	2.70417400	-0.68427000
H	-6.19047200	2.00858100	-1.15566100
H	-5.37197100	3.55569900	-1.35583900
H	-5.95151800	3.05535700	0.24005800
C	0.98879900	-0.90532900	2.80801600
H	1.08712600	-1.26117200	3.83365800
H	0.48695200	0.06165300	2.83834900
H	1.99562100	-0.73181100	2.42012300
C	3.70422800	-1.64118800	-1.01455700
H	3.95428500	-2.64195700	-1.34133200
C	-1.02018400	-3.93982300	0.51379000
H	-1.49922400	-4.71547900	-0.06765000
C	-1.62993600	-2.38094600	-1.29292700
C	0.19418600	-3.23147000	2.44495600
H	0.65509400	-3.46289900	3.39857300
C	-0.43518900	-4.23611900	1.73183700
H	-0.46525700	-5.24681800	2.11914900
F	5.96158600	-1.04144900	-1.29102300
H	2.64456700	5.46864900	1.02099700

C3-GS1-*Z* – S_1 optimized geometry

0 1

N	1.00449400	0.41645100	0.23643800
C	-1.54953700	0.89099400	-0.16172600
C	2.87560500	1.72762300	0.49980900
C	3.22510100	0.57193000	-0.31929400
F	-1.36225500	-1.72742000	-1.89469700
C	1.50798100	1.57506400	0.81442400
C	2.03122700	-0.18373200	-0.45295700
C	-0.59785100	-1.52140200	0.93874700
C	-1.40468600	1.68713300	-1.32610900
C	-2.73380400	1.08411200	0.60581300
C	3.56755900	2.82388200	0.95817700
H	4.61543700	2.96601600	0.72545700
C	-3.66564100	2.04024400	0.23134200
H	-4.54803500	2.17826300	0.84971600
C	4.38362800	0.14380100	-0.91914800

H	5.32220800	0.67688900	-0.84577500
C	-2.36904500	2.63138100	-1.66814600
H	-2.22969700	3.21700900	-2.57203800
C	-3.50781700	2.83258000	-0.90358400
C	0.81987600	2.50832400	1.57871700
H	-0.23191700	2.38424400	1.79314800
F	-2.62177900	-3.42025200	-1.48986100
B	-0.44169600	-0.09054100	0.33887600
C	1.98907100	-1.36698700	-1.19444900
H	1.07144600	-1.92770800	-1.29195700
C	0.12146600	-1.93899800	2.09835200
C	-1.44212800	-2.51035000	0.35375500
C	2.88285600	3.76790300	1.73796300
C	4.31431800	-1.04049100	-1.65334900
C	1.53841900	3.61084800	2.04047400
H	1.03488900	4.35749500	2.64079800
C	-0.23919900	1.51044400	-2.26357100
H	-0.43091300	2.01009300	-3.21414700
H	-0.05399800	0.45401100	-2.46698200
H	0.68482500	1.93333900	-1.85948200
F	-3.23653900	-1.46968400	-0.84365400
C	-3.01164400	0.29562300	1.85965400
H	-3.85338700	0.72602800	2.40426800
H	-2.14377800	0.27578800	2.52269800
H	-3.25578200	-0.74352800	1.63125900
C	-4.54036600	3.86068000	-1.27899900
H	-5.52704200	3.40621000	-1.40127400
H	-4.28180400	4.35858100	-2.21458000
H	-4.63439600	4.62870200	-0.50608400
C	1.01608000	-0.99265400	2.85239600
H	1.28187100	-1.40871600	3.82459000
H	0.52463800	-0.03054600	3.01782400
H	1.94937900	-0.79020600	2.32142000
C	3.15870200	-1.78930000	-1.80482400
H	3.19186700	-2.69529000	-2.39414300
C	-1.59214200	-3.77945300	0.90068500
H	-2.23939000	-4.49701300	0.41635200
C	-2.15910000	-2.27321300	-0.94523000
C	-0.03971500	-3.21580000	2.61731700
H	0.50650700	-3.48544100	3.51495200
C	-0.89711900	-4.14089800	2.03990200
H	-1.01653300	-5.12855900	2.46666700
F	5.43538700	-1.47377100	-2.24222100
H	3.41472100	4.63630700	2.10492500

C3-GS2-*Z* – S_0 optimized geometry

0 1

N	0.52378800	-0.61812100	-0.06492500
C	-2.05397700	-0.21020500	-0.28654400
C	1.72811800	-2.52208000	0.43460800
C	2.59075100	-1.61790200	-0.29330400
F	0.04909900	0.79219900	2.39486800
C	0.48247100	-1.89012000	0.55367600
C	1.84087300	-0.46460900	-0.56846100

C	-0.24812000	1.86698500	-0.24507300
C	-3.11781000	0.31032000	0.48396100
C	-2.35970100	-1.18151200	-1.26814000
C	1.94540300	-3.77798800	0.99445200
H	2.90980300	-4.26287800	0.90027700
C	-3.67214600	-1.60910200	-1.43983800
H	-3.88523200	-2.34714900	-2.20663400
C	3.91160000	-1.73411400	-0.71595300
H	4.50928600	-2.61351700	-0.51411900
C	-4.41140800	-0.16445000	0.29526700
H	-5.20982700	0.23385400	0.91297800
C	-4.71373200	-1.12291000	-0.66275900
C	-0.54811700	-2.49154300	1.27060800
H	-1.50338600	-2.00570400	1.40011000
F	2.08887000	1.30454600	1.90800000
B	-0.57248800	0.31271300	-0.16727100
C	2.40023500	0.57784500	-1.30070300
H	1.84219500	1.46862600	-1.54355000
C	-0.62718400	2.62893800	-1.36752000
C	0.38895600	2.54158600	0.81043500
C	0.91234700	-4.38873500	1.68082900
C	4.44215000	-0.67859600	-1.41845600
C	-0.31892900	-3.74272700	1.81910300
H	-1.11419900	-4.22546700	2.37423200
C	-2.91746000	1.36130800	1.54881700
H	-2.48176800	2.27319200	1.13810700
H	-2.25400400	1.01549500	2.34123600
H	-3.87223000	1.62419300	2.00428500
F	0.90373500	2.63321200	3.11704200
C	-1.32197700	-1.79543600	-2.18072600
H	-1.80326100	-2.21526600	-3.06446400
H	-0.78701100	-2.60715000	-1.68219400
H	-0.57413600	-1.07964300	-2.51993200
C	-6.12795000	-1.58843600	-0.87666400
H	-6.64383600	-0.94219600	-1.59274000
H	-6.69793500	-1.56548400	0.05335400
H	-6.15597900	-2.60444600	-1.27291900
C	-1.30558500	2.00400600	-2.56097500
H	-1.43679200	2.73967700	-3.35425700
H	-2.28697400	1.60626800	-2.29984200
H	-0.72010900	1.17919800	-2.97291900
C	3.71579500	0.46454400	-1.71962500
H	4.18925600	1.25685500	-2.28445400
C	0.64668900	3.90566000	0.76445800
H	1.12612100	4.39359800	1.60191700
C	0.85316300	1.82071700	2.04702100
C	-0.34992800	3.99326100	-1.40509300
H	-0.63818900	4.56292100	-2.28111600
C	0.27882500	4.63415200	-0.35178000
H	0.47789000	5.69747100	-0.39770700
F	5.72352800	-0.75514900	-1.84472500
H	1.05904600	-5.36556800	2.12479900

C3-GS2-*Z* – S_1 optimized geometry

0 1

N	0.53287000	-0.53347000	-0.01461500
C	-2.05173200	-0.29475400	-0.42071400
C	1.88723200	-2.22193900	0.76080100
C	2.54490500	-1.57310600	-0.36714000
F	0.25471300	0.99656400	2.53754800
C	0.66508000	-1.54053600	0.93771200
C	1.65568800	-0.55494300	-0.80030200
C	-0.38315500	1.92906300	-0.12908100
C	-3.19971500	0.17073000	0.27815600
C	-2.22483500	-1.43111200	-1.25330000
C	2.20997900	-3.28240800	1.57576100
H	3.13960100	-3.82371200	1.45139200
C	-3.46330500	-2.05335000	-1.35989000
H	-3.56064500	-2.91572800	-2.01289600
C	3.74147600	-1.76369800	-1.01086000
H	4.45719500	-2.52117500	-0.72036300
C	-4.41838200	-0.48465000	0.14432200
H	-5.27094600	-0.11908200	0.70933900
C	-4.58010500	-1.59949000	-0.67061100
C	-0.24303400	-1.90793700	1.92021200
H	-1.17863600	-1.38107100	2.03756600
F	2.19552900	1.06449100	1.58665000
B	-0.66822700	0.40205100	-0.20338300
C	1.96506400	0.28174500	-1.87618600
H	1.28898900	1.06834900	-2.17761100
C	-0.99859600	2.79524000	-1.08969100
C	0.51756100	2.56590500	0.77391200
C	1.30184000	-3.65524600	2.57577000
C	4.02079700	-0.92146500	-2.08832400
C	0.10092700	-2.97980100	2.74190900
H	-0.58292000	-3.28940700	3.52164100
C	-3.14671300	1.34728800	1.22213800
H	-3.07461400	2.29877100	0.68918000
H	-2.27758800	1.29538300	1.87970400
H	-4.04695800	1.38110400	1.83762100
F	1.57786800	2.65545900	2.89080200
C	-1.09718700	-1.97650800	-2.08995100
H	-1.47455700	-2.67598400	-2.83689400
H	-0.35987800	-2.51395900	-1.48788400
H	-0.56604100	-1.17703700	-2.61282200
C	-5.91970100	-2.26831500	-0.82110500
H	-6.50694800	-1.79976300	-1.61699300
H	-6.50476800	-2.19701000	0.09777300
H	-5.81111000	-3.32418200	-1.07507300
C	-1.96081700	2.28159700	-2.12996600
H	-2.16005300	3.05383000	-2.87394000
H	-2.91536000	1.97533100	-1.69870500
H	-1.55923300	1.40283800	-2.64040900
C	3.16988000	0.07925200	-2.52849000
H	3.46790600	0.69195100	-3.36808800
C	0.83186000	3.91903900	0.69323000
H	1.52123100	4.35078800	1.40567500
C	1.12576300	1.82986700	1.92639900
C	-0.67055500	4.14108600	-1.14154700
H	-1.13658100	4.75894400	-1.90165500
C	0.24817400	4.71580800	-0.27035100
H	0.49268700	5.76814100	-0.33822000

F	5.18506800	-1.09213500	-2.72522200
H	1.54129800	-4.48685400	3.22599300

Catalyst C4

C4-GS1-*E* – S_0 optimized geometry

0 1

N	1.08432400	-1.19443900	-0.22521000
C	0.06659500	1.17646600	0.28105800
C	2.20091800	-2.98391000	-1.06897400
C	3.17505400	-2.03630500	-0.58716800
F	-1.47806400	0.02581200	-2.20741700
C	0.98389300	-2.46140900	-0.82143300
C	2.46123400	-0.93930400	-0.07201600
C	-1.41449500	-1.17241500	0.36788400
C	0.62948200	1.96192800	-0.74623000
C	-0.44278100	1.84186200	1.42190700
C	-0.35423200	3.22243500	1.52217000
H	-0.73269300	3.70946200	2.41530500
C	4.56971200	-2.05176800	-0.53370000
H	5.12428100	-2.89351700	-0.93160100
C	0.67114100	3.34961100	-0.61719100
H	1.09613700	3.93475700	-1.42687600
C	0.19466700	4.00067800	0.50757700
F	-3.62194500	-0.16369500	-2.34461300
B	-0.05242200	-0.38291200	0.12122000
C	3.12101000	0.12772700	0.53140400
H	2.57747600	0.96129200	0.95186000
C	-1.47206300	-2.13171300	1.39898400
C	-2.59342200	-0.93815300	-0.35831800
C	5.22564000	-0.98112500	0.04327700
H	6.30780400	-0.97479200	0.09467100
C	1.21587900	1.39625800	-2.01920600
H	0.95744200	2.03712000	-2.86398300
H	0.87175000	0.39222800	-2.24616000
H	2.30668400	1.36642600	-1.95428200
F	-2.76227000	1.32449900	-1.04983700
C	-1.08054200	1.10188100	2.57288700
H	-1.28019500	1.78498100	3.39867800
H	-0.44351200	0.30366100	2.95615400
H	-2.02919900	0.64942200	2.27879400
C	0.24310100	5.49922300	0.62806500
H	-0.75732800	5.92929000	0.52907400
H	0.87357600	5.94005600	-0.14474400
H	0.63110900	5.80434500	1.60216500
C	-0.27098300	-2.50262300	2.23657100
H	-0.58961200	-2.88404900	3.20704200
H	0.40370900	-1.66578300	2.41084700
H	0.31516500	-3.28603500	1.74922400
C	4.50442400	0.09396700	0.57545200
H	5.03739500	0.91745200	1.03533400
C	-3.77970900	-1.60406500	-0.08393200
H	-4.66114600	-1.40537200	-0.67773300
C	-2.61594700	0.05792400	-1.48051100
C	-2.67403400	-2.78074100	1.67587000
H	-2.70417000	-3.50397000	2.48317600
C	-3.82125100	-2.52597500	0.94696100
H	-4.74298100	-3.04612500	1.17582600

H	2.40142500	-3.93348500	-1.54006600
H	0.00949200	-2.86399400	-1.04385400

C4-GS1-*E* – S_1 optimized geometry

0 1

N	1.04991000	-1.12809500	-0.46189300
C	0.04271700	1.23551300	0.13105300
C	2.27237000	-2.60307000	-1.67174200
C	3.16720300	-1.95418500	-0.80850800
F	-2.00813900	0.21305000	-2.12115900
C	0.99519900	-2.04775700	-1.41929000
C	2.39598700	-1.04165400	-0.04419600
C	-1.38824200	-1.18426100	0.37686200
C	0.77432200	1.97832400	-0.83570500
C	-0.48029200	1.97052000	1.23557700
C	-0.22770800	3.32665100	1.36562700
H	-0.62400500	3.85063100	2.23091600
C	4.55193100	-2.04831000	-0.59134600
H	5.15502500	-2.73234200	-1.17486100
C	1.00233300	3.34118400	-0.66568100
H	1.55785300	3.87701200	-1.43001700
C	0.52158200	4.04033200	0.43096000
F	-4.11913000	0.09184300	-1.73189400
B	-0.13792600	-0.30604000	0.04604500
C	2.95320200	-0.24739900	0.92492700
H	2.35630900	0.44236500	1.50445800
C	-1.27897400	-2.32921600	1.21787200
C	-2.68428100	-0.92050200	-0.14022900
C	5.12350500	-1.24544200	0.37959900
H	6.18785700	-1.29730300	0.56576700
C	1.27349200	1.34489600	-2.10852100
H	1.54967600	2.11105100	-2.83457400
H	0.50692500	0.71056300	-2.55758000
H	2.15934500	0.72349900	-1.94570200
F	-2.90149200	1.42119200	-0.56482900
C	-1.29816500	1.30637900	2.31287300
H	-1.44506000	1.98280600	3.15642700
H	-0.81700800	0.39627500	2.67809500
H	-2.28240200	1.01370300	1.94162300
C	0.79319600	5.50886200	0.61380400
H	-0.12172600	6.05711700	0.85172000
H	1.22458200	5.94703700	-0.28753200
H	1.49459800	5.68392800	1.43543300
C	0.02562500	-2.68913400	1.88037600
H	-0.14128100	-3.37115100	2.71503000
H	0.52879500	-1.79667800	2.26213600
H	0.72130200	-3.17901900	1.19444100
C	4.33722400	-0.36502300	1.12733900
H	4.80650400	0.24566200	1.88803600
C	-3.78706800	-1.70703100	0.17349400
H	-4.75265000	-1.47113100	-0.25179100
C	-2.91725900	0.19198600	-1.12081700
C	-2.39168500	-3.10404600	1.51260700
H	-2.27622400	-3.95345000	2.17774800
C	-3.64843700	-2.80347900	1.00468900

H	-4.50623600	-3.41548500	1.25338600
H	2.48828100	-3.37435300	-2.39391600
H	0.06199900	-2.28345600	-1.90501400

C4-GS2-*E* – S_0 optimized geometry

0 1

N	-0.00357800	1.23321300	0.58595100
C	-1.04452300	-1.10819000	-0.00285400
C	0.41018100	3.27447800	1.49265400
C	-0.80091200	3.36731500	0.71602600
F	1.32430400	0.72206700	-1.87774900
C	0.86152600	2.01086700	1.37301500
C	-1.03335800	2.09466700	0.16468100
C	1.64775000	-0.74651200	0.54222900
C	-1.03113000	-2.01502700	-1.08818000
C	-2.16993100	-1.11690600	0.85139400
C	-3.23108400	-1.98237600	0.59933000
H	-4.07626700	-1.98351400	1.28050600
C	-1.67096100	4.42130300	0.43219800
H	-1.49825400	5.40409200	0.85495000
C	-2.12287900	-2.84412900	-1.31629200
H	-2.09594000	-3.52308600	-2.16252800
C	-3.23800600	-2.84282800	-0.48738900
F	2.90137400	1.88599800	-0.97351800
B	0.17655100	-0.17193200	0.33587600
C	-2.10153300	1.86768300	-0.69838100
H	-2.26742200	0.89879200	-1.14690300
C	1.91338600	-1.67712700	1.56689100
C	2.72276500	-0.36991000	-0.27958000
C	-2.74631300	4.19000600	-0.40427800
H	-3.43188400	4.99590400	-0.63745000
C	0.12603800	-2.11796100	-2.05151000
H	1.06813600	-2.30412500	-1.53460300
H	0.25064700	-1.20363700	-2.63193900
H	-0.03727800	-2.93693100	-2.75200900
F	3.37765300	0.37000300	-2.42656500
C	-2.30215600	-0.23184000	2.07012100
H	-2.90312100	-0.73138000	2.83119800
H	-2.80647800	0.70380400	1.81676700
H	-1.34688600	0.03103500	2.51928000
C	-4.41250700	-3.73947600	-0.76824100
H	-4.08955500	-4.70425900	-1.16323600
H	-5.07407000	-3.28769100	-1.51292900
H	-5.00227100	-3.91589500	0.13214200
C	0.84092200	-2.13015600	2.52525600
H	1.24199200	-2.85356900	3.23473000
H	0.00396200	-2.59398400	2.00251400
H	0.44222500	-1.29257800	3.10228800
C	-2.95322900	2.92526600	-0.96769300
H	-3.79392500	2.76952500	-1.63302800
C	4.00085500	-0.88976000	-0.11090800
H	4.79847700	-0.58767700	-0.77627600
C	2.57562100	0.64348800	-1.38133700
C	3.20114800	-2.18036900	1.73166100
H	3.38789500	-2.89040200	2.52920300

C	4.24104700	-1.79916600	0.90128900
H	5.23293000	-2.21043900	1.04075500
H	1.73575700	1.55512600	1.80715800
H	0.87734100	4.06539200	2.05824200

C4-GS2-*E* – S_1 optimized geometry

0 1

N	0.36308300	0.99441100	0.79154300
C	-1.47045800	-0.77582300	0.14332600
C	1.14834900	2.77638500	1.94808200
C	0.40050700	3.29095200	0.88206000
F	1.65543600	0.55133800	-1.72669700
C	1.07761600	1.36381500	1.84397900
C	-0.08165400	2.17366100	0.15338800
C	1.24585000	-1.41712500	0.33947600
C	-1.84444100	-1.56448400	-0.97787300
C	-2.52341000	-0.28236400	0.95744300
C	-3.85078600	-0.55869100	0.65048900
H	-4.62972000	-0.17868200	1.30538400
C	0.08365600	4.59430600	0.45879800
H	0.44025200	5.45360900	1.01225400
C	-3.18454300	-1.81662900	-1.24976400
H	-3.43714700	-2.41275600	-2.12201800
C	-4.21094400	-1.32091000	-0.45370700
F	3.05196100	1.25091800	-0.23128100
B	0.03325100	-0.45682700	0.42208100
C	-0.84791800	2.31853100	-0.97525800
H	-1.20677700	1.46415900	-1.53040800
C	1.15368600	-2.73071200	0.90324900
C	2.51389900	-1.08611300	-0.22637800
C	-0.69218600	4.74637300	-0.67276000
H	-0.95248100	5.73637500	-1.02244000
C	-0.82160500	-2.12700900	-1.93511300
H	-0.27137800	-2.96635500	-1.50187100
H	-0.07687000	-1.37759400	-2.20801100
H	-1.30638800	-2.48398400	-2.84526500
F	3.74603900	0.06851900	-1.88484200
C	-2.24882700	0.50916300	2.21075000
H	-3.14055800	0.56061600	2.83696100
H	-1.94915400	1.53764400	1.99034200
H	-1.44599500	0.05723400	2.79875400
C	-5.65518800	-1.57917900	-0.78946800
H	-5.78282900	-2.54468400	-1.28255900
H	-6.04661900	-0.81390300	-1.46713100
H	-6.27902800	-1.56938300	0.10624500
C	-0.11873900	-3.22901900	1.53877700
H	0.06170100	-4.16688800	2.06579900
H	-0.90860600	-3.40079700	0.80511800
H	-0.51426900	-2.50010900	2.25020400
C	-1.14588900	3.62626800	-1.37908300
H	-1.74411100	3.77252800	-2.26937600
C	3.61062400	-1.94231100	-0.16228800
H	4.54981200	-1.64220900	-0.60734700
C	2.73133000	0.17454300	-1.00161000
C	2.25833300	-3.56364100	0.94507100

H	2.15700400	-4.53849700	1.41023400
C	3.49650400	-3.18080100	0.43394200
H	4.34795000	-3.84705900	0.48893500
H	1.52184400	0.63049500	2.49714800
H	1.68201200	3.32141100	2.71007100

C4-GS1-*Z* – S_0 optimized geometry

0 1

N	-0.97337700	-1.26624100	0.26032200
C	1.54824000	-0.66324400	0.31448600
C	-1.89658400	-3.30914200	0.62484600
C	-2.92762900	-2.43739500	0.11839300
F	0.29670900	0.80126700	-2.19653900
C	-0.75902500	-2.58904700	0.67776500
C	-2.33230700	-1.18105900	-0.09760800
C	-0.44322900	1.26876900	0.49566000
C	2.03992500	-1.53096300	-0.68483600
C	2.46977900	-0.15779100	1.26373000
C	3.80172000	-0.54168900	1.21667100
H	4.48545200	-0.15613900	1.96634600
C	-4.27687800	-2.63234400	-0.17960300
H	-4.74114400	-3.59745800	-0.01423200
C	3.39280300	-1.86914600	-0.70998900
H	3.75071600	-2.52450700	-1.49779000
C	4.28893800	-1.39607200	0.23256100
F	0.49231700	2.90973400	-2.61088100
B	0.03179000	-0.23835600	0.32530300
C	-3.05769700	-0.12616000	-0.64455100
H	-2.60074900	0.83103700	-0.84788000
C	-1.18751800	1.62805100	1.63662900
C	-0.11609200	2.29045000	-0.40894000
C	-5.00398000	-1.57681800	-0.69688400
H	-6.05246800	-1.70913200	-0.93543100
C	1.18492400	-2.13186000	-1.77858000
H	1.77351300	-2.23694000	-2.69120400
H	0.30783800	-1.53674100	-2.01394400
H	0.83828400	-3.13039300	-1.49956500
F	1.98950400	1.90880600	-1.43258900
C	2.06518400	0.79532400	2.36265400
H	2.89617300	0.95323100	3.05036300
H	1.22345800	0.42256000	2.94732500
H	1.77717400	1.76798100	1.96032400
C	5.74499300	-1.77118100	0.19232200
H	6.36539400	-0.90079600	-0.03688600
H	5.93914900	-2.53057700	-0.56564800
H	6.07778600	-2.15951500	1.15755800
C	-1.63481300	0.61955300	2.66712700
H	-1.81081600	1.10868700	3.62552800
H	-0.91059800	-0.17830000	2.82698400
H	-2.57039200	0.14513000	2.36032800
C	-4.39570100	-0.33851800	-0.93110500
H	-4.97945700	0.47101600	-1.35233400
C	-0.49493800	3.61047800	-0.20771800
H	-0.23701000	4.36505300	-0.93796800
C	0.66413000	1.98333000	-1.65264200

C	-1.54614400	2.95929000	1.83657200
H	-2.10701300	3.22194900	2.72651800
C	-1.20899900	3.94713700	0.92848300
H	-1.50470200	4.97432200	1.10153500
H	-2.00869100	-4.34272900	0.91281000
H	0.22142500	-2.88024700	1.01594400

C4-GS1-*Z* – S_1 optimized geometry

0 1

N	-1.04231500	-1.16947700	0.55674000
C	1.48838700	-0.65908100	0.27861500
C	-2.19565800	-2.99443100	1.24169600
C	-2.99343400	-2.35397000	0.28507300
F	0.57649500	1.08759300	-2.17063500
C	-1.01748000	-2.21743300	1.36980000
C	-2.26044500	-1.22069900	-0.15389700
C	-0.44445900	1.37827200	0.56512000
C	1.77985000	-1.70416400	-0.63366100
C	2.55739000	-0.19456700	1.08979500
C	3.81031200	-0.78634400	1.01123100
H	4.60361300	-0.41990000	1.65655200
C	-4.25824800	-2.62488500	-0.26707600
H	-4.83184800	-3.48011900	0.06694200
C	3.05121400	-2.26806500	-0.68485900
H	3.24626800	-3.05795800	-1.40461600
C	4.08284100	-1.83420200	0.13606200
F	1.04221500	3.18212500	-2.28736500
B	0.04168200	-0.09054100	0.45247100
C	-2.73409200	-0.38008200	-1.12923200
H	-2.16239700	0.47044000	-1.47143100
C	-1.42004100	1.78116600	1.53173700
C	0.04317000	2.42522200	-0.27508500
C	-4.74734200	-1.77486700	-1.24026200
H	-5.71785700	-1.95848400	-1.68124700
C	0.75280500	-2.19798800	-1.62294600
H	1.23653700	-2.73001200	-2.44376500
H	0.18653100	-1.36659300	-2.04519200
H	0.03387300	-2.88772300	-1.17239500
F	2.24443900	1.90025700	-1.05670300
C	2.37373900	0.94014900	2.06440500
H	3.23244000	1.01872600	2.73317600
H	1.47294200	0.80986900	2.66792800
H	2.26569600	1.89318200	1.54187500
C	5.44417900	-2.47449400	0.09189600
H	6.23792400	-1.72928800	0.17758400
H	5.59372000	-3.02471500	-0.83852000
H	5.57522300	-3.18188000	0.91673300
C	-1.99194400	0.81008500	2.53090700
H	-2.51196400	1.34435800	3.32668500
H	-1.20592100	0.20262000	2.98698600
H	-2.71229200	0.12306500	2.07909200
C	-3.99410800	-0.67688900	-1.66914000
H	-4.39226600	-0.03493500	-2.44443900
C	-0.36673700	3.74627700	-0.13968100
H	0.02855200	4.49898400	-0.80742300

C	0.96822200	2.14475800	-1.42220700
C	-1.81739300	3.10497100	1.63762000
H	-2.53974800	3.37103400	2.40220500
C	-1.29727200	4.10008500	0.81970700
H	-1.61462800	5.12940300	0.92687200
H	-2.40842700	-3.90267200	1.78285700
H	-0.17724100	-2.39107400	2.02264600

C4-GS2-*Z* – S_0 optimized geometry

0 1

N	-0.49915300	-1.23522000	-0.21068200
C	1.90620100	-0.27519800	-0.03776100
C	-1.11412000	-3.14691700	-1.27175900
C	-2.23094400	-2.69877400	-0.47785300
F	-0.66374500	0.81922000	-2.16398000
C	-0.11188500	-2.26835500	-1.07759800
C	-1.83001100	-1.51233700	0.16323600
C	-0.32350500	1.23254600	0.62778600
C	2.71844300	0.65740500	-0.72590400
C	2.54836200	-1.35608400	0.60908000
C	3.93250500	-1.49400800	0.53434100
H	4.40294300	-2.32184400	1.05545200
C	-3.50658700	-3.21890700	-0.25632400
H	-3.81950200	-4.13123800	-0.75041900
C	4.09343100	0.46843300	-0.79205200
H	4.69416700	1.19026700	-1.33601800
C	4.72407500	-0.60439400	-0.17403600
F	-2.74106300	1.05417900	-1.62994700
B	0.34142000	-0.10925800	0.09534700
C	-2.67920000	-0.85539200	1.04948700
H	-2.37784000	0.04432000	1.56496600
C	-0.06905600	1.67075400	1.94303700
C	-1.15894100	2.03219000	-0.16726200
C	-4.35605300	-2.55499100	0.60827200
H	-5.35026200	-2.94353600	0.79359300
C	2.15858300	1.87003400	-1.42917400
H	1.56186200	2.48867000	-0.75819400
H	1.52049600	1.59192600	-2.26798300
H	2.96846100	2.48685600	-1.81860400
F	-1.62233200	2.73768300	-2.37295700
C	1.81672700	-2.39340600	1.43288100
H	2.47415000	-2.77945100	2.21292600
H	1.50668700	-3.24181900	0.81797300
H	0.92067800	-2.00616300	1.91340700
C	6.21272100	-0.79193200	-0.27862700
H	6.73690300	0.16445800	-0.23581200
H	6.47673300	-1.26521900	-1.22867100
H	6.59077500	-1.42774900	0.52284600
C	0.78638700	0.86942400	2.89126400
H	0.91234100	1.39838200	3.83564200
H	1.77534100	0.67427000	2.47569200
H	0.32806400	-0.09683700	3.11700000
C	-3.94068800	-1.38708400	1.25694300
H	-4.61775400	-0.88612800	1.93831500
C	-1.72125100	3.21203600	0.30590300

H	-2.34886400	3.80848800	-0.34295000
C	-1.53895000	1.65769100	-1.57298000
C	-0.64629100	2.84949500	2.40675700
H	-0.44431400	3.16733000	3.42327200
C	-1.46546000	3.62162800	1.60048800
H	-1.89847600	4.53948100	1.97786900
H	0.87477400	-2.24814000	-1.50950700
H	-1.08309300	-4.01637000	-1.90966300

C4-GS2-*Z* – S_1 optimized geometry

0 1

N	-0.51486200	-1.04067700	-0.41263900
C	1.91343900	-0.19167500	0.00663900
C	-1.43406200	-2.64306900	-1.71674000
C	-2.15167300	-2.64930200	-0.50960000
F	-0.95304800	1.14667400	-2.33236000
C	-0.45129400	-1.63277700	-1.59763800
C	-1.57009800	-1.64938000	0.30556100
C	-0.32189300	1.42500400	0.48726000
C	2.80959300	0.74377000	-0.57375800
C	2.46991800	-1.40946100	0.47534400
C	3.82883900	-1.66952800	0.33968900
H	4.22486800	-2.60545000	0.72334500
C	-3.23596200	-3.39878000	-0.02832800
H	-3.69551300	-4.16096700	-0.64465600
C	4.16255200	0.44436600	-0.69114700
H	4.82075100	1.17431900	-1.15356500
C	4.69839200	-0.75986700	-0.24906400
F	-2.74212900	0.39752600	-1.37735200
B	0.37843500	0.10634100	0.07249400
C	-2.02891000	-1.37911800	1.56759800
H	-1.58604800	-0.60475600	2.17817600
C	0.13865400	2.12802300	1.64762500
C	-1.44633600	2.00943500	-0.16885900
C	-3.70485900	-3.13530400	1.24676100
H	-4.54024800	-3.69731500	1.64228900
C	2.33905000	2.07440400	-1.10870000
H	2.08359400	2.76987100	-0.30480100
H	1.44185500	1.96535800	-1.71960400
H	3.11839100	2.54007800	-1.71409800
F	-2.69025300	2.40208600	-2.14642300
C	1.62833700	-2.43279600	1.19547300
H	2.25922200	-3.14886900	1.72407900
H	0.99100500	-3.00324800	0.51501000
H	0.96935500	-1.95738900	1.92644800
C	6.16062100	-1.07301000	-0.41974800
H	6.77097000	-0.16996500	-0.35955300
H	6.35476400	-1.53199900	-1.39422000
H	6.50899800	-1.77115600	0.34357600
C	1.31185600	1.63577400	2.45566300
H	1.39488300	2.19856100	3.38640500
H	2.25639200	1.73260700	1.91731200
H	1.20439700	0.57562700	2.69865700
C	-3.10877600	-2.14642000	2.03154000
H	-3.48862700	-1.96313700	3.02848300

C	-2.10059000	3.13638900	0.32260900
H	-2.94927000	3.53789300	-0.21408600
C	-1.94675900	1.49532800	-1.48070700
C	-0.52679900	3.25128800	2.10824500
H	-0.16449100	3.73712200	3.00808100
C	-1.65533300	3.75939300	1.46979300
H	-2.16443000	4.63303900	1.85625900
H	0.27978500	-1.33112000	-2.32951200
H	-1.57731400	-3.27878200	-2.57587000

Catalyst C5

C5-GS1-*E* – S_0 optimized geometry

0 1

N	0.52599500	-0.45872800	-0.04772900
C	-1.27425700	1.44631800	0.06510500
C	2.36207500	-1.74797300	-0.57909200
C	2.82703100	-0.44581200	-0.13357500
F	-2.40144500	-0.62000100	-1.97221900
C	0.95668000	-1.72094800	-0.50663700
C	1.69511700	0.30114800	0.16570200
C	-1.84859600	-1.16255600	0.74862300
C	-0.98040400	2.14264900	-1.13002300
C	-2.02534000	2.11541100	1.05682300
C	2.99824900	-2.90402100	-1.03931900
H	4.07390800	-2.96597000	-1.10830000
C	-2.43512300	3.42755100	0.85464100
H	-2.99168700	3.93009900	1.63914300
C	4.12787700	0.11581000	0.04612900
C	-1.43718100	3.44543700	-1.30269800
H	-1.21388900	3.95795100	-2.23301000
C	-2.16097800	4.11017800	-0.32358500
C	0.19053100	-2.80414000	-0.92689700
H	-0.88740100	-2.77006700	-0.91711000
F	-4.36445100	-1.50521100	-1.84977200
B	-0.83505300	-0.05393400	0.22453200
C	1.78692100	1.60727300	0.69538100
H	0.90030400	2.16536000	0.95282800
C	-1.54416800	-1.84669600	1.94281100
C	-3.07661400	-1.45296800	0.13432000
C	2.23766400	-3.99254900	-1.42407000
H	2.72848600	-4.88974800	-1.78076100
C	4.21162500	1.44149600	0.55227200
C	0.84445600	-3.93877200	-1.37375600
H	0.26117100	-4.79223500	-1.69722500
C	-0.17368500	1.55051000	-2.26264300
H	-0.39318900	2.07813700	-3.19144400
H	-0.37834100	0.49485800	-2.42278300
H	0.89812600	1.65314600	-2.07474300
F	-4.01068300	0.42762500	-0.97423400
C	-2.39844900	1.47016000	2.37002500
H	-2.79061500	2.21749500	3.06018000
H	-1.54792000	0.99036500	2.85536700
H	-3.16831100	0.70836800	2.23351300
C	-2.65880700	5.51263200	-0.54117500
H	-3.66917900	5.50227900	-0.96012200
H	-2.02047200	6.05742100	-1.23815000
H	-2.69993900	6.06925300	0.39637800
C	-0.24476000	-1.64525300	2.68504600
H	-0.32892600	-2.02317000	3.70398600
H	0.05311100	-0.59801200	2.74324600
H	0.57141000	-2.18403800	2.19782600
C	3.02209200	2.15196200	0.87196700
H	3.11381700	3.15496400	1.27253100
C	-3.97515300	-2.36742700	0.66648000

H	-4.90319800	-2.57640800	0.15237500
C	-3.46512500	-0.78821100	-1.15379900
C	-2.46238000	-2.74860100	2.47567100
H	-2.21973200	-3.25629900	3.40228100
C	-3.66827500	-3.01282800	1.85089100
H	-4.36371500	-3.72310600	2.28019800
C	5.33569400	-0.56120900	-0.24530400
H	5.30925100	-1.56816500	-0.63175400
C	5.48050800	2.03468300	0.74349700
H	5.52543900	3.04664800	1.13032500
C	6.55098600	0.04038900	-0.04993400
H	7.46043000	-0.50034300	-0.28323200
C	6.62964800	1.35337400	0.44979100
H	7.59642000	1.81815700	0.59991500

C5-GS1-*E* – S_1 optimized geometry

0 1

N	0.53197200	-0.43860300	-0.09050500
C	-1.31224100	1.42517800	-0.11667600
C	2.32655300	-1.60187000	-0.95582100
C	2.81741700	-0.47808600	-0.17505300
F	-2.93369500	-0.71546900	-1.74465800
C	0.91916800	-1.53057400	-0.88797700
C	1.66017400	0.17630100	0.32873800
C	-1.77393000	-1.15127800	0.91760200
C	-0.92417000	2.04199100	-1.33371800
C	-2.02370800	2.23208100	0.81485000
C	2.91077500	-2.62692200	-1.68238000
H	3.98300400	-2.73615100	-1.75640300
C	-2.26900300	3.57026100	0.54324300
H	-2.79673600	4.16485000	1.28350800
C	4.09747500	0.02613400	0.13573700
C	-1.19592300	3.38648200	-1.56813600
H	-0.89382900	3.82422500	-2.51514100
C	-1.85993100	4.17730800	-0.64150400
C	0.09828900	-2.43093800	-1.53211900
H	-0.97699100	-2.34596000	-1.47446000
F	-4.86236900	-1.39036700	-1.08082900
B	-0.90814200	-0.04014100	0.24928700
C	1.74096300	1.32524300	1.16211400
H	0.83731600	1.79572800	1.52047500
C	-1.26754200	-1.97385200	1.96910500
C	-3.11568300	-1.42694500	0.52114800
C	2.08995900	-3.55156300	-2.33723400
H	2.54460000	-4.35300100	-2.90490000
C	4.16676000	1.18284400	0.97260300
C	0.71154600	-3.45178600	-2.26910000
H	0.09311200	-4.17162900	-2.78977800
C	-0.26024200	1.25958400	-2.43739900
H	-0.28682200	1.81823500	-3.37421300
H	-0.76249400	0.30412700	-2.59711700
H	0.78960800	1.04352100	-2.22144400
F	-4.13341700	0.52032900	-0.43441600
C	-2.51255500	1.68577500	2.13139700
H	-2.83774100	2.49519600	2.78688400

H	-1.73500500	1.11438900	2.64338700
H	-3.35686300	1.00789800	1.99040800
C	-2.12101700	5.63715400	-0.89589600
H	-3.12546000	5.92386500	-0.57671000
H	-2.01902300	5.87952200	-1.95489100
H	-1.41559100	6.26679300	-0.34464900
C	0.11941600	-1.78198000	2.52251700
H	0.23466500	-2.32395300	3.46172600
H	0.32830000	-0.72613500	2.71251100
H	0.89099500	-2.14809700	1.84074800
C	2.97145300	1.80002100	1.46668200
H	3.07648100	2.67427500	2.09741700
C	-3.89612400	-2.39194300	1.14822800
H	-4.90672600	-2.56658400	0.80660900
C	-3.74651100	-0.75125400	-0.66256600
C	-2.06486100	-2.93627500	2.57063200
H	-1.64937800	-3.52176000	3.38396100
C	-3.38034700	-3.14993700	2.18247800
H	-3.98904400	-3.89893100	2.67276200
C	5.30721400	-0.54881900	-0.33037800
H	5.27573600	-1.41877300	-0.96841300
C	5.42747000	1.70765900	1.30481000
H	5.47672600	2.58474400	1.93879500
C	6.51711000	-0.01274700	0.01360800
H	7.43153400	-0.46303800	-0.35108800
C	6.58013500	1.12523500	0.83896800
H	7.54330400	1.54223800	1.10522100

C5-GS2-*E* – S_0 optimized geometry

0 1

N	-0.25736600	-0.35882000	-0.34055300
C	1.45190600	1.62680100	-0.23343300
C	-2.11878000	-1.55196600	-0.99052600
C	-2.55791000	-0.36812300	-0.27241500
F	0.72814000	-0.72356500	2.34104400
C	-0.71127400	-1.52347900	-0.99681400
C	-1.41070800	0.32011000	0.09719400
C	2.26111900	-0.99560400	-0.06579500
C	2.31536300	2.24738400	0.69818300
C	0.95068200	2.41097400	-1.29814300
C	-2.78248100	-2.60682200	-1.62265400
H	-3.86054200	-2.66522700	-1.63755900
C	1.29698100	3.75511700	-1.39539600
H	0.91003600	4.33548300	-2.22684800
C	-3.84410100	0.13121700	0.09646400
C	2.61370400	3.59968600	0.57644700
H	3.26012200	4.06151300	1.31579400
C	2.11791400	4.37430000	-0.46453800
C	0.02618700	-2.50847600	-1.64636800
H	1.10451300	-2.48303700	-1.67131100
F	0.17656600	-2.70557400	1.68506400
B	1.10886800	0.09103100	-0.18923300
C	-1.46488200	1.49080000	0.88446900
H	-0.56161900	1.99138500	1.19756100
C	3.30618600	-1.04876800	-1.00843000

C	2.30343000	-1.90838100	1.00161300
C	-2.04841800	-3.59673000	-2.24892100
H	-2.56069200	-4.41582600	-2.73856300
C	-3.89354700	1.32974500	0.85974400
C	-0.65450800	-3.54374500	-2.26237600
H	-0.09161000	-4.32158900	-2.76392200
C	2.92528100	1.50821200	1.86470000
H	3.53044900	2.18637300	2.46635800
H	3.56993800	0.69347300	1.53135200
H	2.16604100	1.07334500	2.51407500
F	1.66944800	-2.45396700	3.21435800
C	0.04830300	1.86383100	-2.38131900
H	0.08447000	2.51035700	-3.25853100
H	-0.99145300	1.82124100	-2.04857900
H	0.32368600	0.85889900	-2.69951100
C	2.49037000	5.82558100	-0.59605100
H	3.45147000	5.93357300	-1.10698700
H	2.58655800	6.30000600	0.38190500
H	1.74683000	6.37575700	-1.17412000
C	3.34892800	-0.12532300	-2.20036600
H	4.16166200	-0.40430400	-2.87076100
H	3.49903300	0.91162000	-1.89697600
H	2.42139200	-0.16394800	-2.77547700
C	-2.68534000	1.97563500	1.24255500
H	-2.75119600	2.87482600	1.84422800
C	3.32816600	-2.83582200	1.13755900
H	3.33549700	-3.51352400	1.98007300
C	1.22591300	-1.94693300	2.05102800
C	4.31968900	-1.99327000	-0.86671300
H	5.11072100	-2.02913000	-1.60703900
C	4.33965900	-2.88031100	0.19561700
H	5.14136100	-3.60173700	0.29176000
C	-5.06870000	-0.48830400	-0.24752200
H	-5.06733100	-1.39901800	-0.82603100
C	-5.14725400	1.85878700	1.24265900
H	-5.16669900	2.77315800	1.82515000
C	-6.26865300	0.04940400	0.13729200
H	-7.19172000	-0.44469200	-0.14156500
C	-6.31367900	1.23671700	0.89086800
H	-7.26837100	1.65209300	1.18969400

C5-GS2-*E* – S_1 optimized geometry

0 1

N	-0.21205300	-0.24867100	-0.44039000
C	1.73268500	1.50555800	-0.29913800
C	-2.13452100	-1.10630000	-1.38327800
C	-2.49427800	-0.13764400	-0.36306100
F	0.28090900	-0.99832400	2.40274200
C	-0.72550800	-1.13407900	-1.40630000
C	-1.26388700	0.33019400	0.17782200
C	2.15344500	-1.21070500	0.19732400
C	2.57102300	2.08072300	0.69470800
C	1.30129400	2.35923300	-1.34711300
C	-2.83477500	-1.93409500	-2.24648400
H	-3.91457400	-1.96772700	-2.25540000

C	1.67088500	3.69919600	-1.37128400
H	1.32786700	4.32215700	-2.19227200
C	-3.71454900	0.38457900	0.11757700
C	2.91480000	3.42612700	0.63312800
H	3.53658700	3.84203900	1.42077900
C	2.47738500	4.26067700	-0.38979000
C	-0.01392100	-1.94384500	-2.26227700
H	1.06658100	-1.95585000	-2.24974200
F	-0.61776500	-2.52230800	1.16042400
B	1.27276200	0.01421300	-0.18048600
C	-1.21442200	1.29644100	1.21915200
H	-0.26080000	1.61965200	1.60816700
C	3.45122600	-1.34639000	-0.39264700
C	1.76193900	-2.27980500	1.05534600
C	-2.12541100	-2.75996600	-3.12495800
H	-2.67083200	-3.40696600	-3.79960800
C	-3.65097100	1.35741700	1.16155700
C	-0.74209000	-2.76121800	-3.13669800
H	-0.20977900	-3.40502400	-3.82516900
C	3.08311700	1.28507100	1.87053900
H	3.49055600	1.95095700	2.63287700
H	3.87508300	0.58994500	1.58016800
H	2.29397500	0.68098400	2.32124500
F	0.50984800	-3.07818200	2.90174200
C	0.47900700	1.83982100	-2.49839000
H	0.47412400	2.55458700	-3.32246500
H	-0.56244100	1.66178000	-2.21855000
H	0.87602700	0.89312100	-2.87279500
C	2.89097300	5.70656100	-0.44624900
H	3.86948800	5.81900800	-0.92345200
H	2.96822200	6.13720700	0.55412700
H	2.17811000	6.30204500	-1.01911400
C	4.01115700	-0.31291900	-1.33654900
H	4.91287600	-0.69147900	-1.81963000
H	4.26715200	0.61852400	-0.82860200
H	3.28661300	-0.05039700	-2.11117700
C	-2.38557600	1.78370900	1.68714300
H	-2.39003800	2.51982300	2.48159200
C	2.54923100	-3.40974800	1.25607200
H	2.20334000	-4.19138400	1.91835200
C	0.50371200	-2.21833300	1.86302300
C	4.21651800	-2.47997400	-0.16872200
H	5.18195600	-2.55876200	-0.65716400
C	3.77788400	-3.52420200	0.63858000
H	4.39133900	-4.40327800	0.78941600
C	-4.98626900	0.00059500	-0.37652300
H	-5.05483000	-0.72444400	-1.17313600
C	-4.84682600	1.89297200	1.66621700
H	-4.79532600	2.63038700	2.45830100
C	-6.13262200	0.54169700	0.13860900
H	-7.09622600	0.23750100	-0.24983100
C	-6.06469900	1.49482700	1.16978100
H	-6.97715500	1.91749100	1.57136500

C5-GS1-*Z* – S_0 optimized geometry

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0 1
 N                  0.48149600    0.51538200    0.17535200
 C                 -2.11819600    0.79195800   -0.00654400
 C                  2.23238100    2.00169100    0.37722900
 C                  2.76687800    0.71306900   -0.02773600
 F                 -1.41257300   -1.48742400   -2.01368600
 C                  0.83673600    1.84834700    0.47919000
 C                  1.68408900   -0.14972600   -0.13443400
 C                 -0.94697100   -1.57831900    0.77512400
 C                 -2.21475200    1.52778300   -1.21001700
 C                 -3.22339600    0.80706200    0.87257800
 C                  2.80552100    3.24258500    0.66935800
 H                  3.87108900    3.40126200    0.59808100
 C                 -4.35599900    1.54753500    0.55658400
 H                 -5.18460100    1.56375900    1.25724300
 C                  4.08555400    0.25059600   -0.32137100
 C                 -3.38049600    2.22894700   -1.50116900
 H                 -3.44109500    2.77538300   -2.43698500
 C                 -4.46137600    2.25857600   -0.63181000
 C                  0.02500000    2.89657200    0.90380600
 H                 -1.04187800    2.77242200    1.00838000
 F                 -2.34278900   -3.43333100   -2.01975100
 B                 -0.83636100   -0.06939500    0.28353400
 C                  1.83501800   -1.47865400   -0.58685100
 H                  0.98139500   -2.12390100   -0.71902400
 C                 -0.40841100   -1.91961300    2.03222400
 C                 -1.62366200   -2.58534500    0.06866900
 C                  1.99586900    4.29095300    1.06397700
 H                  2.43746400    5.25387300    1.28956400
 C                  4.23440500   -1.10005100   -0.73992000
 C                  0.61699800    4.11518200    1.18509800
 H                 -0.00403200    4.94211000    1.50748100
 C                 -1.09843000    1.61296200   -2.22508600
 H                 -1.49994300    1.89998900   -3.19754600
 H                 -0.56521200    0.67365900   -2.34899500
 H                 -0.36640600    2.37144300   -1.93648800
 F                 -3.41747000   -1.74106600   -1.23992800
 C                 -3.23150300    0.05896500    2.18422200
 H                 -4.08731500    0.36314100    2.78725900
 H                 -2.33314900    0.24325000    2.77433000
 H                 -3.30304000   -1.01883500    2.02678900
 C                 -5.71719600    3.01069400   -0.97730300
 H                 -6.42882200    2.35747600   -1.49052600
 H                 -5.50745700    3.85152700   -1.63995600
 H                 -6.21083500    3.39174400   -0.08197900
 C                  0.36287300   -0.93674700    2.88053300
 H                  0.41101400   -1.28489400    3.91235100
 H                 -0.08016100    0.05932100    2.88653300
 H                  1.38858200   -0.82852900    2.51951800
 C                  3.08762600   -1.93036200   -0.87083800
 H                  3.22544400   -2.94773400   -1.21811600
 C                 -1.77515100   -3.87042300    0.57053700
 H                 -2.28723800   -4.62280100   -0.01333100
 C                 -2.20195500   -2.31351200   -1.28945600
 C                 -0.58298800   -3.20838700    2.53194000
 H                 -0.17521400   -3.45109100    3.50667000
 C                 -1.25803200   -4.18047900    1.81575300
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H	-1.37577500	-5.17738100	2.22164500
C	5.25067200	1.04742100	-0.22161500
H	5.17415900	2.07604300	0.09478500
C	5.52378100	-1.59802300	-1.03747400
H	5.61900500	-2.63008200	-1.35610400
C	6.48705700	0.53578000	-0.51520100
H	7.36312400	1.16729200	-0.42811400
C	6.63044500	-0.80174500	-0.92835200
H	7.61336000	-1.19451400	-1.15817400

C5-GS1-*Z* – S_1 optimized geometry

0 1

N	0.52341100	0.42058100	0.34616900
C	-2.00128100	0.87321700	-0.23502200
C	2.35654300	1.76240000	0.74660200
C	2.78301400	0.57666500	0.01990400
F	-1.66212200	-1.75159400	-1.93072300
C	0.96553800	1.61872200	0.93173300
C	1.60299600	-0.18112100	-0.20817700
C	-1.11382900	-1.52096200	0.94624000
C	-1.78092800	1.65826200	-1.39649300
C	-3.24344000	1.05617400	0.43625300
C	2.98067300	2.89937600	1.23098100
H	4.03965200	3.06969900	1.10137000
C	-4.16016700	1.99144700	-0.02108000
H	-5.09061400	2.11988100	0.52463700
C	4.02470900	0.09886900	-0.44745900
C	-2.73030700	2.58161100	-1.82318800
H	-2.53286300	3.15708800	-2.72293400
C	-3.92788000	2.77367100	-1.14961200
C	0.20097800	2.55945900	1.58755200
H	-0.86446500	2.42544700	1.70770700
F	-2.91351000	-3.46904000	-1.61283400
B	-0.92029800	-0.09229300	0.34771000
C	1.61642100	-1.39982200	-0.93857800
H	0.69519400	-1.93399900	-1.11553100
C	-0.49342000	-1.91157600	2.17043600
C	-1.89848400	-2.52596000	0.31048000
C	2.21709300	3.86412900	1.90019800
H	2.70433600	4.75319500	2.27896800
C	4.02838600	-1.13352000	-1.17159900
C	0.85590800	3.69686800	2.07784400
H	0.28355800	4.45331800	2.59926600
C	-0.54291300	1.49067100	-2.23855100
H	-0.67198300	1.96796000	-3.21109200
H	-0.31914300	0.43546100	-2.40534200
H	0.33686800	1.94338600	-1.77235400
F	-3.61553100	-1.52854000	-1.02646200
C	-3.60236300	0.27779600	1.67564600
H	-4.48396600	0.70550500	2.15566500
H	-2.78208400	0.27319400	2.39707300
H	-3.82046900	-0.76608200	1.44191100
C	-4.93385300	3.79488000	-1.60682200
H	-5.95248600	3.40516100	-1.54710200
H	-4.74741800	4.10132100	-2.63733300

H	-4.89579500	4.69399800	-0.98385400
C	0.31798000	-0.93979000	2.98544900
H	0.49279600	-1.33248000	3.98768000
H	-0.19646200	0.01962700	3.08119300
H	1.29555200	-0.73718000	2.54177200
C	2.80688900	-1.84551800	-1.40462400
H	2.85759300	-2.76773400	-1.97036900
C	-2.08000000	-3.78975000	0.86129500
H	-2.67884000	-4.52078200	0.33635100
C	-2.51667200	-2.30997600	-1.04124600
C	-0.68283900	-3.18248400	2.69321900
H	-0.21320000	-3.43199800	3.63879900
C	-1.47708000	-4.12734200	2.05849600
H	-1.62045100	-5.11046600	2.48845200
C	5.25773900	0.76847200	-0.23992700
H	5.27766200	1.69419500	0.31487000
C	5.24881900	-1.63495800	-1.65554100
H	5.24816900	-2.56896700	-2.20454300
C	6.42700700	0.25209900	-0.72573000
H	7.36000100	0.77495900	-0.55785500
C	6.42487800	-0.95940900	-1.44145000
H	7.35626400	-1.35936000	-1.82233300

C5-GS2-*Z* – S_0 optimized geometry

0 1

N	0.22662000	-0.39452400	0.04090400
C	-2.35055300	-0.61541000	-0.37719000
C	1.80213800	-1.94720000	0.68871800
C	2.47404200	-0.88675700	-0.04208600
F	-0.74143600	0.89439700	2.41859900
C	0.43530600	-1.61604800	0.71418300
C	1.49716400	0.03476900	-0.39605600
C	-1.11069000	1.83486700	-0.26451200
C	-3.56522600	-0.34934400	0.29472700
C	-2.33765800	-1.65200900	-1.33892800
C	2.23233800	-3.11051100	1.33352400
H	3.27263900	-3.39942900	1.34037200
C	-3.49326000	-2.38601100	-1.58670200
H	-3.46381100	-3.16996500	-2.33670700
C	3.83413700	-0.67514300	-0.42152000
C	-4.68920800	-1.12506200	0.03350300
H	-5.60530900	-0.91834700	0.57741500
C	-4.67800400	-2.14854000	-0.90521400
C	-0.48737900	-2.39830200	1.40176400
H	-1.53000200	-2.12303300	1.44961500
F	1.14865300	1.86115100	2.02396800
B	-1.05093700	0.24962200	-0.16919100
C	1.80364000	1.18230100	-1.15893400
H	1.03712500	1.88374900	-1.44811400
C	-1.59657900	2.47065000	-1.42390100
C	-0.72855700	2.65408400	0.81152900
C	1.31102500	-3.90536500	1.98938700
H	1.64188500	-4.80706900	2.49007200
C	4.13834500	0.49507800	-1.16914600

C	-0.03741600	-3.54719800	2.02729900
H	-0.74432900	-4.17101700	2.56073300
C	-3.70525700	0.74163000	1.32880600
H	-4.71886300	0.75372100	1.72949800
H	-3.50312800	1.72629400	0.90465600
H	-3.01846100	0.60266300	2.16328500
F	-0.37654300	2.89198800	3.13866000
C	-1.11528400	-2.01594800	-2.15108500
H	-1.41015600	-2.57539200	-3.03925000
H	-0.43143800	-2.64624800	-1.57798400
H	-0.54862100	-1.14614000	-2.48180900
C	-5.91927600	-2.94602400	-1.19779300
H	-6.55119900	-2.42622800	-1.92369600
H	-6.51525600	-3.09643700	-0.29616800
H	-5.67403100	-3.92335400	-1.61543400
C	-2.01646200	1.68882400	-2.64352800
H	-2.26299900	2.36350800	-3.46313000
H	-2.88933100	1.06755500	-2.43966800
H	-1.22094800	1.02670600	-2.99232400
C	3.09797900	1.39689500	-1.52257500
H	3.35371000	2.27595000	-2.10287300
C	-0.81806500	4.03873600	0.75181100
H	-0.52810500	4.63615200	1.60513800
C	-0.17827700	2.07766200	2.08767900
C	-1.66782400	3.86053400	-1.47405100
H	-2.03310800	4.33446300	-2.37792500
C	-1.28717400	4.64486100	-0.39911100
H	-1.35836800	5.72379400	-0.45579300
C	4.89617300	-1.55537500	-0.10536600
H	4.70044500	-2.45547700	0.45639200
C	5.47367100	0.74292500	-1.56198600
H	5.68740900	1.64098200	-2.13084900
C	6.18042400	-1.28836100	-0.50046200
H	6.97483100	-1.97897400	-0.24370000
C	6.47810400	-0.12633100	-1.23628300
H	7.49767000	0.07405700	-1.54218000

C5-GS2-*Z* – S_1 optimized geometry

0 1

N	0.20597500	-0.31142900	0.08610900
C	-2.32293000	-0.68253500	-0.52138100
C	1.82192100	-1.66834200	1.02060400
C	2.42466400	-0.85433000	-0.01738000
F	-0.60184600	1.11801400	2.53223200
C	0.46262400	-1.29737200	1.06005200
C	1.36508700	-0.06636300	-0.55473200
C	-1.23778000	1.86761900	-0.18834800
C	-3.60009200	-0.48875700	0.07275000
C	-2.16368500	-1.83339400	-1.33576200
C	2.27368100	-2.65779000	1.88242400
H	3.30103700	-2.99179300	1.87965800
C	-3.21574700	-2.72224300	-1.52639800
H	-3.06041400	-3.58791100	-2.16374800
C	3.73034400	-0.72153000	-0.53715400
C	-4.62396600	-1.40408100	-0.14225800

H	-5.58159000	-1.23890400	0.34321300
C	-4.46022700	-2.53081400	-0.94062700
C	-0.43557900	-1.86921500	1.93232100
H	-1.47201000	-1.56547900	1.94364000
F	1.33813200	1.68265900	1.76178900
B	-1.15468000	0.31696600	-0.22801600
C	1.57120800	0.84282100	-1.62883500
H	0.74410200	1.42485400	-2.00757900
C	-1.96120900	2.55872600	-1.21385100
C	-0.58420800	2.70586300	0.76298200
C	1.37292500	-3.24726300	2.77267000
H	1.72200300	-4.01852200	3.44685800
C	3.92237200	0.19475100	-1.61573200
C	0.04415700	-2.85798800	2.79938600
H	-0.63837100	-3.32259600	3.49953500
C	-3.89084800	0.67442200	0.98990800
H	-4.82166400	0.50644600	1.53400700
H	-3.99306400	1.61434100	0.44153600
H	-3.08742300	0.82523300	1.71264700
F	0.21318900	3.06105600	2.96472100
C	-0.87314200	-2.11577700	-2.06127000
H	-1.02179900	-2.87453200	-2.83078600
H	-0.09610000	-2.48665700	-1.38732700
H	-0.48106500	-1.21682900	-2.54354000
C	-5.59688800	-3.48733900	-1.18136900
H	-6.24129300	-3.13812200	-1.99415800
H	-6.22426000	-3.59070800	-0.29370800
H	-5.23146100	-4.47796900	-1.45717700
C	-2.69756400	1.82282800	-2.30397300
H	-3.00732000	2.51690200	-3.08633400
H	-3.58902600	1.31409700	-1.93275700
H	-2.06925300	1.05002200	-2.75310700
C	2.81954000	0.95255800	-2.13613300
H	3.01620400	1.63363000	-2.95508000
C	-0.58237900	4.09430700	0.66526200
H	-0.07019600	4.68190400	1.41486900
C	0.07977200	2.14659200	1.98184200
C	-1.94736500	3.94247700	-1.28141100
H	-2.48172100	4.42765400	-2.09132300
C	-1.25387700	4.72407300	-0.36246200
H	-1.25129400	5.80354800	-0.44348800
C	4.84950900	-1.44176000	-0.05047700
H	4.72763600	-2.12970200	0.77214900
C	5.20726200	0.34642800	-2.15935900
H	5.34982100	1.04201900	-2.97756500
C	6.08953600	-1.27069900	-0.60372800
H	6.93462200	-1.82744700	-0.21943000
C	6.27184300	-0.37111400	-1.66799000
H	7.25643000	-0.24239200	-2.09978300

10.3 Delta-SCF calculated geometries for compound C2

S0 optimized geometries

GS1-conf1

N	0.624132	0.127466	0.041477
C	-1.850400	0.961213	-0.083325
C	2.672660	1.208616	0.000400
C	2.901670	-0.198257	-0.232300
F	-1.800590	-1.543671	-1.868785
C	1.280006	1.381045	0.152419
C	1.640464	-0.830840	-0.195558
C	-1.179860	-1.526971	0.888882
C	-1.839387	1.612367	-1.343675
C	-2.898324	1.272212	0.819567
C	3.546657	2.284245	0.112331
H	4.619796	2.158777	0.000132
C	-3.869502	2.208906	0.472552
H	-4.651401	2.450954	1.190361
C	4.061535	-0.923480	-0.478711
H	5.035999	-0.444611	-0.511281
C	-2.850397	2.520445	-1.665486
H	-2.834824	2.998652	-2.643648
C	-3.870503	2.837613	-0.772632
C	0.764154	2.633344	0.462433
H	-0.297232	2.788067	0.617692
F	-3.100478	-3.270400	-1.664701
B	-0.775977	-0.132767	0.248828
C	1.535489	-2.191495	-0.455825
H	0.577877	-2.697715	-0.479730
C	-0.649798	-1.862472	2.157936
C	-2.110259	-2.416841	0.321037
C	3.020086	3.545553	0.388008
C	3.955297	-2.297081	-0.697516
C	1.637464	3.714860	0.568164
H	1.224032	4.689162	0.800225
C	-0.768546	1.392847	-2.385587
H	-1.167923	1.596130	-3.383444
H	-0.358695	0.382129	-2.378746
H	0.070988	2.080753	-2.222772
F	-3.783450	-1.326733	-0.985007
C	-2.996541	0.635871	2.184422
H	-3.726451	1.167159	2.801344
H	-2.038765	0.644882	2.712452
H	-3.316465	-0.410053	2.113034
C	-4.959190	3.804180	-1.147611
H	-5.836568	3.265559	-1.527519
H	-4.629475	4.491389	-1.932035
H	-5.286940	4.388170	-0.282085
C	0.369275	-0.998862	2.860008
H	0.403638	-1.242711	3.925043
H	0.160906	0.070400	2.760538
H	1.371244	-1.166412	2.445294
C	2.698310	-2.923684	-0.692826
H	2.607314	-3.985873	-0.886450
C	-2.520279	-3.581714	0.966880
H	-3.232914	-4.249725	0.495268
C	-2.694498	-2.139236	-1.036157
C	-1.075837	-3.026647	2.801192
H	-0.669683	-3.264287	3.781472
C	-2.002718	-3.881784	2.219077

H	-2.318569	-4.782757	2.736677
O	5.133406	-2.951840	-0.924766
O	3.931550	4.560670	0.478655
C	3.441174	5.871003	0.779093
H	2.942240	5.893892	1.756093
H	4.320147	6.516800	0.804037
H	2.749602	6.223754	0.003741
C	5.076826	-4.361174	-1.166750
H	4.491459	-4.586489	-2.066983
H	6.110409	-4.676794	-1.316111
H	4.651561	-4.894567	-0.307366

GS1-conf2

N	0.587281	0.005917	0.031937
C	-1.787544	1.091436	-0.072305
C	2.735497	0.868614	0.016742
C	2.816930	-0.548973	-0.240227
F	-2.005636	-1.365585	-1.917152
C	1.367161	1.183167	0.168425
C	1.501303	-1.045358	-0.220799
C	-1.380237	-1.472759	0.843848
C	-1.712148	1.758446	-1.321823
C	-2.794619	1.494193	0.840418
C	3.715840	1.846766	0.146979
H	4.770794	1.613394	0.034551
C	-3.664167	2.532305	0.512628
H	-4.414290	2.842855	1.237938
C	3.909302	-1.383857	-0.494626
H	4.913104	-0.974604	-0.504680
C	-2.625157	2.770272	-1.625540
H	-2.563133	3.259565	-2.596362
C	-3.604449	3.176824	-0.722995
C	0.982598	2.476944	0.497436
H	-0.057616	2.738503	0.652566
F	-3.493993	-2.936017	-1.737294
B	-0.832418	-0.114296	0.235677
C	1.254003	-2.387260	-0.512087
H	0.248611	-2.788940	-0.553344
C	-0.887522	-1.894347	2.102393
C	-2.401565	-2.243954	0.257835
C	3.321286	3.151232	0.440944
C	3.655728	-2.730476	-0.738981
C	1.962874	3.460268	0.621727
H	1.652089	4.468534	0.868160
C	-0.669763	1.448354	-2.369920
H	-1.052115	1.694694	-3.364806
H	-0.354115	0.404447	-2.371552
H	0.229145	2.056156	-2.205147
F	-3.945426	-0.942425	-1.011645
C	-2.954541	0.848350	2.194553
H	-3.619154	1.444792	2.825524
H	-1.999162	0.743057	2.716591
H	-3.387034	-0.155159	2.107788
C	-4.589028	4.255762	-1.078922
H	-5.505896	3.817021	-1.492574
H	-4.180660	4.935239	-1.832566

H	-4.876045	4.837573	-0.197757
C	0.219020	-1.163318	2.822221
H	0.226867	-1.435173	3.880939
H	0.128631	-0.075605	2.748800
H	1.196940	-1.428357	2.400823
C	2.335435	-3.219172	-0.754840
H	2.175882	-4.270208	-0.976004
C	-2.933410	-3.373305	0.876933
H	-3.714197	-3.949475	0.392369
C	-2.956624	-1.872751	-1.089626
C	-1.436128	-3.021328	2.719002
H	-1.057348	-3.324518	3.692174
C	-2.449819	-3.757535	2.119795
H	-2.859785	-4.631729	2.616891
O	4.619999	-3.664276	-0.992259
O	4.332260	4.065848	0.548146
C	3.978157	5.414669	0.869095
H	3.479262	5.472467	1.844639
H	4.918809	5.965984	0.907722
H	3.330246	5.849392	0.097617
C	5.979768	-3.219061	-0.993980
H	6.259482	-2.801625	-0.018442
H	6.582612	-4.104576	-1.199835
H	6.149281	-2.468954	-1.776939

GS1-conf3

N	0.577012	0.131537	0.094159
C	-1.841512	1.110526	-0.047200
C	2.676406	1.102719	0.065713
C	2.831357	-0.307932	-0.195254
F	-1.905170	-1.349464	-1.896054
C	1.300410	1.343601	0.228559
C	1.538593	-0.875290	-0.165327
C	-1.336481	-1.434193	0.873251
C	-1.773482	1.783734	-1.293831
C	-2.882254	1.465676	0.847738
C	3.618844	2.128843	0.189254
H	4.673235	1.913219	0.059373
C	-3.791240	2.464623	0.506401
H	-4.567204	2.739523	1.218814
C	3.950864	-1.088104	-0.462611
H	4.949238	-0.660987	-0.491422
C	-2.725245	2.754995	-1.611741
H	-2.667438	3.249503	-2.580161
C	-3.737700	3.115084	-0.726564
C	0.849528	2.619204	0.570424
H	-0.201057	2.825699	0.738078
F	-3.309778	-2.998470	-1.754770
B	-0.838820	-0.051743	0.276240
C	1.361429	-2.222955	-0.452381
H	0.378349	-2.677506	-0.481935
C	-0.851207	-1.833607	2.141851
C	-2.311067	-2.249270	0.267859
C	3.155141	3.405328	0.491411
C	3.771451	-2.449063	-0.709562
C	1.780532	3.638636	0.687431

H	1.458426	4.643789	0.942622
C	-0.701270	1.523200	-2.325154
H	-1.079276	1.752096	-3.325864
H	-0.337230	0.495199	-2.322152
H	0.165978	2.171969	-2.147365
F	-3.889110	-1.032165	-1.044611
C	-3.036067	0.811473	2.198699
H	-3.740633	1.374279	2.817081
H	-2.086501	0.752770	2.738333
H	-3.417118	-0.211927	2.103696
C	-4.762136	4.151245	-1.096565
H	-5.666509	3.672500	-1.492955
H	-4.383410	4.829373	-1.866597
H	-5.062895	4.740567	-0.224852
C	0.211573	-1.057021	2.879712
H	0.214847	-1.329952	3.938179
H	0.075899	0.025846	2.805878
H	1.206038	-1.279492	2.472837
C	2.483331	-3.009606	-0.710555
H	2.336290	-4.061300	-0.925474
C	-2.807868	-3.398962	0.878802
H	-3.553244	-4.008364	0.379236
C	-2.849567	-1.907155	-1.093799
C	-1.364456	-2.981467	2.750006
H	-0.992696	-3.267308	3.731085
C	-2.334949	-3.760020	2.132603
H	-2.718663	-4.649357	2.623796
O	4.912218	-3.160289	-0.958327
O	3.954536	4.503953	0.634823
C	5.361177	4.319135	0.449815
H	5.582014	3.958220	-0.562746
H	5.812307	5.301737	0.594631
H	5.767984	3.615687	1.187379
C	4.778157	-4.556896	-1.240148
H	4.174515	-4.723483	-2.141022
H	5.792036	-4.923123	-1.407971
H	4.331203	-5.091890	-0.392812

GS1-conf4

N	0.531676	0.048729	0.057414
C	-1.834034	1.153167	-0.043922
C	2.680429	0.901049	0.066606
C	2.757610	-0.509559	-0.221918
F	-2.052465	-1.266196	-1.941078
C	1.317897	1.216579	0.222075
C	1.439479	-1.001758	-0.216027
C	-1.451581	-1.432855	0.823300
C	-1.740175	1.847053	-1.277231
C	-2.846744	1.544553	0.867891
C	3.677424	1.870796	0.220614
H	4.719740	1.600076	0.096379
C	-3.702338	2.598541	0.555610
H	-4.456583	2.900061	1.280467
C	3.847009	-1.344307	-0.492299
H	4.852983	-0.940231	-0.491494
C	-2.640344	2.874670	-1.566659

H	-2.564211	3.384933	-2.525578
C	-3.623698	3.270873	-0.664275
C	0.935553	2.508558	0.584712
H	-0.103657	2.770705	0.745117
F	-3.556795	-2.825852	-1.804492
B	-0.891160	-0.065646	0.247480
C	1.187113	-2.336082	-0.535871
H	0.180199	-2.732910	-0.586471
C	-0.970522	-1.884121	2.075863
C	-2.471651	-2.186051	0.212124
C	3.282458	3.164330	0.546036
C	3.587810	-2.683931	-0.766180
C	1.920873	3.471374	0.732182
H	1.652991	4.487916	1.004266
C	-0.692326	1.549544	-2.323609
H	-1.067986	1.813036	-3.316684
H	-0.380710	0.504602	-2.340037
H	0.207822	2.151557	-2.144694
F	-3.994477	-0.843835	-1.039853
C	-3.027502	0.868773	2.204694
H	-3.693995	1.456479	2.841846
H	-2.079326	0.742421	2.735153
H	-3.468051	-0.128330	2.089417
C	-4.593067	4.368963	-1.002893
H	-5.525395	3.948650	-1.400740
H	-4.184040	5.041663	-1.762082
H	-4.853842	4.954848	-0.116167
C	0.132896	-1.173702	2.820830
H	0.129346	-1.467332	3.873744
H	0.048637	-0.084260	2.769164
H	1.113381	-1.435291	2.403317
C	2.265491	-3.167131	-0.794609
H	2.102239	-4.212718	-1.037717
C	-3.012831	-3.326636	0.801533
H	-3.792340	-3.888549	0.298538
C	-3.014160	-1.781660	-1.130915
C	-1.528444	-3.022398	2.662689
H	-1.158806	-3.349146	3.631767
C	-2.540233	-3.740673	2.039093
H	-2.957551	-4.624093	2.513235
O	4.548668	-3.616413	-1.037760
O	4.140459	4.213059	0.722955
C	5.537226	3.953030	0.554972
H	5.754271	3.604461	-0.462757
H	6.040758	4.904557	0.731133
H	5.890822	3.209801	1.280823
C	5.910306	-3.177690	-1.025928
H	6.189256	-2.783301	-0.040587
H	6.509756	-4.061168	-1.249755
H	6.085655	-2.411205	-1.791588

GS2-conf1

N	-0.289735	0.247573	-0.178754
C	2.250842	-0.252893	-0.520795
C	-1.451922	2.241604	0.009062
C	-2.375640	1.221734	-0.429092

F	0.349211	-0.588059	2.474434
C	-0.191988	1.621668	0.147615
C	-1.645885	0.016631	-0.523018
C	0.438261	-2.224449	0.127044
C	3.384115	-0.669407	0.222712
C	2.469431	0.522348	-1.690526
C	-1.624163	3.588495	0.308924
H	-2.590358	4.074970	0.210077
C	3.768050	0.872698	-2.062009
H	3.916111	1.456565	-2.969043
C	-3.727894	1.269506	-0.748282
H	-4.295869	2.192870	-0.678699
C	4.663490	-0.277293	-0.170516
H	5.517842	-0.589377	0.427644
C	4.878718	0.494520	-1.311062
C	0.891513	2.340869	0.635588
H	1.859294	1.876734	0.787613
F	-1.742078	-1.176265	2.335070
B	0.790345	-0.706681	-0.164581
C	-2.266733	-1.137579	-0.983951
H	-1.728408	-2.070650	-1.101219
C	0.719414	-3.217913	-0.837850
C	-0.145460	-2.642238	1.339484
C	-0.523637	4.317178	0.759088
C	-4.355099	0.099060	-1.173971
C	0.723925	3.693278	0.928236
H	1.575629	4.250158	1.300276
C	3.265966	-1.503286	1.474006
H	2.717423	-2.432096	1.290183
H	2.733574	-0.966905	2.265321
H	4.257576	-1.762972	1.853818
F	-0.395763	-2.238350	3.666404
C	1.353258	0.986110	-2.597543
H	1.750762	1.227693	-3.587164
H	0.874112	1.890856	-2.203760
H	0.565083	0.238660	-2.720891
C	6.270291	0.867949	-1.740314
H	6.710993	0.070962	-2.352513
H	6.925461	1.014414	-0.876345
H	6.269519	1.781900	-2.341264
C	1.335064	-2.864530	-2.167319
H	1.344239	-3.733175	-2.830592
H	2.364804	-2.511731	-2.046300
H	0.779044	-2.063772	-2.667439
C	-3.624784	-1.093966	-1.297585
H	-4.101335	-2.002477	-1.646231
C	-0.461365	-3.977970	1.586357
H	-0.906943	-4.270285	2.531348
C	-0.476445	-1.664585	2.439041
C	0.391560	-4.550729	-0.582780
H	0.600700	-5.300271	-1.342148
C	-0.195902	-4.933896	0.616603
H	-0.441981	-5.975825	0.798740
O	-0.758576	5.637302	1.027769
O	-5.687136	0.212445	-1.463004
C	0.336097	6.425365	1.505181
H	1.152437	6.456199	0.772626

H	-0.063512	7.430513	1.647570
H	0.713951	6.042801	2.461695
C	-6.376573	-0.964404	-1.894669
H	-6.339763	-1.748842	-1.128330
H	-7.411788	-0.659061	-2.054126
H	-5.959563	-1.347888	-2.834478

GS2-conf2

N	-0.322971	0.060615	-0.180610
C	2.231687	0.486772	-0.495912
C	-2.104193	1.523795	0.017199
C	-2.608184	0.262511	-0.470122
F	0.566686	-0.585514	2.470320
C	-0.710068	1.373183	0.178357
C	-1.509295	-0.610494	-0.568392
C	1.217524	-2.012986	0.074830
C	3.431915	0.484945	0.258490
C	2.170413	1.312881	-1.649405
C	-2.736663	2.719144	0.343609
H	-3.809377	2.846534	0.229001
C	3.263560	2.107773	-1.995993
H	3.202738	2.723968	-2.891674
C	-3.898033	-0.142339	-0.828313
H	-4.725973	0.552130	-0.742213
C	4.492920	1.311956	-0.109781
H	5.397466	1.311152	0.496023
C	4.430018	2.132424	-1.234844
C	0.049435	2.405837	0.712815
H	1.114981	2.298246	0.881525
F	-1.218059	-1.810409	2.231097
B	1.021459	-0.459680	-0.172123
C	-1.683465	-1.899124	-1.074096
H	-0.854275	-2.586314	-1.193966
C	1.840706	-2.818100	-0.905126
C	0.798856	-2.642630	1.264335
C	-1.963927	3.767326	0.842337
C	-4.066503	-1.441215	-1.298144
C	-0.580545	3.607492	1.031956
H	0.019117	4.412012	1.440617
C	3.601960	-0.356120	1.498686
H	3.378154	-1.409893	1.307879
H	2.933179	-0.025746	2.299563
H	4.627991	-0.287114	1.869670
F	0.355912	-2.431172	3.589040
C	0.969914	1.369347	-2.565583
H	1.266320	1.744785	-3.548918
H	0.203126	2.047060	-2.170351
H	0.491304	0.396426	-2.703536
C	5.602202	2.982468	-1.639012
H	6.305101	2.402941	-2.250760
H	6.152095	3.341798	-0.763927
H	5.282118	3.843689	-2.232547
C	2.310536	-2.236195	-2.213462
H	2.632529	-3.028586	-2.893855
H	3.149204	-1.547994	-2.063383
H	1.515294	-1.668799	-2.709188

C	-2.961872	-2.304503	-1.423675
H	-3.129019	-3.305023	-1.811178
C	0.966601	-4.010599	1.475202
H	0.637986	-4.466732	2.402961
C	0.133395	-1.868753	2.374528
C	1.996434	-4.188223	-0.685670
H	2.464915	-4.796216	-1.455744
C	1.563785	-4.785713	0.491447
H	1.695577	-5.852555	0.645773
O	-2.645240	4.916271	1.136112
O	-5.265187	-1.976223	-1.679100
C	-1.900280	6.014428	1.670860
H	-1.128952	6.352000	0.967254
H	-2.625007	6.814773	1.827682
H	-1.434494	5.750019	2.628593
C	-6.418086	-1.135073	-1.581395
H	-6.317347	-0.250030	-2.222438
H	-7.258628	-1.740410	-1.923658
H	-6.590287	-0.819405	-0.544499

GS2-conf3

N	-0.282594	0.165308	-0.146685
C	2.285552	0.501546	-0.472201
C	-2.007289	1.691200	0.061434
C	-2.562624	0.449533	-0.419995
F	0.593018	-0.503023	2.498624
C	-0.624162	1.490011	0.212919
C	-1.493225	-0.467318	-0.525260
C	1.187064	-1.959699	0.102580
C	3.492799	0.440588	0.269810
C	2.245622	1.349912	-1.610388
C	-2.607011	2.911631	0.389596
H	-3.676388	3.039850	0.266803
C	3.361831	2.115999	-1.948589
H	3.315419	2.751119	-2.831825
C	-3.858842	0.082410	-0.765384
H	-4.687650	0.780371	-0.687509
C	4.576527	1.241967	-0.088040
H	5.485176	1.198064	0.509930
C	4.532157	2.089490	-1.194064
C	0.178890	2.497984	0.747060
H	1.240475	2.351830	0.911207
F	-1.217271	-1.694196	2.286674
B	1.043362	-0.401120	-0.145806
C	-1.718311	-1.745217	-1.021194
H	-0.915318	-2.462283	-1.144121
C	1.768733	-2.785996	-0.885108
C	0.769062	-2.572365	1.300611
C	-1.791254	3.925389	0.882606
C	-4.084791	-1.213384	-1.228060
C	-0.411197	3.710390	1.064961
H	0.187495	4.518057	1.475302
C	3.653167	-0.447137	1.478752
H	3.459545	-1.496544	1.235454
H	2.959993	-0.170122	2.278279
H	4.669336	-0.372263	1.874776

F	0.360525	-2.338589	3.629571
C	1.044691	1.461878	-2.521005
H	1.353954	1.826517	-3.504512
H	0.310437	2.172665	-2.121975
H	0.523033	0.511559	-2.659406
C	5.727378	2.912516	-1.585985
H	6.410962	2.324798	-2.211653
H	6.290386	3.237883	-0.705972
H	5.431098	3.794560	-2.161023
C	2.225500	-2.220603	-2.205215
H	2.524463	-3.021977	-2.885609
H	3.075630	-1.542637	-2.074496
H	1.428555	-1.646051	-2.690613
C	-3.018394	-2.117669	-1.360973
H	-3.184847	-3.120353	-1.736308
C	0.903548	-3.943679	1.515057
H	0.577015	-4.387121	2.449704
C	0.134580	-1.778280	2.414708
C	1.891904	-4.158613	-0.662004
H	2.330205	-4.782503	-1.437127
C	1.464877	-4.738629	0.526068
H	1.571990	-5.807683	0.684145
O	-2.233842	5.168178	1.238689
O	-5.382531	-1.512112	-1.541471
C	-3.630810	5.435158	1.084378
H	-4.233084	4.762408	1.708023
H	-3.775336	6.465332	1.412928
H	-3.938193	5.336712	0.035482
C	-5.666123	-2.831813	-2.015253
H	-5.398288	-3.588342	-1.266906
H	-6.742663	-2.858243	-2.190550
H	-5.137837	-3.039971	-2.954282

GS2-conf4

N	-0.271520	0.069859	-0.192048
C	2.204900	0.851187	-0.460252
C	-2.238460	1.251407	0.078407
C	-2.564055	-0.047811	-0.455145
F	0.653506	-0.542625	2.444046
C	-0.839726	1.296418	0.222240
C	-1.351984	-0.748442	-0.601018
C	1.539003	-1.779957	0.013075
C	3.396096	0.966370	0.300604
C	2.034576	1.723401	-1.568240
C	-3.044226	2.331699	0.456038
H	-4.120319	2.272892	0.338321
C	3.010347	2.677199	-1.860782
H	2.867847	3.328664	-2.721458
C	-3.787413	-0.623080	-0.816060
H	-4.707115	-0.062756	-0.691263
C	4.333894	1.950331	-0.010692
H	5.229980	2.037870	0.601139
C	4.160766	2.817658	-1.088313
C	-0.226340	2.409517	0.797208
H	0.845324	2.449567	0.955483
F	-0.920278	-2.017582	2.147644

B	1.132382	-0.261716	-0.187743
C	-1.344044	-2.025036	-1.163284
H	-0.424789	-2.575917	-1.324121
C	2.279888	-2.454259	-0.983712
C	1.204285	-2.502298	1.176041
C	-2.418984	3.454256	0.989756
C	-3.771912	-1.912622	-1.338125
C	-1.021394	3.482875	1.164016
H	-0.574118	4.367935	1.606381
C	3.690808	0.072235	1.479174
H	3.718182	-0.982040	1.185709
H	2.931745	0.167585	2.260667
H	4.659260	0.327363	1.917242
F	0.723458	-2.434087	3.501464
C	0.841351	1.665576	-2.493818
H	1.091384	2.124753	-3.454292
H	-0.010676	2.216544	-2.077074
H	0.497423	0.645628	-2.684062
C	5.206645	3.841246	-1.432242
H	5.983376	3.398760	-2.068793
H	5.700741	4.221326	-0.533005
H	4.773993	4.683703	-1.979505
C	2.680140	-1.763142	-2.261956
H	3.110860	-2.478102	-2.967548
H	3.419231	-0.977842	-2.070480
H	1.822172	-1.285187	-2.747147
C	-2.555396	-2.598589	-1.515814
H	-2.582058	-3.595765	-1.944768
C	1.563980	-3.839097	1.344207
H	1.295669	-4.368860	2.252008
C	0.423541	-1.873229	2.302811
C	2.626796	-3.795030	-0.807664
H	3.183801	-4.303507	-1.590783
C	2.273372	-4.487573	0.343665
H	2.554057	-5.529623	0.464988
O	-3.073019	4.583865	1.394752
O	-4.886408	-2.603464	-1.724868
C	-4.496009	4.605111	1.252058
H	-4.965468	3.813683	1.850143
H	-4.817871	5.580399	1.619931
H	-4.789702	4.493462	0.200498
C	-6.149626	-1.953469	-1.560205
H	-6.205081	-1.037178	-2.161805
H	-6.899035	-2.665151	-1.909434
H	-6.334929	-1.711697	-0.505848

T_1 optimized geometries

GS1-conf1

N	0.636813	0.101614	0.200083
C	-1.844216	0.822230	-0.227609
C	2.633138	1.237058	0.111064
C	2.860854	-0.127402	-0.334130
F	-2.123343	-1.953722	-1.511761
C	1.247932	1.314986	0.427116
C	1.596175	-0.775909	-0.258035
C	-1.180041	-1.487128	1.212735
C	-1.646046	1.380256	-1.520729
C	-2.955577	1.302762	0.524096
C	3.446268	2.333713	0.268407
H	4.508164	2.310713	0.042305
C	-3.795340	2.281945	-0.000901
H	-4.626067	2.644660	0.603924
C	3.968800	-0.809622	-0.776394
H	4.947885	-0.345962	-0.852337
C	-2.513026	2.356790	-2.015278
H	-2.344144	2.754838	-3.015514
C	-3.597565	2.823797	-1.274128
C	0.678428	2.495969	0.911749
H	-0.377577	2.542660	1.155316
F	-3.531451	-3.455109	-0.843360
B	-0.850614	-0.206070	0.399453
C	1.443967	-2.112923	-0.633933
H	0.476583	-2.600076	-0.578078
C	-0.471889	-1.805520	2.417213
C	-2.203437	-2.414522	0.836057
C	2.865324	3.532755	0.747176
C	3.814251	-2.166525	-1.148062
C	1.497900	3.607025	1.067026
H	1.067655	4.529164	1.438124
C	-0.526691	0.914357	-2.418151
H	-0.734644	1.173940	-3.460576
H	-0.386989	-0.169677	-2.351623
H	0.432555	1.378573	-2.152807
F	-3.940740	-1.364768	-0.459407
C	-3.230894	0.807204	1.920259
H	-3.988682	1.426938	2.409365
H	-2.318269	0.816463	2.528490
H	-3.587848	-0.229007	1.919700
C	-4.543524	3.852087	-1.833244
H	-5.435626	3.375327	-2.260012
H	-4.071394	4.436365	-2.628925
H	-4.888018	4.540412	-1.054341
C	0.589527	-0.887271	2.966274
H	0.799892	-1.127637	4.012158
H	0.269003	0.160344	2.907019
H	1.534951	-0.963627	2.414894
C	2.563469	-2.805153	-1.078756
H	2.456521	-3.843149	-1.369161
C	-2.534581	-3.522125	1.617684
H	-3.321368	-4.197558	1.299573
C	-2.933499	-2.285797	-0.471607
C	-0.809236	-2.924569	3.170909

H	-0.270957	-3.115015	4.097367
C	-1.842970	-3.782712	2.792348
H	-2.101808	-4.642249	3.403174
O	4.949591	-2.766217	-1.561809
O	3.727478	4.563314	0.863733
C	3.229484	5.825177	1.341402
H	2.831409	5.724723	2.357172
H	4.089938	6.494127	1.344451
H	2.456100	6.214583	0.670249
C	4.889190	-4.145001	-1.966184
H	4.215189	-4.267948	-2.821176
H	5.906881	-4.407712	-2.254537
H	4.561682	-4.778046	-1.134121

GS1-conf2

N	0.589811	-0.025024	0.174192
C	-1.799336	0.960803	-0.241492
C	2.694561	0.894346	0.137401
C	2.779590	-0.468582	-0.359133
F	-2.346731	-1.772352	-1.587121
C	1.323857	1.108422	0.450910
C	1.455031	-0.979675	-0.313938
C	-1.383817	-1.438505	1.148792
C	-1.533497	1.532878	-1.516763
C	-2.859094	1.535152	0.519090
C	3.618427	1.890647	0.342192
H	4.673974	1.765085	0.119593
C	-3.584549	2.614841	0.020917
H	-4.375936	3.045795	0.633547
C	3.825866	-1.243126	-0.820455
H	4.834412	-0.847496	-0.855571
C	-2.286415	2.611372	-1.984542
H	-2.067945	3.018684	-2.971416
C	-3.320009	3.170648	-1.233837
C	0.880168	2.321917	0.980882
H	-0.167028	2.471756	1.221549
F	-3.918707	-3.116465	-0.946548
B	-0.923123	-0.181748	0.361156
C	1.163920	-2.281523	-0.744057
H	0.149902	-2.664457	-0.711819
C	-0.717927	-1.848013	2.350033
C	-2.493326	-2.251573	0.752318
C	3.164951	3.125715	0.868764
C	3.527783	-2.555030	-1.243962
C	1.811864	3.333266	1.185437
H	1.478673	4.280215	1.591911
C	-0.463447	0.976282	-2.422463
H	-0.637659	1.282206	-3.458536
H	-0.437434	-0.117757	-2.383315
H	0.537142	1.332248	-2.142414
F	-4.094805	-0.998241	-0.537899
C	-3.197853	1.029202	1.897355
H	-3.876379	1.719281	2.408235
H	-2.293211	0.904102	2.504586
H	-3.679280	0.044989	1.860530
C	-4.146026	4.309978	-1.766995

H	-5.053761	3.940034	-2.261608
H	-3.588555	4.895983	-2.504333
H	-4.467188	4.979409	-0.962267
C	0.427232	-1.051423	2.921045
H	0.617080	-1.343292	3.957673
H	0.205639	0.022987	2.896867
H	1.359600	-1.197058	2.362051
C	2.208481	-3.056892	-1.205056
H	2.036654	-4.072617	-1.546696
C	-2.938040	-3.334441	1.512536
H	-3.786861	-3.921475	1.178946
C	-3.196865	-2.026234	-0.556477
C	-1.170325	-2.940082	3.082426
H	-0.658631	-3.200424	4.006868
C	-2.282702	-3.683558	2.684802
H	-2.630006	-4.523447	3.278842
O	4.452334	-3.419276	-1.709813
O	4.133018	4.050247	1.031695
C	3.770253	5.337703	1.560720
H	3.351937	5.237641	2.568365
H	4.698412	5.907723	1.598624
H	3.051329	5.837096	0.901910
C	5.823510	-2.990145	-1.776240
H	6.198138	-2.735078	-0.778697
H	6.375364	-3.842538	-2.172147
H	5.929008	-2.133043	-2.450354

GS1-conf3

N	0.576292	0.093790	0.229936
C	-1.853130	0.971191	-0.198431
C	2.636346	1.108124	0.212005
C	2.788880	-0.248610	-0.285038
F	-2.280224	-1.768373	-1.561800
C	1.256033	1.256432	0.513046
C	1.487892	-0.822952	-0.252026
C	-1.338180	-1.414651	1.181201
C	-1.607209	1.557809	-1.470412
C	-2.939940	1.495917	0.559627
C	3.525010	2.143758	0.422430
H	4.578356	2.025142	0.195649
C	-3.710456	2.543717	0.061287
H	-4.522774	2.937795	0.671394
C	3.861129	-0.979241	-0.737747
H	4.868002	-0.574392	-0.780154
C	-2.405124	2.603635	-1.938652
H	-2.200595	3.023400	-2.923246
C	-3.465293	3.114310	-1.190837
C	0.751418	2.452091	1.044595
H	-0.302973	2.554949	1.277881
F	-3.792244	-3.185527	-0.935372
B	-0.929375	-0.133413	0.405199
C	1.262173	-2.131660	-0.681862
H	0.266344	-2.560756	-0.657914
C	-0.658474	-1.804711	2.381478
C	-2.409461	-2.273060	0.774042
C	3.009537	3.348237	0.945965

C	3.631947	-2.310453	-1.164886
C	1.638131	3.488872	1.252547
H	1.299040	4.436637	1.658334
C	-0.509509	1.051606	-2.372757
H	-0.693729	1.350040	-3.409276
H	-0.433415	-0.040080	-2.333965
H	0.472579	1.452959	-2.088783
F	-4.062157	-1.080830	-0.509205
C	-3.262202	0.971120	1.934854
H	-3.976382	1.626492	2.442779
H	-2.356800	0.888643	2.548160
H	-3.694989	-0.035147	1.893041
C	-4.338049	4.219023	-1.722516
H	-5.249380	3.814232	-2.181823
H	-3.818337	4.804600	-2.487094
H	-4.654434	4.896120	-0.922139
C	0.446920	-0.962015	2.964361
H	0.639526	-1.248074	4.002118
H	0.181241	0.102211	2.940247
H	1.389702	-1.068098	2.413512
C	2.345335	-2.874226	-1.138980
H	2.180726	-3.891755	-1.471693
C	-2.806435	-3.381949	1.522766
H	-3.626904	-4.003862	1.181496
C	-3.119811	-2.067830	-0.534366
C	-1.062544	-2.923238	3.101950
H	-0.542942	-3.168202	4.026238
C	-2.138828	-3.712771	2.693601
H	-2.449436	-4.573199	3.278481
O	4.737726	-2.959482	-1.583345
O	3.763063	4.438276	1.194024
C	5.172396	4.379991	0.911469
H	5.345980	4.188875	-0.153204
H	5.562867	5.361398	1.180164
H	5.657246	3.607588	1.518612
C	4.606044	-4.318975	-2.033770
H	3.944130	-4.375515	-2.905091
H	5.612620	-4.631608	-2.311048
H	4.224769	-4.957198	-1.229065

GS1-conf4

N	0.537573	0.006322	0.214684
C	-1.840141	1.029831	-0.186250
C	2.648732	0.906074	0.231218
C	2.726732	-0.439092	-0.313491
F	-2.399350	-1.633930	-1.650102
C	1.279713	1.119965	0.540381
C	1.398167	-0.939487	-0.301511
C	-1.462653	-1.425884	1.108597
C	-1.563114	1.645541	-1.438220
C	-2.902624	1.581319	0.587395
C	3.591577	1.884830	0.472469
H	4.636686	1.719141	0.237115
C	-3.621204	2.680144	0.122508
H	-4.415495	3.092271	0.744316
C	3.770962	-1.207101	-0.789056

H	4.784034	-0.821332	-0.797209
C	-2.309483	2.742194	-1.873186
H	-2.082855	3.183095	-2.843595
C	-3.346871	3.277953	-1.110635
C	0.841511	2.321253	1.113544
H	-0.205663	2.472498	1.353432
F	-3.992948	-2.985151	-1.082804
B	-0.978841	-0.142497	0.380685
C	1.100178	-2.220606	-0.782718
H	0.082253	-2.594732	-0.776774
C	-0.816742	-1.895581	2.299114
C	-2.578358	-2.207065	0.666194
C	3.142699	3.099024	1.037807
C	3.466234	-2.501939	-1.262830
C	1.782741	3.302618	1.354176
H	1.495182	4.252556	1.793131
C	-0.487127	1.118276	-2.354405
H	-0.648454	1.465530	-3.379477
H	-0.467857	0.023444	-2.358112
H	0.512287	1.456825	-2.049835
F	-4.151277	-0.883976	-0.589238
C	-3.253406	1.027759	1.944267
H	-3.930084	1.703836	2.475891
H	-2.353359	0.874467	2.551893
H	-3.741895	0.049176	1.869086
C	-4.166814	4.437113	-1.609153
H	-5.087342	4.087632	-2.094885
H	-3.613864	5.029800	-2.344433
H	-4.466620	5.095477	-0.787095
C	0.333069	-1.140519	2.915059
H	0.508035	-1.479032	3.940103
H	0.127328	-0.062948	2.934986
H	1.269019	-1.276470	2.359380
C	2.142865	-2.990853	-1.259256
H	1.964679	-3.991445	-1.639842
C	-3.046611	-3.314150	1.375817
H	-3.899182	-3.874456	1.007656
C	-3.264187	-1.919838	-0.639768
C	-1.292491	-3.010673	2.980019
H	-0.795021	-3.315540	3.898590
C	-2.410487	-3.721411	2.539705
H	-2.776300	-4.580154	3.094351
O	4.390291	-3.357127	-1.745210
O	3.956173	4.136824	1.317169
C	5.359422	4.011751	1.025521
H	5.518844	3.849976	-0.046189
H	5.803657	4.960223	1.326953
H	5.803345	3.193070	1.602407
C	5.766553	-2.940259	-1.775380
H	6.127622	-2.723229	-0.763982
H	6.316091	-3.784611	-2.191197
H	5.891656	-2.062341	-2.418611

GS2-conf1

N	-0.306373	0.237221	-0.138901
C	2.167690	-0.327405	-0.781898

C	-1.429257	2.222167	0.147171
C	-2.330948	1.270661	-0.479470
F	0.254547	-0.405360	2.634842
C	-0.200479	1.528565	0.331232
C	-1.582307	0.071413	-0.633690
C	0.474074	-2.212993	0.393441
C	3.402464	-0.646094	-0.144900
C	2.234275	0.481832	-1.951196
C	-1.555759	3.531888	0.544628
H	-2.478264	4.092068	0.423830
C	3.459413	0.950311	-2.426249
H	3.476739	1.558231	-3.330414
C	-3.636406	1.336168	-0.904457
H	-4.238233	2.234557	-0.804012
C	4.607246	-0.157828	-0.649664
H	5.533051	-0.400152	-0.128521
C	4.663340	0.646386	-1.789993
C	0.903437	2.152725	0.916425
H	1.834464	1.613877	1.055705
F	-1.851328	-0.693547	2.150652
B	0.810152	-0.811414	-0.179828
C	-2.143634	-1.062876	-1.223356
H	-1.564359	-1.973695	-1.334742
C	0.907543	-3.383637	-0.315340
C	-0.320326	-2.462454	1.559230
C	-0.435344	4.162947	1.133862
C	-4.205516	0.184341	-1.496146
C	0.779259	3.476508	1.316120
H	1.629325	3.969822	1.771260
C	3.448780	-1.473150	1.114941
H	3.221018	-2.528758	0.922155
H	2.703915	-1.128955	1.840163
H	4.440960	-1.422585	1.573792
F	-0.939514	-1.816353	3.763120
C	0.998868	0.809324	-2.752019
H	1.268656	1.136479	-3.760560
H	0.408304	1.613981	-2.295314
H	0.340518	-0.063899	-2.834332
C	5.979102	1.133584	-2.333843
H	6.437043	0.381568	-2.989765
H	6.692385	1.336406	-1.528318
H	5.852261	2.046918	-2.923188
C	1.730028	-3.277978	-1.573248
H	1.800582	-4.251539	-2.066809
H	2.746414	-2.919653	-1.376262
H	1.285073	-2.555902	-2.268911
C	-3.461935	-0.999301	-1.655353
H	-3.908033	-1.874829	-2.111043
C	-0.722755	-3.745950	1.935141
H	-1.332292	-3.886458	2.821861
C	-0.703490	-1.359610	2.501840
C	0.507428	-4.651899	0.089253
H	0.830357	-5.512691	-0.492868
C	-0.320497	-4.848889	1.197536
H	-0.634162	-5.847747	1.485133
O	-0.640922	5.446821	1.493253
O	-5.490691	0.328897	-1.879563

C	0.437217	6.167187	2.114988
H	1.295542	6.240314	1.437921
H	0.041134	7.161579	2.320506
H	0.736096	5.683330	3.051427
C	-6.152963	-0.787664	-2.498091
H	-6.197361	-1.640394	-1.811526
H	-7.161029	-0.439162	-2.722332
H	-5.642718	-1.075444	-3.423939

GS2-conf2

N	-0.337511	0.052494	-0.170714
C	2.186856	0.408807	-0.761104
C	-2.081410	1.514604	0.142127
C	-2.585712	0.337100	-0.543008
F	0.372491	-0.463427	2.592110
C	-0.693067	1.281660	0.345159
C	-1.467057	-0.520627	-0.711075
C	1.241764	-1.993816	0.303995
C	3.447116	0.509561	-0.103017
C	1.983103	1.241449	-1.897824
C	-2.660527	2.684454	0.572928
H	-3.716696	2.898064	0.437183
C	2.974491	2.126733	-2.321232
H	2.791240	2.742334	-3.201479
C	-3.835351	-0.025676	-1.006632
H	-4.686758	0.632557	-0.876632
C	4.413210	1.407511	-0.556309
H	5.358870	1.478187	-0.019484
C	4.200923	2.230869	-1.663986
C	0.114473	2.223844	0.983326
H	1.171483	2.034490	1.137127
F	-1.491821	-1.448459	2.036545
B	1.074564	-0.541898	-0.215380
C	-1.589514	-1.756097	-1.360184
H	-0.729368	-2.405672	-1.484019
C	2.066801	-2.911237	-0.429766
C	0.570592	-2.549304	1.441316
C	-1.838614	3.640901	1.216694
C	-3.953783	-1.273496	-1.652285
C	-0.467145	3.408526	1.418303
H	0.150711	4.146326	1.915209
C	3.764884	-0.307070	1.124286
H	3.925378	-1.365150	0.882946
H	2.938027	-0.280747	1.842010
H	4.670601	0.067049	1.611142
F	-0.276394	-2.242795	3.643515
C	0.721763	1.153155	-2.719815
H	0.872399	1.599633	-3.707236
H	-0.119692	1.678147	-2.249221
H	0.412072	0.109589	-2.854043
C	5.272920	3.166965	-2.153078
H	5.961801	2.653880	-2.836961
H	5.871616	3.554538	-1.322405
H	4.844261	4.014342	-2.697050
C	2.814613	-2.477812	-1.663529
H	3.225937	-3.346341	-2.186017
H	3.640117	-1.795637	-1.432053

H	2.153330	-1.930519	-2.346675
C	-2.836193	-2.119924	-1.825361
H	-2.985751	-3.068035	-2.331813
C	0.639317	-3.905274	1.767926
H	0.105499	-4.283511	2.633684
C	-0.190123	-1.686006	2.403765
C	2.132130	-4.253395	-0.073808
H	2.743490	-4.924190	-0.674077
C	1.412672	-4.769003	1.007406
H	1.465758	-5.824502	1.256307
O	-2.483402	4.760469	1.604332
O	-5.112433	-1.754483	-2.146680
C	-1.731061	5.788006	2.272365
H	-0.938248	6.171940	1.620892
H	-2.448951	6.578688	2.489935
H	-1.300557	5.407027	3.205044
C	-6.303807	-0.961061	-2.005720
H	-6.197087	-0.005449	-2.530817
H	-7.099372	-1.548349	-2.464011
H	-6.530681	-0.788121	-0.947911

GS2-conf3

N	-0.299381	0.134133	-0.100355
C	2.227034	0.408746	-0.719534
C	-1.987806	1.655228	0.229670
C	-2.539536	0.499012	-0.455166
F	0.405966	-0.405185	2.652439
C	-0.609011	1.371021	0.419590
C	-1.453761	-0.400200	-0.635335
C	1.219146	-1.962107	0.359739
C	3.492952	0.478543	-0.069032
C	2.038748	1.239630	-1.859465
C	-2.535156	2.846287	0.665254
H	-3.587920	3.058570	0.518519
C	3.051631	2.094748	-2.294387
H	2.880042	2.710214	-3.177061
C	-3.794234	0.173745	-0.912315
H	-4.648814	0.833502	-0.794221
C	4.480776	1.346741	-0.533530
H	5.431206	1.395038	-0.002681
C	4.284252	2.168798	-1.644968
C	0.239539	2.286231	1.057654
H	1.290528	2.061437	1.203880
F	-1.488766	-1.336934	2.108494
B	1.091313	-0.507370	-0.160151
C	-1.624370	-1.624088	-1.281918
H	-0.786966	-2.301927	-1.411745
C	2.014053	-2.904282	-0.376492
C	0.537850	-2.496817	1.501721
C	-1.675108	3.764137	1.301816
C	-3.967583	-1.071708	-1.563308
C	-0.304788	3.476666	1.491563
H	0.309365	4.218710	1.991597
C	3.795567	-0.339607	1.161151
H	3.931818	-1.402078	0.923739
H	2.971782	-0.292050	1.881216

H	4.711007	0.015959	1.643700
F	-0.286872	-2.165139	3.708433
C	0.769795	1.181533	-2.672319
H	0.927377	1.612577	-3.665503
H	-0.051910	1.737306	-2.202108
H	0.427326	0.146663	-2.792681
C	5.378325	3.072985	-2.145299
H	6.053265	2.535872	-2.824585
H	5.987622	3.454299	-1.319456
H	4.969584	3.924877	-2.697405
C	2.766234	-2.494839	-1.615617
H	3.149414	-3.375901	-2.138612
H	3.612520	-1.836130	-1.391381
H	2.116463	-1.930543	-2.295939
C	-2.891184	-1.956471	-1.747584
H	-3.035215	-2.905692	-2.248779
C	0.569489	-3.853818	1.829709
H	0.029853	-4.215513	2.698939
C	-0.192045	-1.611417	2.467791
C	2.042957	-4.246949	-0.018574
H	2.631979	-4.935814	-0.620737
C	1.314306	-4.740452	1.067069
H	1.338796	-5.796585	1.317681
O	-2.074788	4.962879	1.772255
O	-5.229144	-1.314945	-1.973954
C	-3.456466	5.334390	1.624790
H	-4.105947	4.629687	2.155659
H	-3.539994	6.324397	2.072835
H	-3.734089	5.380495	0.565923
C	-5.504844	-2.555595	-2.646936
H	-5.287683	-3.406975	-1.992350
H	-6.569043	-2.528729	-2.880693
H	-4.921380	-2.631916	-3.571081

GS2-conf4

N	-0.283818	0.027025	-0.135078
C	2.162623	0.765623	-0.697458
C	-2.209089	1.217741	0.240900
C	-2.546840	0.022971	-0.514487
F	0.469140	-0.533756	2.600194
C	-0.805520	1.163710	0.444495
C	-1.323133	-0.665317	-0.718877
C	1.573619	-1.795303	0.247314
C	3.388993	1.024839	-0.019684
C	1.848492	1.599820	-1.806969
C	-2.956666	2.272799	0.725849
H	-4.028390	2.311469	0.566912
C	2.705488	2.631669	-2.189318
H	2.441776	3.244426	-3.050981
C	-3.733951	-0.476852	-1.011430
H	-4.666962	0.051814	-0.852985
C	4.218806	2.068176	-0.430251
H	5.139529	2.256176	0.121428
C	3.899050	2.888918	-1.513603
C	-0.133833	2.171549	1.147226
H	0.938268	2.119265	1.304029
F	-1.220854	-1.760199	1.972164

B	1.197457	-0.359363	-0.200974
C	-1.276086	-1.866609	-1.435868
H	-0.336139	-2.387195	-1.588023
C	2.532355	-2.540429	-0.519479
C	0.987222	-2.503095	1.346891
C	-2.273332	3.288731	1.428577
C	-3.681870	-1.691221	-1.729307
C	-0.877985	3.228060	1.632328
H	-0.404697	4.034127	2.183600
C	3.810158	0.220887	1.184485
H	4.127926	-0.792965	0.911054
H	2.980646	0.100342	1.889216
H	4.645467	0.705556	1.699150
F	0.095045	-2.443285	3.551364
C	0.616235	1.362314	-2.643173
H	0.701675	1.865953	-3.610687
H	-0.293379	1.739200	-2.158015
H	0.462049	0.291189	-2.820985
C	4.827769	3.986305	-1.958375
H	5.593296	3.600577	-2.644386
H	5.352363	4.432386	-1.107241
H	4.285295	4.777236	-2.485371
C	3.214910	-1.937712	-1.719758
H	3.741787	-2.710078	-2.287535
H	3.939419	-1.164125	-1.441220
H	2.485533	-1.446771	-2.375368
C	-2.461341	-2.368805	-1.935519
H	-2.478675	-3.297757	-2.496316
C	1.257316	-3.848425	1.606021
H	0.781742	-4.346479	2.444611
C	0.100434	-1.815913	2.342507
C	2.797163	-3.873691	-0.229388
H	3.506191	-4.413539	-0.853837
C	2.156868	-4.546370	0.814628
H	2.366736	-5.593259	1.011592
O	-2.879142	4.374104	1.950585
O	-4.765033	-2.289282	-2.264512
C	-4.302304	4.512072	1.795137
H	-4.827199	3.680727	2.278523
H	-4.558376	5.448822	2.289911
H	-4.573028	4.565355	0.734859
C	-6.049958	-1.663757	-2.100218
H	-6.060577	-0.672682	-2.567033
H	-6.758280	-2.319127	-2.606789
H	-6.309560	-1.584962	-1.038706

T_1 optimized geometries

GS1-conf1

N	0.640210	0.101683	0.205079
C	-1.844440	0.808034	-0.241484
C	2.639447	1.233154	0.124197
C	2.860672	-0.121891	-0.347651
F	-2.111293	-1.986031	-1.477885
C	1.255837	1.307308	0.453315
C	1.593651	-0.768336	-0.277513
C	-1.180668	-1.469603	1.243519
C	-1.638070	1.357607	-1.538391
C	-2.964493	1.292189	0.497807
C	3.451759	2.331068	0.285871
H	4.509977	2.314664	0.042156
C	-3.800239	2.266736	-0.041431
H	-4.635418	2.633645	0.554542
C	3.965519	-0.803936	-0.801808
H	4.947699	-0.344982	-0.866928
C	-2.503267	2.327105	-2.047250
H	-2.328373	2.716754	-3.049704
C	-3.594502	2.798242	-1.317690
C	0.690681	2.482022	0.956907
H	-0.364215	2.526043	1.206875
F	-3.520319	-3.477451	-0.789047
B	-0.852325	-0.204752	0.407799
C	1.436522	-2.098785	-0.672421
H	0.468414	-2.584940	-0.616676
C	-0.472502	-1.773837	2.452058
C	-2.204838	-2.402683	0.878110
C	2.876027	3.521097	0.787634
C	3.804790	-2.151686	-1.196138
C	1.510695	3.590156	1.121768
H	1.083567	4.506901	1.509489
C	-0.512000	0.886095	-2.423899
H	-0.707467	1.147654	-3.468196
H	-0.378636	-0.198733	-2.357028
H	0.446370	1.345218	-2.147731
F	-3.937022	-1.381350	-0.449629
C	-3.252377	0.809668	1.895797
H	-4.010954	1.437406	2.373221
H	-2.344588	0.819279	2.511101
H	-3.614697	-0.224607	1.901652
C	-4.538422	3.819051	-1.892769
H	-5.418943	3.335090	-2.335351
H	-4.057463	4.407162	-2.680333
H	-4.902127	4.504121	-1.119851
C	0.593696	-0.852109	2.984667
H	0.814927	-1.085606	4.029829
H	0.272669	0.195116	2.922356
H	1.532740	-0.932608	2.423372
C	2.550926	-2.787087	-1.133520
H	2.439288	-3.819953	-1.440083
C	-2.539627	-3.496540	1.677455
H	-3.326244	-4.176225	1.368086
C	-2.927260	-2.299745	-0.436115
C	-0.814499	-2.878798	3.223338

H	-0.277223	-3.056260	4.152897
C	-1.851819	-3.739194	2.858002
H	-2.114538	-4.587498	3.482664
O	4.936635	-2.750514	-1.622839
O	3.737872	4.552024	0.910068
C	3.242371	5.806185	1.409471
H	2.853636	5.691469	2.427382
H	4.101779	6.476514	1.413932
H	2.462346	6.203719	0.750779
C	4.868550	-4.122128	-2.048709
H	4.192182	-4.228913	-2.904096
H	5.884317	-4.385263	-2.343570
H	4.540026	-4.766994	-1.226080

GS1-conf2

N	0.590967	-0.024233	0.172606
C	-1.803615	0.949213	-0.256308
C	2.698354	0.890163	0.145988
C	2.778370	-0.462261	-0.375233
F	-2.340528	-1.802803	-1.559668
C	1.328489	1.100754	0.470115
C	1.451598	-0.970524	-0.337082
C	-1.382933	-1.423161	1.173416
C	-1.532634	1.513825	-1.535124
C	-2.869036	1.528544	0.495455
C	3.621940	1.886943	0.357153
H	4.675150	1.767942	0.119937
C	-3.590405	2.605607	-0.013340
H	-4.383746	3.041554	0.593104
C	3.822054	-1.235969	-0.847541
H	4.833085	-0.845726	-0.872025
C	-2.283486	2.588060	-2.013505
H	-2.061375	2.988268	-3.002420
C	-3.320558	3.152722	-1.270846
C	0.888010	2.306860	1.018105
H	-0.158526	2.454115	1.264266
F	-3.912401	-3.137793	-0.900401
B	-0.926057	-0.179504	0.364967
C	1.156483	-2.264882	-0.786014
H	0.141594	-2.646152	-0.755928
C	-0.713730	-1.819735	2.377321
C	-2.492728	-2.242459	0.787355
C	3.172249	3.111980	0.905562
C	3.519059	-2.538159	-1.292146
C	1.820346	3.314468	1.233793
H	1.489359	4.255122	1.656353
C	-0.459700	0.950339	-2.432690
H	-0.623922	1.257951	-3.469853
H	-0.440926	-0.143858	-2.394348
H	0.540503	1.299941	-2.144152
F	-4.093175	-1.013366	-0.529835
C	-3.215037	1.035337	1.876371
H	-3.896933	1.730046	2.376271
H	-2.313756	0.917061	2.489891
H	-3.695375	0.050470	1.847086
C	-4.144038	4.287994	-1.815371
H	-5.048824	3.914151	-2.312598

H	-3.583026	4.869623	-2.553473
H	-4.470198	4.961983	-1.016513
C	0.434735	-1.018277	2.933725
H	0.635733	-1.305082	3.969639
H	0.210962	0.055526	2.907518
H	1.360992	-1.164910	2.365186
C	2.197347	-3.035928	-1.261076
H	2.021847	-4.045661	-1.618292
C	-2.935843	-3.315489	1.562301
H	-3.783952	-3.908114	1.236843
C	-3.193421	-2.039993	-0.526874
C	-1.165476	-2.901498	3.124590
H	-0.651914	-3.150727	4.051014
C	-2.279775	-3.648846	2.738680
H	-2.626752	-4.480709	3.344066
O	4.440054	-3.399877	-1.771191
O	4.140561	4.035775	1.076513
C	3.779451	5.313970	1.627946
H	3.367556	5.197683	2.636537
H	4.707023	5.884764	1.669096
H	3.055751	5.822935	0.981727
C	5.812953	-2.976157	-1.828362
H	6.187095	-2.738951	-0.826177
H	6.361862	-3.824346	-2.237244
H	5.923723	-2.108480	-2.488072

GS1-conf3

N	0.580485	0.092040	0.238383
C	-1.852429	0.957513	-0.209205
C	2.642731	1.102095	0.228481
C	2.789984	-0.243249	-0.296131
F	-2.266280	-1.801238	-1.530330
C	1.263703	1.245430	0.543062
C	1.487358	-0.815848	-0.268346
C	-1.339075	-1.400612	1.211993
C	-1.599363	1.535329	-1.485186
C	-2.946786	1.487014	0.537331
C	3.530808	2.138207	0.445699
H	4.581263	2.027571	0.201851
C	-3.713670	2.530514	0.025324
H	-4.529503	2.929548	0.627353
C	3.859295	-0.971908	-0.763147
H	4.868353	-0.571494	-0.796361
C	-2.395984	2.574737	-1.967321
H	-2.186485	2.986004	-2.954396
C	-3.461952	3.090322	-1.230324
C	0.762568	2.432689	1.096273
H	-0.290551	2.531410	1.337911
F	-3.783084	-3.206255	-0.888149
B	-0.929721	-0.133548	0.415708
C	1.257492	-2.116466	-0.717909
H	0.261185	-2.544904	-0.693585
C	-0.660628	-1.778536	2.417052
C	-2.412196	-2.262651	0.813548
C	3.019237	3.331693	0.994097
C	3.624902	-2.292460	-1.213842
C	1.649747	3.466017	1.315100

H	1.313383	4.406721	1.739190
C	-0.495997	1.022792	-2.376458
H	-0.666828	1.324757	-3.414191
H	-0.427812	-0.069471	-2.339457
H	0.485322	1.416768	-2.080618
F	-4.056463	-1.094183	-0.505388
C	-3.279118	0.976064	1.915203
H	-3.994952	1.638436	2.411520
H	-2.378135	0.897144	2.535362
H	-3.714498	-0.029303	1.880794
C	-4.333191	4.188252	-1.777263
H	-5.237481	3.776809	-2.244668
H	-3.807744	4.772067	-2.539272
H	-4.661629	4.867779	-0.983898
C	0.450685	-0.934739	2.985922
H	0.653228	-1.216662	4.022888
H	0.186229	0.129686	2.960519
H	1.387189	-1.044696	2.425552
C	2.336165	-2.853290	-1.193243
H	2.167518	-3.864530	-1.542696
C	-2.814687	-3.358413	1.578517
H	-3.635633	-3.983503	1.244258
C	-3.113652	-2.081102	-0.503263
C	-1.071194	-2.883551	3.153791
H	-0.553350	-3.117725	4.081816
C	-2.151793	-3.673384	2.756255
H	-2.467636	-4.523106	3.353820
O	4.727279	-2.938653	-1.647958
O	3.772995	4.419431	1.253732
C	5.179723	4.367971	0.958557
H	5.344760	4.197110	-0.110963
H	5.571783	5.344478	1.242430
H	5.670338	3.584550	1.546746
C	4.588337	-4.288646	-2.122940
H	3.922807	-4.326855	-2.992581
H	5.592519	-4.600211	-2.410072
H	4.207793	-4.940628	-1.328886

GS1-conf4

N	0.536910	0.006787	0.209346
C	-1.846319	1.018689	-0.202136
C	2.651037	0.898897	0.242666
C	2.724678	-0.433562	-0.329131
F	-2.395590	-1.668683	-1.625850
C	1.282044	1.109853	0.558577
C	1.393994	-0.930043	-0.327577
C	-1.461401	-1.413297	1.130290
C	-1.563498	1.629932	-1.456394
C	-2.913680	1.574623	0.564570
C	3.594531	1.875150	0.497499
H	4.638272	1.715590	0.251847
C	-3.626637	2.673335	0.091968
H	-4.421856	3.090483	0.709126
C	3.766997	-1.199720	-0.815714
H	4.782462	-0.820147	-0.811125
C	-2.306545	2.724700	-1.899192
H	-2.075911	3.160755	-2.870774

C	-3.346507	3.265309	-1.142846
C	0.846100	2.302615	1.150793
H	-0.201107	2.452187	1.392409
F	-3.988519	-3.011828	-1.037304
B	-0.982992	-0.141662	0.380348
C	1.092422	-2.202039	-0.829345
H	0.073642	-2.574218	-0.827453
C	-0.809900	-1.869067	2.323162
C	-2.577159	-2.202313	0.699602
C	3.148389	3.077971	1.085977
C	3.457763	-2.482959	-1.313567
C	1.788732	3.277986	1.407902
H	1.502997	4.220709	1.863311
C	-0.485394	1.096296	-2.365860
H	-0.635585	1.448720	-3.390812
H	-0.475536	0.001347	-2.373620
H	0.514075	1.425107	-2.051727
F	-4.150492	-0.902590	-0.581995
C	-3.271333	1.031598	1.923723
H	-3.951014	1.712095	2.445710
H	-2.374594	0.883832	2.537524
H	-3.759006	0.052315	1.854564
C	-4.162469	4.423237	-1.649457
H	-5.081289	4.072651	-2.137768
H	-3.605664	5.012123	-2.384858
H	-4.465292	5.085073	-0.831324
C	0.344073	-1.107959	2.922987
H	0.532124	-1.442186	3.947058
H	0.135248	-0.031035	2.941920
H	1.273270	-1.243118	2.356164
C	2.132302	-2.967056	-1.319822
H	1.950756	-3.960375	-1.717505
C	-3.042327	-3.300151	1.425392
H	-3.894297	-3.867207	1.066281
C	-3.261894	-1.938080	-0.611978
C	-1.283709	-2.974333	3.020711
H	-0.782891	-3.267600	3.941181
C	-2.403760	-3.690345	2.593718
H	-2.768007	-4.541457	3.160999
O	4.378819	-3.334172	-1.810594
O	3.963123	4.110473	1.383383
C	5.365722	3.988783	1.088766
H	5.524699	3.848400	0.013931
H	5.812070	4.930054	1.409145
H	5.808487	3.157652	1.648587
C	5.756506	-2.922812	-1.830764
H	6.117085	-2.726565	-0.814898
H	6.303408	-3.761232	-2.261839
H	5.886631	-2.033137	-2.456738

GS2-conf1

N	-0.305146	0.238048	-0.139848
C	2.163824	-0.336947	-0.798630
C	-1.433736	2.217968	0.159523
C	-2.327558	1.273842	-0.486276
F	0.271900	-0.380638	2.643319
C	-0.205862	1.522706	0.348178

C	-1.574676	0.077128	-0.649755
C	0.484031	-2.206204	0.417963
C	3.404481	-0.652518	-0.168826
C	2.221516	0.470923	-1.970206
C	-1.560184	3.527317	0.562530
H	-2.479062	4.091415	0.432152
C	3.442049	0.940337	-2.454379
H	3.452304	1.545841	-3.360206
C	-3.631906	1.338887	-0.917588
H	-4.238827	2.232503	-0.805690
C	4.603976	-0.160895	-0.682012
H	5.533673	-0.398347	-0.165670
C	4.650844	0.640403	-1.824928
C	0.894012	2.143144	0.944384
H	1.824772	1.603687	1.084852
F	-1.833759	-0.663057	2.153360
B	0.814416	-0.813369	-0.176794
C	-2.130561	-1.052060	-1.254222
H	-1.550226	-1.962138	-1.367810
C	0.912029	-3.384928	-0.282828
C	-0.309249	-2.444405	1.587426
C	-0.445831	4.152326	1.166006
C	-4.193156	0.194176	-1.527321
C	0.767279	3.463386	1.353369
H	1.614076	3.952945	1.818593
C	3.462722	-1.474074	1.093969
H	3.235257	-2.531055	0.909162
H	2.723383	-1.127755	1.823912
H	4.458645	-1.419311	1.544092
F	-0.934797	-1.772622	3.782226
C	0.980068	0.793853	-2.762901
H	1.242419	1.127160	-3.771331
H	0.387731	1.592694	-2.298769
H	0.326375	-0.082776	-2.845839
C	5.961706	1.129207	-2.378261
H	6.414386	0.378446	-3.039314
H	6.681404	1.330581	-1.578152
H	5.829710	2.043437	-2.965089
C	1.726782	-3.295373	-1.547119
H	1.794083	-4.275628	-2.027711
H	2.744478	-2.934263	-1.362836
H	1.276741	-2.583382	-2.249952
C	-3.445144	-0.986025	-1.695731
H	-3.886182	-1.857428	-2.164027
C	-0.711214	-3.723306	1.977251
H	-1.317990	-3.854454	2.867242
C	-0.691209	-1.330976	2.517241
C	0.510592	-4.648364	0.135291
H	0.829414	-5.515052	-0.440275
C	-0.312374	-4.833973	1.249073
H	-0.625598	-5.829717	1.547653
O	-0.652165	5.434868	1.532579
O	-5.477150	0.338857	-1.916979
C	0.421941	6.148552	2.168082
H	1.286006	6.225204	1.498602
H	0.026094	7.142238	2.377700
H	0.712724	5.657594	3.103464

C	-6.131336	-0.771994	-2.553372
H	-6.177526	-1.633406	-1.877771
H	-7.139178	-0.424346	-2.779989
H	-5.614437	-1.047078	-3.479419

GS2-conf2

N	-0.335401	0.055219	-0.170881
C	2.188490	0.401725	-0.775644
C	-2.083741	1.509613	0.154021
C	-2.582272	0.342092	-0.549219
F	0.379591	-0.442495	2.601615
C	-0.695739	1.275404	0.361739
C	-1.460110	-0.511039	-0.725800
C	1.247449	-1.985570	0.323541
C	3.452733	0.506637	-0.122861
C	1.978783	1.230366	-1.914951
C	-2.663294	2.679411	0.588526
H	-3.717260	2.897656	0.443038
C	2.966614	2.115403	-2.345570
H	2.779051	2.726510	-3.227960
C	-3.830420	-0.020656	-1.019776
H	-4.685450	0.630732	-0.879246
C	4.413486	1.406452	-0.582437
H	5.360323	1.482775	-0.048567
C	4.195124	2.224913	-1.692843
C	0.108678	2.213378	1.009562
H	1.165612	2.024235	1.165118
F	-1.487509	-1.420146	2.041036
B	1.080298	-0.540511	-0.211855
C	-1.578144	-1.739180	-1.389894
H	-0.716729	-2.386618	-1.516827
C	2.068969	-2.910864	-0.405773
C	0.571522	-2.533730	1.462170
C	-1.845534	3.628802	1.244899
C	-3.942845	-1.258644	-1.682899
C	-0.474766	3.394113	1.451870
H	0.140939	4.127761	1.957536
C	3.777496	-0.301742	1.107899
H	3.936363	-1.361643	0.874171
H	2.954854	-0.269962	1.830317
H	4.685961	0.076082	1.586647
F	-0.284958	-2.213083	3.658519
C	0.714962	1.135896	-2.731892
H	0.859574	1.583020	-3.719881
H	-0.126036	1.657520	-2.257144
H	0.408722	0.091311	-2.865094
C	5.263105	3.161367	-2.189025
H	5.953170	2.645641	-2.869779
H	5.861230	3.556508	-1.361524
H	4.831115	4.003325	-2.738681
C	2.817837	-2.489878	-1.643266
H	3.229610	-3.363998	-2.155904
H	3.643178	-1.805232	-1.419451
H	2.157130	-1.950557	-2.333328
C	-2.821954	-2.099590	-1.864536
H	-2.967528	-3.041564	-2.383476
C	0.635033	-3.887606	1.796118

H	0.099004	-4.259033	2.663429
C	-0.189441	-1.662723	2.416726
C	2.127538	-4.251456	-0.042789
H	2.736157	-4.927991	-0.639328
C	1.406068	-4.758427	1.041001
H	1.455275	-5.812676	1.295771
O	-2.491203	4.746794	1.638170
O	-5.098959	-1.737862	-2.186769
C	-1.741189	5.767344	2.318669
H	-0.944369	6.155948	1.674775
H	-2.459036	6.557282	2.539254
H	-1.315880	5.378230	3.250446
C	-6.293353	-0.951366	-2.036784
H	-6.189402	0.012513	-2.547279
H	-7.085908	-1.534599	-2.505438
H	-6.523430	-0.794719	-0.977043

GS2-conf3

N	-0.300287	0.135698	-0.096699
C	2.225810	0.400447	-0.730737
C	-1.993368	1.649119	0.244025
C	-2.538849	0.502589	-0.458953
F	0.412461	-0.384225	2.666606
C	-0.615023	1.363470	0.439731
C	-1.449407	-0.392333	-0.646544
C	1.224237	-1.953959	0.384208
C	3.497317	0.471100	-0.088483
C	2.031144	1.229517	-1.872160
C	-2.541181	2.839837	0.683517
H	-3.591650	3.056805	0.527194
C	3.041500	2.081909	-2.316036
H	2.864926	2.694622	-3.199580
C	-3.791509	0.177402	-0.924562
H	-4.649673	0.830877	-0.797429
C	4.481209	1.338838	-0.561196
H	5.434264	1.389855	-0.035413
C	4.278467	2.157249	-1.674327
C	0.230639	2.274864	1.086790
H	1.281481	2.049771	1.234678
F	-1.483109	-1.312544	2.118162
B	1.094576	-0.505901	-0.152531
C	-1.615243	-1.609558	-1.306721
H	-0.776950	-2.286364	-1.437173
C	2.016057	-2.902834	-0.348246
C	0.542190	-2.481673	1.529307
C	-1.685064	3.751200	1.332144
C	-3.958359	-1.058570	-1.592715
C	-0.315577	3.461797	1.527216
H	0.296288	4.200345	2.035207
C	3.808377	-0.339990	1.144192
H	3.944641	-1.403699	0.912883
H	2.989050	-0.289078	1.869143
H	4.726348	0.019754	1.618669
F	-0.293023	-2.134693	3.730095
C	0.757469	1.169387	-2.676988
H	0.906060	1.607713	-3.668332
H	-0.063518	1.717481	-2.197147

H	0.419649	0.133626	-2.802274
C	5.369619	3.059099	-2.184124
H	6.038546	2.519861	-2.867747
H	5.985818	3.440593	-1.363535
H	4.957878	3.910590	-2.734605
C	2.764820	-2.507029	-1.594021
H	3.142673	-3.394625	-2.109708
H	3.614599	-1.849376	-1.380515
H	2.114529	-1.947441	-2.277685
C	-2.878582	-1.938501	-1.783427
H	-3.018099	-2.882032	-2.296511
C	0.574515	-3.835542	1.867686
H	0.035847	-4.190676	2.740139
C	-0.189699	-1.589083	2.486855
C	2.043954	-4.243028	0.019494
H	2.630759	-4.936766	-0.579170
C	1.318469	-4.728068	1.110640
H	1.343756	-5.782185	1.369456
O	-2.086132	4.947641	1.808948
O	-5.218122	-1.300992	-2.011726
C	-3.466590	5.320585	1.656769
H	-4.119336	4.611715	2.178131
H	-3.552703	6.307016	2.112210
H	-3.738486	5.375159	0.596749
C	-5.486450	-2.533387	-2.701918
H	-5.269961	-3.392722	-2.057489
H	-6.549584	-2.507005	-2.940663
H	-4.898325	-2.596375	-3.624193

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N	-0.282966	0.031200	-0.137440
C	2.165979	0.760531	-0.710499
C	-2.212418	1.210594	0.251934
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F	0.473623	-0.509593	2.610176
C	-0.808948	1.156096	0.459738
C	-1.317834	-0.653416	-0.735598
C	1.576779	-1.785992	0.267116
C	3.397118	1.020546	-0.039215
C	1.846548	1.593831	-1.820323
C	-2.961395	2.262803	0.744167
H	-4.031828	2.305656	0.577611
C	2.701863	2.623817	-2.209142
H	2.434495	3.234606	-3.070999
C	-3.730061	-0.471405	-1.026793
H	-4.666047	0.048920	-0.858450
C	4.223460	2.063948	-0.455342
H	5.145994	2.254424	0.092360
C	3.898925	2.882136	-1.539408
C	-0.140161	2.158458	1.172730
H	0.932027	2.106664	1.330074
F	-1.221329	-1.725866	1.974497
B	1.202051	-0.355440	-0.197700
C	-1.266337	-1.845476	-1.467670
H	-0.325040	-2.362930	-1.623039
C	2.532319	-2.540455	-0.495891
C	0.985038	-2.486358	1.368932

C	-2.281591	3.270351	1.460221
C	-3.672402	-1.673861	-1.762267
C	-0.886592	3.208831	1.667346
H	-0.415478	4.009864	2.227778
C	3.824715	0.221992	1.166260
H	4.142766	-0.792661	0.896480
H	2.998728	0.103568	1.875507
H	4.661724	0.710202	1.674704
F	0.077085	-2.411943	3.566946
C	0.610360	1.354608	-2.649667
H	0.686933	1.864050	-3.614834
H	-0.297176	1.724369	-2.155702
H	0.459837	0.283899	-2.832735
C	4.825722	3.977933	-1.990877
H	5.588430	3.589722	-2.678704
H	5.353899	4.426231	-1.143158
H	4.281336	4.767216	-2.518333
C	3.217333	-1.951699	-1.701873
H	3.739259	-2.732302	-2.262845
H	3.946731	-1.180104	-1.431179
H	2.490591	-1.462663	-2.361724
C	-2.448896	-2.343993	-1.976987
H	-2.462329	-3.265365	-2.550295
C	1.250470	-3.830242	1.637413
H	0.772086	-4.321269	2.478481
C	0.096240	-1.789810	2.355777
C	2.790887	-3.873161	-0.197157
H	3.497518	-4.419938	-0.818220
C	2.148655	-4.536389	0.851360
H	2.355031	-5.582600	1.055402
O	-2.889568	4.350597	1.991999
O	-4.753069	-2.269611	-2.306781
C	-4.312142	4.488505	1.834095
H	-4.837464	3.650377	2.305314
H	-4.571270	5.418645	2.339688
H	-4.580037	4.554553	0.773746
C	-6.040376	-1.652272	-2.133268
H	-6.055180	-0.653948	-2.584378
H	-6.746007	-2.302470	-2.650218
H	-6.300810	-1.590952	-1.070737