Synthesis of CCl_3-substituted amides, ketones, indenes by intermolecular reactions of β-CCl_3-enones or β-CCl_3-β-hydroxy ketones with various nucleophiles in CF_3SO_3H

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Contents

1. Experimental part

General information. The NMR spectra of solutions of compounds in $CDCl_3$ or $(CD_3)_2CO$ were recorded on Bruker 400 spectrometer at 25°C at 400, 101 and 376 MHz for ^1H and ^{13}C, and ^{19}F NMR spectra respectively. The residual proton-solvent peaks $CDCl_3$ (δ 7.26 ppm) or $(CD_3)_2CO$ (δ 2.05 ppm) for ^1H NMR spectra, and the carbon signals of $CDCl_3$ (δ 77.0 ppm) or $(CD_3)_2CO$ (δ 29.84 and 206.26 ppm) for ^{13}C NMR spectra were used as references. ^{19}F NMR spectra were indirectly referred to the signal of $CFCl_3$ (δ 0.0 ppm). HRMS were carried out at instruments Bruker maXis HRMS-ESI-QTOF and Varian 902-MS MALDI Mass Spectrometer. Preparative TLC was performed on silica gel (Merck Co., 5−40 μm) with hexane-ethyl acetate mixture elution. HPLC was carried out on instrument Shimadzu LC-20AP using column Agilent Zorbax prepHT XDB-C18, 5 μm, 21.2 × 150 mm; under the following conditionsC: temperature – 40 °C, flow rate – 12mL/min, mobile phase – water (A)/acetonitrile (B), both + 0.1% TFA; elution program: 5 min 20% B, then linear gradient of B 20-98% within 35 min.

Single-crystal X-ray analyses of compounds **3a**, **3e**, **3j**, **4e**, **4g**, **5fb** were performed using a single-crystal diffractometer SuperNova, Single source at offset/far, HyPix3000. The crystals were kept at 100(5) K during data collection. Using Olex2,[1] the structures were solved with the ShelXT[2] structure solution program using Intrinsic Phasing and refined with the ShelXL[3] refinement package using Least Squares minimization. Supporting crystallographic data for this paper have been deposited at the Cambridge Crystallographic Data Centre (CCDC 2491771 for **3a**, 2491772 for **3e**, 2491778 for **3j**, 2491779 for **4e**, 2491780 for **4g**, and 2491781 for **5fb**) and can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

DFT calculations. All computations were carried out at the DFT/HF hybrid level of theory using hybrid exchange functional B3LYP by using GAUSSIAN 2009 program packages.[4] The geometries optimization were performed using the 6-311+G(2d,2p) basis set (standard 6-311G basis set added with polarization (d,p) and diffuse functions). Optimizations were performed on all degrees of freedom and solvent phase optimized structures were verified as true minima with no imaginary frequencies. The Hessian matrix was calculated analytically for the optimized structures in order to prove the location of correct minima and to estimate the thermodynamic parameters. Solvent-phase calculations used the Polarizable Continuum Model (PCM, solvent=water).

Starting compounds **1** and **2** were synthesized and characterized by ourselves previously.[5]

General procedure for the synthesis of CCl_3-amides 3 by the reaction of compounds 1 or 2 with nitriles in TfOH. The solution of hydroxyketone **1** (0.1-0.2 mmol) or enone **2** (0.1-0.2 mmol) and nitrile (0.1 ml, excess) in 1 ml of TfOH was stirred at room temperature for 2 days (**3g-i**), 1 week (**3a**, **3d-f**, **3ea**, **3eb**) or 30 days (**3b-c**, **3j**). Then, the reaction mixture was quenched with water (30 ml). The reaction product was extracted with CH_2Cl_2 (2×20 ml). The combined organic phases were consequently washed with saturated aqueous solution of Na_2CO_3 (20 ml), water (2×20

ml) and dried with Na_2SO_4. The solvent was removed in vacuum. The reaction product was crystallized from chloroform-hexane mixture (**3a**, **3d-e**, **3h-i**), methanol-hexane mixture (**3f**, **3ea**), or purified by preparative TCL using hexane-ethyl acetate mixture in a ratio of 1:1 (vol.) as an eluent (**3b-c**, **3j**, **3eb**). Compound **3g** was obtained without purification.

General procedure for the synthesis of CCl_3-ketones 4 by reaction of compounds 1 or 2 with cyclohexane or durene (1,2,4,5-tetramethylbezene) in TfOH. The solution of hydroxyketone **1** (0.1-0.2 mmol) or enone **2** (0.1-0.2 mmol) and cyclohexane (0.1 ml, excess) or durene (13.4-26.8 mg, 0.1-0.2 mmol, 1 equiv.) in 1 ml of TfOH was stirred at room temperature for 3 days (**4a**, **4d-4f**) or for 2 h (**4g-i**). Then, the reaction mixture was quenched with water (30 ml). The reaction product was extracted with CH_2Cl_2 (2×20 ml). The combined organic phases were consequently washed with saturated aqueous solution of Na_2CO_3 (20 ml), water (2×20 ml) and dried with Na_2SO_4. The solvent was removed in vacuum. The reaction product was purified with TCL using hexane-ethyl acetate mixture in a ratio of 1:1 (vol.) as an eluent.

General procedure for the synthesis of CCl_3-ketones 5 by reaction of compounds 1 or 2 with arenes in TfOH. The solution of hydroxyketone **1** (0.1-0.2 mmol) or enone **2** (0.1-0.2 mmol) and corresponding arene (0.1 ml, excess) in 1 ml of TfOH was stirred at room temperature for 7 days (**5a**, **5d-f, 5aa, 5da, 5ea**) or for 4 days (**5ab,db-fb, 5l**). Then, the reaction mixture was quenched with water (30 ml). The reaction product was extracted with CH_2Cl_2 (2×20 ml). The combined organic phases were consequently washed with saturated aqueous solution of Na_2CO_3 (20 ml), water (2×20 ml) and dried with Na_2SO_4. The solvent was removed in vacuum. The reaction product was purified with TCL using hexane-ethyl acetate mixture in a ratio of 1:1 (vol.) as an eluent (**5a**, **5d-5f, 5aa, 5da, 5ea**) or crystallized from chloroform-hexane mixture (**5ab, 5db-fb, 5l**).

General procedure for the synthesis of CCl_3-indenes 6 by reaction of compounds 2 with *o*-xylene or pseudocumene in TfOH. The solution of hydroxyketone enone **2** (0.1-0.4 mmol) and arene (0.1 ml, excess) in 1 ml of TfOH was stirred at room temperature for 7 days. Then, the reaction mixture was quenched with water (30 ml). The reaction product was extracted with CH_2Cl_2 (2×20 ml). The combined organic phases were consequently washed with saturated aqueous solution of Na_2CO_3 (20 ml), water (2×20 ml) and dried with Na_2SO_4. The solvent was removed in vacuum. The reaction product was purified with TCL using hexane-ethyl acetate mixture in a ratio of 1:1 (vol.) as an eluent to yield mixture of isomers. Compound **6d** was separated from its isomer **6da** using HPLC.

N-(1,1,1-Trichloro-4-phenyl-4-oxobutan-2-yl)acetamide (3a). It was obtained from (*E*)-4,4,4-trichloro-1-phenylbut-2-en-1-one **(2a)** (28 mg, 0.1 mmol) and acetonitrile (0.1 ml) in 7 days. Yield of 25 mg (73%). Colorless solid, m.p 181-183°C (chloroform-hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.98 d (2H, J=7.4 Hz), 7.63 t (1H, J=7.4 Hz), 7.51 t (1H, J=7.4 Hz), 6.09 d (1H, J=9.5 Hz), 5.58 td (1H, J=9.5, 3.2 Hz), 3.84 dd (1H, J=16.2, 3.2 Hz), 3.38 dd (1H, J=16.2, 9.5 Hz),

2.05 s (3H, Me). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 195.3, 169.5, 136.2, 133.8, 128.9, 128.3, 102.4, 60.5, 40.2, 23.3. HRMS (ESI), m/z: $[M+Na]^+$ Calcd. for $C_{12}H_{12}Cl_3NO_2Na$ 329.9826; Found 329.9820.

N-(1,1,1-Trichloro-4-(2-methylphenyl)-4-oxobutan-2-yl)acetamide (3b). It was obtained from 4,4,4-trichloro-3-hydroxy-1-(2-methylphenyl)butan-1-one **(1b)** (32 mg, 0.1 mmol) and acetonitrile (0.1 ml) in 30 days. Yield of 15 mg (42%). Colorless solid, m.p 144-146°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.69 d (1H, J=7.6 Hz), 7.43 t (1H, J=7.5 Hz), 7.26-7.35 m (2H), 6.17 d (1H, J=9.5 Hz), 5.49 td (1H, J=9.5, 3.3 Hz), 3.80 dd (1H, J=16.0, 3.3 Hz), 3.27 dd (1H, J=16.0, 9.5 Hz), 2.50 s (3H, Me), 2.05 s (3H, Me). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 198.7, 169.4, 139.1, 136.6, 132.4, 132.1, 128.7, 125.9, 102.3, 60.6, 42.9, 23.2, 21.4. HRMS (ESI), m/z: $[M+Na]^+$ Calcd. for $C_{13}H_{14}Cl_3NO_2Na$ 343.9982; Found 343.9980.

N-(1,1,1-Trichloro-4-(4-methylphenyl)-4-oxobutan-2-yl)acetamide (3c). It was obtained from 4,4,4-trichloro-3-hydroxy-1-(4-methylphenyl)butan-1-one **(1c)** (32 mg, 0.1 mmol) and acetonitrile (0.1 ml) in 30 days. Yield of 8 mg (23%). Colorless solid, m.p. 147-150°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.88 d (2H, J=8.1 Hz), 7.31 d (2H, J=8.1 Hz), 6.06 d (1H, J=9.5 Hz), 5.56td (1H, J=9.5, 3.3 Hz), 3.81 dd (1H, J=16.1, 3.3 Hz), 3.33 dd (1H, J=16.1, 9.5 Hz), 2.44 s (3H, Me), 2.05 s (3H, Me). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 195.0, 169.4, 144.8, 133.7, 129.6, 128.4, 102.4, 60.6, 40.0, 23.3, 21.7. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{13}H_{15}Cl_3NO_2$ 322.0163; Found 322.0158.

N-(1,1,1-Trichloro-4-(4-fluorophenyl)-4-oxobutan-2-yl)acetamide (3d). It was obtained from (*E*)-4,4,4-trichloro-1-(4-fluorophenyl)but-2-en-1-one **(2d)** (50 mg, 0.2 mmol) and acetonitrile (0.1 ml) in 7 days. Yield of 23 mg (37%). Colorless solid, m.p 162-163°C (chloroform-hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 8.02 dd (2H, J=8.7, 5.3 Hz), 7.18 t (2H, J=8.7 Hz), 6.12 d (1H, J=9.5 Hz), 5.58 td (1H, J=9.5, 3.2 Hz), 3.84 dd (1H, J=16.3, 3.2 Hz), 3.38 dd (1H, J=16.3, 9.5 Hz), 2.05 s (3H, Me). ^{13}C NMR (CDCl3, 101 MHz) δ, ppm: 193.6, 169.5, 166.1 d (*J* = 256.2 Hz), 132.6 d (*J* = 3.0 Hz), 131.0 d (*J* = 9.4 Hz), 116.1 d (*J* = 22.0 Hz), 102.2, 60.5, 40.2, 23.2. ^{19}F NMR ($CDCl_3$, 376 MHz) δ, ppm: -103.7. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{12}H_{12}Cl_3FNO_2$ 325.9912; Found 325.9911.

N-(4-(4-Chlorophenyl)-1,1,1-trichloro-4-oxobutan-2-yl)acetamide (3e). It was obtained from (*E*)-4,4,4-trichloro-1-(4-chlorophenyl)but-2-en-1-one **(2e)** (50 mg, 0.2 mmol) and acetonitrile (0.1 ml) in 7 days. Yield of 31 mg (52%). Colorless solid, m.p 152-153°C (Chloroform-hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.93 d (2H, J=8.5 Hz), 7.49 d (2H, J=8.5 Hz), 5.99 d (1H, J=9.5 Hz), 5.56 td (1H, J=9.5, 3.2 Hz), 3.82 dd (1H, J=16.2, 3.2 Hz), 3.33 dd (1H, J=16.2, 9.5 Hz), 2.06 s (3H, Me). ^{13}C NMR (CDCl3, 101 MHz) δ, ppm: 194.1, 169.4, 140.4, 134.4, 129.7, 129.3, 102.2, 60.4, 40.2, 23.3. HRMS (ESI), m/z: $[M+Na]^+$ Calcd. for $C_{12}H_{11}Cl_4NO_2Na$ 363.9436; Found 363.9434.

N-(4-(4-Bromophenyl)-1,1,1-trichloro-4-oxobutan-2-yl)acetamide (3f). It was obtained from 1-(4-bromophenyl)-4,4,4-trichloro-3-hydroxybutan-1-one **(1f)** (30 mg, 0.1 mmol) and acetonitrile (0.1 ml) in 7 days. Yield of 32 mg (95%). Colorless solid, m.p 159-161°C. (methanol-hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.84 d (2H, J=8.5 Hz), 7.65 d (2H, J=8.5 Hz), 6.18 d (1H, J=9.5 Hz), 5.55 td (1H, J=9.5, 3.1 Hz), 3.80 dd (1H, J=16.3, 3.1 Hz), 3.35 dd (1H, J=16.3, 9.5 Hz), 2.05 s (3H, Me). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 194.2, 169.6, 134.8, 132.2, 129.7, 129.1, 102.2, 60.4, 40.2, 23.2. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{12}H_{12}BrCl_3NO_2$ 385.9112; Found 385.9107.

N-(1,1,1-Trichloro-4-(4-(trifluoromethyl)phenyl)-4-oxobutan-2-yl)acetamide (3g). It was obtained from 4,4,4-trichloro-3-hydroxy-1-(4-(trifluoromethyl)phenyl)butan-1-one **(1g)** (31 mg, 0.1 mmol) and acetonitrile (0.1 ml) in 2 days. Yield of 32 mg (94%). Colorless solid, m.p. 149-151°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 8.09 d (2H, J=8.1 Hz), 7.77 d (2H, J=8.1 Hz), 6.20 d (1H, J=9.5 Hz), 5.57 td (1H, J=9.5, 3.1 Hz), 3.86 dd (1H, J=16.5, 3.1 Hz), 3.42 dd (1H, J=16.5, 9.5 Hz), 2.05 s (3H, Me). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 194.3, 169.6, 138.7, 135.0 d (J = 32.7 Hz), 128.6, 126.0 q (J = 3.7 Hz), 123.4 d (J = 272.8 Hz), 102.1, 60.3, 40.7, 23.2. ^{19}F NMR ($CDCl_3$, 376 MHz) δ, ppm: -63.2. HRMS, m/z: $[M+H]^+$ Calcd. for $C_{13}H_{12}Cl_3F_3NO_2$ 375.9880; Found 375.9879.

N-(1,1,1-Trichloro-4-(3-nitrophenyl)-4-oxobutan-2-yl)acetamide (3h). It was obtained from 4,4,4-trichloro-3-hydroxy-1-(3-nitrophenyl)butan-1-one **(1h)** (40 mg, 0.1 mmol) and acetonitrile (0.1 ml) in 2 days. Yield of 27 mg (60%). Colorless solid, m.p 163°C (Chloroform-hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 8.80 t (1H, J=1.9 Hz), 8.49 ddd (1H, J=8.1, 2.3, 1.0 Hz), 8.33 dt (1H, J=7.8, 1.4 Hz), 7.75 t (1H, J=8.0 Hz), 6.06 d (1H, J=9.5 Hz), 5.60 td (1H, J=9.5, 3.1 Hz), 3.91 dd (1H, J=16.5, 3.1 Hz), 3.45 dd (1H, J=16.5, 9.5 Hz), 2.08 s (3H, Me). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 193.1, 169.6, 148.6, 137.3, 133.8, 130.3, 128.0, 123.1, 101.9, 60.3, 40.8, 23.3. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{12}H_{12}Cl_3N_2O_4$ 352.9857; Found 352.9853.

N-(1,1,1-Trichloro-4-(4-nitrophenyl)-4-oxobutan-2-yl)acetamide (3i). It was obtained from 4,4,4-trichloro-3-hydroxy-1-(4-nitrophenyl)butan-1-one **(1i)** (40 mg, 0.1 mmol) and acetonitrile (0.1 ml) in 2 days. Yield of 26 mg (58%). Colorless solid, m.p 163-164°C (Chloroform-hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 8.36 d (2H, J=8.9 Hz), 8.15 d (2H, J=8.9 Hz), 6.12 d (1H, J=9.5 Hz), 5.57 td (1H, J=9.5, 3.2 Hz), 3.90 dd (1H, J=16.5, 3.2 Hz), 3.44 dd (1H, J=16.5, 9.5 Hz), 2.07 s (3H, Me). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 193.8, 169.6, 150.7, 140.4, 129.3, 124.1, 101.9, 60.3, 41.0, 23.2. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{12}H_{12}Cl_3N_2O_4$ 352.9857; Found 352.9851.

N-(1,1,1-Trichloro-4-(2,4,5-trimethylphenyl)-4-oxobutan-2-yl)acetamide (3j). It was obtained from 4,4,4-trichloro-3-hydroxy-1-(2,4,5-trimethylphenyl)butan-1-one **(1j)** (32 mg, 0.1 mmol) and acetonitrile (0.1 ml) in 30 days. Yield of 7 mg (20%). Colorless solid, m.p. 177-179°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.47 s (1H), 7.06 s (1H), 6.03 d (1H, J=9.5 Hz), 5.48td (1H, J=9.5, 3.3 Hz), 3.80 dd (1H, J=16.1, 3.3 Hz), 3.23 dd (1H, J=16.1, 9.5 Hz), 2.45 s (3H, Me), 2.31 s

(3H, Me), 2.29 s (3H, Me), 2.06 s (3H, Me). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 198.2, 169.3, 141.6, 136.9, 134.0, 133.9, 133.8, 130.3, 102.4, 60.8, 42.6, 23.3, 21.0, 19.8, 19.4. HRMS (ESI), m/z: $[M+Na]^+$ Calcd. for $C_{15}H_{18}Cl_3NO_2Na$ 372.0295; Found 372.0290.

N-(4-(4-Chlorophenyl)-1,1,1-trichloro-4-oxobutan-2-yl)propionamide (3ea). It was obtained from (*E*)-4,4,4-trichloro-1-(4-chlorophenyl)but-2-en-1-one **(2e)** (30 mg, 0.1 mmol) and propionitrile (0.1 ml) in 7 days. Yield of 19 mg (51%). Colorless solid, m.p. 173-175°C (Methanol-hexane). ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.92 d (2H, J=8.5 Hz), 7.49 d (2H, J=8.5 Hz), 6.01 d (1H, J=9.5 Hz), 5.56 td (1H, J=9.5, 3.2 Hz), 3.81 dd (1H, J=16.2, 3.2 Hz), 3.34 dd (1H, J=16.2, 9.5 Hz), 2.27 qd (2H, J=7.6, 1.5 Hz), 1.17 t (3H, J=7.6 Hz). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 194.1, 173.2, 140.4, 134.5, 129.7, 129.3, 102.2, 60.3, 40.3, 29.7, 9.6. HRMS (ESI), m/z: $[M+Na]^+$ Calcd. for $C_{13}H_{13}Cl_4NO_2Na$ 377.9593; Found 377.9590.

2,2,2-Tricloro-N-(4-(4-chlorophenyl)-1,1,1-trichloro-4-oxobutan-2-yl)acetamide (3eb). It was obtained from (*E*)-4,4,4-trichloro-1-(4-chlorophenyl)but-2-en-1-one **(2e)** (30 mg, 0.1 mmol) and trichloroacetonitrile (0.1 ml) in 7 days. Yield of 11 mg (23%). Pale-red solid, m.p. 108-110°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.94 d (2H, J=8.5 Hz), 7.51 d (2H, J=8.5 Hz), 5.49 ddd (1H, J=9.6, 8.4, 3.5 Hz), 3.82 dd (1H, J=17.2, 3.5 Hz), 3.59 dd (1H, J=17.2, 8.4 Hz). ^{13}C NMR (CDCl3, 101 MHz) δ, ppm: 193.4, 161.3, 140.7, 134.3, 129.6, 129.34, 129.31, 101.1, 62.4, 39.5. HRMS, m/z: $[M+H]^+$ Calcd. for $C_{12}H_9Cl_7NO_2$ 443.8447; Found 443.8450.

4,4,4-Trichloro-1-phenylbutan-1-one (4a). It was obtained from (*E*)-4,4,4-trichloro-1-phenylbut-2-en-1-one **(2a)** (50 mg, 0.2 mmol) and cyclohexane (0.1 ml) in 3 days. Yield of 40 mg (80%). Pale-yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 8.03 d (2H, J=7.3 Hz), 7.63 t (1H, J=7.3 Hz), 7.52 t (2H, J=7.3 Hz), 3.51 t (2H, J= 8.0 Hz), 3.23 t (2H, J= 8.0 Hz). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 196.7, 136.3, 133.6, 128.8, 128.1, 99.4, 49.4, 35.8. HRMS (ESI), m/z: $[M+Na]^+$ Calcd. for $C_{10}H_9Cl_3ONa$ 272.9611; Found 272.9606.

4,4,4-Trichloro-1-(4-fluorophenyl)butan-1-one (4d). It was obtained from (*E*)-4,4,4-trichloro-1-(4-fluorophenyl)but-2-en-1-one **(2d)** (50 mg, 0.2 mmol) and cyclohexane (0.1 ml) in 3 days. Yield of 43 mg (86%). Pale-yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 8.06 dd (2H, J = 8.9, 5.3 Hz), 7.19 t (2H, J = 8.9 Hz), 3.48 t (2H, J= 8.0 Hz), 3.21 t (2H, J= 8.0 Hz). ^{13}C NMR (CDCl3, 101 MHz) δ, ppm: 195.1, 166.0 d (*J* = 255.5 Hz), 132.8 d (*J* = 3.0 Hz), 130.8 d (*J* = 9.4 Hz), 115.9 d (*J* = 21.9 Hz), 99.3, 49.3, 35.7. ^{19}F NMR ($CDCl_3$, 376 MHz) δ, ppm: -104.3. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{10}H_9Cl_3FO$ 268.9698; Found 268.9693.

4,4,4-Trichloro-1-(4-chlorophenyl)butan-1-one (4e). It was obtained from (*E*)-4,4,4-trichloro-1-(4-chlorophenyl)but-2-en-1-one **(2e)** (50 mg, 0.2 mmol) and cyclohexane (0.1 ml) in 3 days. Yield of 45 mg (90%). Pale-yellow prisms, m.p. 86-88°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.97 d (2H, J=8.6 Hz), 7.50 d (2H, J=8.6 Hz), 3.48 t (2H, J= 8.0 Hz), 3.22 t (2H, J= 8.0 Hz).

^{13}C NMR (CDCl3, 101 MHz) δ, ppm: 195.5, 140.1, 134.6, 129.5, 129.1, 99.2, 49.3, 35.8. HRMS (ESI), m/z: $[M-Cl]^+$ Calcd. for $C_{10}H_8Cl_3O$ 248.9635; Found 248.9638.

1-(4-Bromophenyl)-4,4,4-trichlorobutan-1-one (4f). It was obtained from 1-(4-bromophenyl)-4,4,4-trichloro-3-hydroxybutan-1-one **(1f)** (30 mg, 0.1 mmol) and cyclohexane (0.1 ml) in 3 days. Yield of 22 mg (74%). Colorless solid, m.p. 87-90°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.89 d (2H, J=8.6 Hz), 7.67 d (2H, J=8.6 Hz), 3.47 t (2H, J= 8.0 Hz), 3.22 t (2H, J= 8.0 Hz). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 195.7, 135.0, 132.1, 129.6, 128.8, 99.2, 49.3, 35.8. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{10}H_9BrCl_3O$ 328.8897; Found 328.8893.

4,4,4-Trichloro-1-(4-(trifluoromethyl)phenyl)butan-1-one (4g). It was obtained from 4,4,4-trichloro-1-(4-(trifluoromethyl)-3-hydroxy-phenylbutan-1-one **(1g)** (31 mg, 0.1 mmol) and cyclohexane (0.1 ml) in 2 hours. Yield of 20 mg (68%). Colorless solid, m.p. 85-87°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 8.14 d (2H, J=8.1 Hz), 7.79 d (2H, J=8.1 Hz), 3.53 t (2H, J= 8.0 Hz), 3.24 t (2H, J= 8.0 Hz). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 195.7, 138.9, 134.9 d (J = 32.9 Hz), 128.5, 125.9 q (J = 3.6 Hz), 123.5 d (J = 272.9 Hz), 99.0, 49.2, 36.1. ^{19}F NMR ($CDCl_3$, 376 MHz) δ, ppm: -63.2. MALDI, m/z: $[M+H]^+$ Calcd. for $C_{11}H_9Cl_3F_3O$ 318.9665; Found 318.9668.

4,4,4-Trichloro-1-(3-nitrophenyl)butan-1-one (4h) and (*E*)-4,4,4-trichloro-1-(4-nitrophenyl)but-2-en-1-one (2h) (see properties of **2h** in our previous work[23]). They were obtained from 4,4,4-trichloro-3-hydroxy-1-(3-nitrophenyl)butan-1-one **(1h)** (30 mg, 0.1 mmol) and cyclohexane (0.1 ml) in 2 h in total yield of 26 mg (91%) with **4h**/**2h** ratio of 10 : 1. Colorless solid. m.p. 72-74°C. Compound **4h**: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: (selected signals from spectrum of compound mixture) 3.56 t (2H, J= 8.0 Hz), 3.26 t (2H, J= 8.0 Hz). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: selected signals from spectrum of compound mixture 194.5, 148.6, 137.5, 133.6, 130.1, 127.8, 123.0, 98.9, 49.0, 36.1. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{10}H_9Cl_3NO_3$ 295.9643; Found 295.9645.

4,4,4-Trichloro-1-(4-nitrophenyl)butan-1-one (4i). It was obtained from 4,4,4-trichloro-3-hydroxy-1-(4-nitrophenyl)butan-1-one **(1i)** (30 mg, 0.1 mmol) and cyclohexane (0.1 ml) in 2 hours. Yield of 23 mg (81%). Colorless solid, m.p. 72-74°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 8.37 d (2H, J=8.9 Hz), 8.19 d (2H, J=8.9 Hz), 3.56 t (2H, J= 8.0 Hz), 3.25 t (2H, J= 8.0 Hz). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 195.2, 150.7, 140.6, 129.2, 124.0, 98.9, 49.0, 36.4. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{10}H_9Cl_3NO_3$ 295.9643; Found 295.9646.

4,4,4-Trichloro-1,3-diphenylbutan-1-one (5a). It was obtained from (*E*)-4,4,4-trichloro-1-phenylbut-2-en-1-one **(2a)** (30 mg, 0.1 mmol) and benzene (0.1 ml) in 7 days. Yield of 25 mg (64%). Colorless needles, m.p. 129-131°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.96 d (2H, J=7.2 Hz), 7.54-7.62 m (3H), 7.48 t (2H, J=7.6 Hz), 7.31=7.38 m (3H), 4.64 dd (1H, J=7.9, 4.5 Hz), 3.92-4.04 m (2H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 195.7, 136.9, 136.5, 133.5, 130.3, 128.7, 128.5,

128.2, 128.1, 103.4, 60.6, 41.9. HRMS (ESI), m/z: $[M+Na]^+$ Calcd. for $C_{16}H_{13}Cl_3ONa$ 348.9924; Found 348.9934.

4,4,4-Trichloro-1-(4-fluorophenyl)-3-phenylbutan-1-one (5d). It was obtained from (*E*)-4,4,4-trichloro-1-(4-fluorophenyl)but-2-en-1-one **(2d)** (20 mg, 0.1 mmol) and benzene (0.1 ml) in 7 days. Yield of 19 mg (73%). Colorless needles, m.p. 73-75°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.95-8.02 m (2H), 7.52-7.58 m (2H), 7.32-7.39 m (3H), 7.15 t (2H, J=8.6 Hz), 4.62 dd (1H, J=7.6, 4.8 Hz), 3.88-4.00 m (2H). ^{13}C NMR (CDCl3, 101 MHz) δ, ppm: 194.1, 165.9 d (*J* = 255.5 Hz), 136.9, 132.9 d (*J* = 3.1 Hz), 130.8 d (*J* = 9.4 Hz), 130.2, 128.5, 128.2, 115.8 d (*J* = 21.9 Hz), 103.3, 60.7, 41.8. ^{19}F NMR ($CDCl_3$, 376 MHz) δ, ppm: -104.4. HRMS (ESI), m/z: $[M+Ag]^+$ Calcd. for $C_{16}H_{12}Cl_3FOAg$ 450.8983; Found 450.8983.

1-(4-Chlorophenyl)-4,4,4-trichloro-3-phenylbutan-1-one (5e). It was obtained from (*E*)-4,4,4-trichloro-1-(4-chlorophenyl)but-2-en-1-one **(2e)** (30 mg, 0.1 mmol) and benzene (0.1 ml) in 7 days. Yield of 21 mg (55%). Colorless needles, m.p. 125-127°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.90 d (2H, J=8.6 Hz), 7.51-7.58 m (2H), 7.44 d (2H, J=8.6 Hz), 7.30-7.39 m (3H), 4.61 dd (1H, J=7.3, 5.0 Hz), 3.88-4.00 m (2H). ^{13}C NMR (CDCl3, 101 MHz) δ, ppm: 194.5, 140.0, 136.8, 134.8, 130.2, 129.5, 129.0, 128.6, 128.2, 103.2, 60.6, 41.8. HRMS (ESI), m/z: $[M+Ag]^+$ Calcd. for $C_{16}H_{12}Cl_4OAg$ 466.8687; Found 466.8695.

1-(4-Bromophenyl)-4,4,4-trichloro-3-phenylbutan-1-one (5f). It was obtained from 1-(4-bromophenyl)-4,4,4-trichloro-3-hydroxybutan-1-one **(1f)** (30 mg, 0.1 mmol) and benzene (0.1 ml) in 7 days. Yield of 12 mg (32%). Colorless needles, m.p. 155-157°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.82 d (2H, J=8.6 Hz), 7.62 d (2H, J=8.6 Hz), 7.52-7.56 m (2H), 7.32-7.38 m (3H), 4.61 dd (1H, J=7.2, 5.2 Hz), 3.88-3.99 m (2H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 194.7, 147.3, 136.8, 135.2, 132.0, 130.2, 129.6, 128.6, 128.2, 103.0, 60.6, 41.8. HRMS (ESI), m/z: $[M+Na]^+$ Calcd. for $C_{16}H_{12}BrCl_3ONa$ 426.9029; Found 426.9029.

4,4,4-Trichloro-3-(2,4-dimethylphenyl)-1-phenylbutan-1-one (5aa). It was obtained from (*E*)-4,4,4-trichloro-1-phenylbut-2-en-1-one **(2a)** (30 mg, 0.1 mmol) and *m*-xylene (0.1 ml) in 7 days. Yield of 16 mg (38%). Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.95 d (2H, J=7.2 Hz), 7.58 t (1H, J=7.4), 7.44-7.53 m (3H), 7.05 d (1H, J=2.0 Hz), 6.99 dd (1H, J= 8.1, 2.0), 4.95 dd (1H, J=9.4, 3.0 Hz), 3.88-4.06 m (2H), 2.62 s (3H, Me), 2.29 s (3H, Me). ^{13}C NMR (CDCl3, 101 MHz) δ, ppm: 196.1, 139.2, 137.8, 136.5, 133.4, 132.9, 131.6, 128.7, 128.1, 126.7, 126.5, 104.2, 54.7, 42.9, 21.0, 20.7. MALDI, m/z: $[M+H]^+$ Calcd. for $C_{18}H_{18}Cl_3O$ 355.0418; Found 355.0423.

4,4,4-Trichloro-3-(2,4-dimethylphenyl)-1-(4-fluorophenyl)butan-1-one (5da). It was obtained from (*E*)-4,4,4-trichloro-1-(4-fluorophenyl)but-2-en-1-one **(2d)** (20 mg, 0.1 mmol) and *m*-xylene (0.1 ml) in 7 days. Yield of 9 mg (30%). Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.98 dd (2H, J=8.8, 5.4 Hz), 7.49 d (1H, J=8.0 Hz), 7.14 t (2H, J=8.6 Hz), 7.05 s (1H), 6.99 d (1H, J=8.1 Hz), 4.63 dd (1H, J=9.3, 3.1 Hz), 3.98 dd (1H, J=17.6, 9.3 Hz), 3.88 dd (1H, J=17.6, 3.1 Hz),

2.62 s (3H), 2.29 s (3H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 194.5, 165.9 d (J = 255.5 Hz), 139.2, 137.9, 132.9 d (J = 2.1 Hz), 131.6, 130.7 d (J = 9.4 Hz), 128.7, 126.6, 126.5, 115.8 d (J = 22.0 Hz), 104.1, 54.7, 42.8, 21.0, 20.6. ^{19}F NMR ($CDCl_3$, 376 MHz) δ, ppm: -104.6. MALDI, m/z: $[M+H]^+$ Calcd. for $C_{18}H_{17}Cl_3FO$ 373.0324; Found 373.0325.

4,4,4-Trichloro-1-(4-chlorophenyl)-3-(2,5-dimethylphenyl)butan-1-one (5ea). It was obtained from (*E*)-4,4,4-trichloro-1-(4-chlorophenyl)but-2-en-1-one **(2e)** (30 mg, 0.1 mmol) and *p*-xylene (0.1 ml) in 7 days. Yield of 10 mg (24%). Yellow oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.89 d (2H, J=8.6 Hz), 7.45 d (2H, J=8.6 Hz), 7.38 s (1H), 7.11 d (1H, J=7.7 Hz), 7.03 d (1H, J=7.7 Hz), 4.94 dd (1H, J=8.6, 3.7 Hz), 3.86-4.00 m (2H), 2.60 s (3H), 2.30 s (3H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 194.8, 139.9, 136.2, 135.6, 135.1, 134.8, 130.6, 129.5, 129.01, 128.99, 127.4, 103.9, 54.8, 42.9, 29.7, 20.3. MALDI, m/z: $[M+H]^+$ Calcd. for $C_{18}H_{17}Cl_4O$ 389.0028; Found 389.0027.

4,4,4-Trichloro-3-(4-hydroxyphenyl)-1-phenylbutan-1-one (5ab). It was obtained from (*E*)-4,4,4-trichloro-1-phenylbut-2-en-1-one **(2a)** (60 mg, 0.2 mmol) and anisole (0.1 ml) in 4 days. Yield of 36 mg (44%). White solid. m.p. 172-174°C (chloroform-hexane). ^{1}H NMR ($(CD_3)_2CO$, 400 MHz) δ, ppm: 8.46 s (1H), 8.04 d (2H, J=7.4 Hz), 7.64 t (2H, J=7.4 Hz), 7.53 t (1H, J=7.4 Hz), 7.45 d (2H, J=8.5 Hz), 6.81 d (2H, J=8.5 Hz), 4.54 dd (1H, J=9.4, 2.8 Hz), 4.16 dd (1H, J=17.6, 9.4 Hz), 3.93 dd (1H, J=17.6, 2.8 Hz). ^{13}C NMR ($(CD_3)_2CO$, 101 MHz) δ, ppm: 195.5, 157.5, 136.8, 133.3, 131.7, 128.7, 128.0, 127.7, 114.7, 104.3, 60.3, 41.4. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{16}H_{14}Cl_3O_2$ 343.0054; Found 343.0061.

4,4,4-Trichloro-3-(4-hydroxyphenyl)-1-(4-fluorophenyl)butan-1-one (5db). It was obtained from (*E*)-4,4,4-trichloro-1-(4-fluorophenyl)but-2-en-1-one **(2d)** (60 mg, 0.2 mmol) and anisole (0.1 ml) in 4 days. Yield of 49 mg (60%). Colorless solid, m.p. 176-178°C (Chloroform-hexane). ^{1}H NMR ($(CD_3)_2CO$, 400 MHz) δ, ppm: 8.13 dd (2H, J=8.8, 5.5 Hz), 7.45 d (2H, J=8.6 Hz), 7.28 t (2H, J=8.8 Hz), 6.81 d (2H, J=8.6 Hz), 4.53 dd (1H, J=9.5, 3.0 Hz), 4.16 dd (1H, J=17.6, 9.5 Hz), 3.92 dd (1H, J=17.6, 3.0 Hz). ^{13}C NMR ($(CD_3)_2CO$, 101 MHz) δ, ppm: 194.1, 165.7 d (J = 252.7 Hz), 157.5, 133.4 d (J = 3.0 Hz), 131.7, 131.0 d (J = 9.4 Hz), 127.7, 115.6 d (J = 22.0 Hz), 114.7, 104.2, 60.3, 41.4. ^{19}F NMR ($(CD_3)_2CO$, 376 MHz) δ, ppm: -107.2. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{16}H_{13}Cl_3FO_2$ 360.9960; Found 360.9967.

1-(4-Chlorophenyl)-4,4,4-trichloro-3-(4-hydroxyphenyl)butan-1-one (5eb). It was obtained from (*E*)-4,4,4-trichloro-1-(4-chlorophenyl)but-2-en-1-one **(2e)** (60 mg, 0.2 mmol) and anisole (0.1 ml) in 4 days. Yield of 35 mg (44%). Colorless solid, m.p. 148-149°C (Chloroform-hexane). ^{1}H NMR ($(CD_3)_2CO$, 400 MHz) δ, ppm: 8.47 s (1H), 8.05 d (2H, J=8.6 Hz), 7.56 d (2H, J=8.6 Hz), 7.45 d (2H, J=8.6 Hz), 6.81 d (2H, J=8.6 Hz), 4.52 dd (1H, J=9.5, 3.0 Hz), 4.16 dd (1H, J=17.6, 9.5 Hz), 3.93 dd (1H, J=17.6, 3.0 Hz). ^{13}C NMR ($(CD_3)_2CO$, 101 MHz) δ, ppm: 194.6,

157.6, 139.0, 135.3, 131.7, 129.9, 128.8, 127.6, 114.8, 104.1, 60.3, 41.4. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{16}H_{13}Cl_4O_2$ 376.9664; Found 376.9665.

1-(4-Bromophenyl)-4,4,4-trichloro-3-(4-hydroxyphenyl)butan-1-one (5fb). It was obtained from 1-(4-bromophenyl)-4,4,4-trichloro-3-hydroxybutan-1-one **(1f)** (60 mg, 0.2 mmol) and anisole (0.1 ml) in 4 days. Yield of 46 mg (63%). Colorless solid, m.p. 154-156°C (chloroform-hexane). ^{1}H NMR ($(CD_3)_2CO$, 400 MHz) δ, ppm: 8.48 s (OH), 7.97 d (2H, J=8.6 Hz), 7.71 d (2H, J=8.6), 7.45 d (2H, J=8.6 Hz), 6.81 d (2H, J=8.6 Hz), 4.52 dd (1H, J=9.5, 3.0 Hz), 4.15 dd (1H, J=17.7, 9.5 Hz), 3.93 dd (1H, J=17.7, 3.0 Hz). ^{13}C NMR ($(CD_3)_2CO$, 101 MHz) δ, ppm: 194.8, 157.6, 135.7, 131.9, 131.7, 130.0, 127.7, 127.6, 114.8, 104.1, 60.3, 41.4. HRMS (ESI), m/z: $[M+H]^+$ Calcd. for $C_{16}H_{13}BrCl_3O_2$ 420.9159; Found 420.9161.

4,4,4-Trichloro-3-(4-hydroxyphenyl)-1-(naphthalen-2-yl)butan-1-one (5l). It was obtained from (*E*)-4,4,4-trichloro-1-(naphthalen-2-yl)but-2-en-1-one **(2l)** (60 mg, 0.2 mmol) and anisole (0.1 ml) in 4 days. Yield of 24 mg (30%). Colorless solid, m.p. 110-112°C (chloroform-hexane). ^{1}H NMR ($(CD_3)_2CO$, 400 MHz) δ, ppm: 8.78 s (1H), 8.48 s (OH), 8.14 d (1H, J=7.4 Hz), 7.95-8.04 m (3H), 7.66 dddd (2H, J=18.8, 8.1, 6.9, 1.4 Hz), 7.49 d (2H, J=8.7 Hz), 6.81 d (2H, J=8.6 Hz), 4.60 dd (1H, J=9.6, 2.9 Hz), 4.33 dd (1H, J=17.5, 9.6 Hz), 4.05 dd (1H, J=17.5, 2.8 Hz). ^{13}C NMR ($(CD_3)_2CO$, 101 MHz) δ, ppm: 195.5, 157.6, 135.7, 134.1, 132.7, 131.7, 130.1, 129.7, 128.7, 128.4, 127.74, 127.71, 126.9, 123.6, 114.8, 104.3, 60.4, 41.4. MALDI, m/z: $[M+H]^+$ Calcd. for $C_{20}H_{16}Cl_3O_2$ 393.0210; Found 393.0214.

5,6-Dimethyl-3-phenyl-1-(trichloromethyl)-1*H*-indene (6a) and 6,7-dimethyl-3-phenyl-1-(trichloromethyl)-1H-indene (6aa). They were obtained from (*E*)-4,4,4-trichloro-1-phenylbut-2-en-1-one **(2a)** (30 mg, 0.1 mmol) and *o*-xylene (0.1 ml) in 7 days in total yield of 13 mg (32%) with **6a/6aa** ratio of 7 : 1. Pale yellow oil. Compound **6a**: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: (selected signals from spectrum of isomer mixture) 6.56 d (1H, J=2.1 Hz), 4.60 d (1H, J=2.1 Hz), 2.38 s (3H, Me), 2.34 s (3H, Me). Compound **6aa**: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: (selected signals from spectrum of isomer mixture) 6.51 d (1H, J=2.1 Hz), 4.58 d (1H, J=2.1 Hz), 2.37 s (3H, Me), 2.31 s (3H, Me). For mixture of isomers: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.82 s (1H), 7.64 d (2H, J=7.1Hz), 7.51 d (2H, J=7.1 Hz), 7.45 t (1H, J=7.1 Hz), 7.33 s (1H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 148.4, 142.5, 139.1, 136.7, 134.9, 134.5, 129.1, 128.7, 128.4, 127.8, 127.0, 122.2, 100.1, 67.3, 20.23, 20.18. MALDI, m/z: $[M+H]^+$ Calcd. for $C_{18}H_{16}Cl_3$ 337.0312; Found 337.0314.

5,6-Dimethyl-3-(4-fluorophenyl)-1-(trichloromethyl)-1H-indene (6d) and 6,7-dimethyl-3-(4-fluorophenyl)-1-(trichloromethyl)-1*H*-indene (6da). They were obtained from (*E*)-4,4,4-trichloro-1-(4-fluorophenyl)but-2-en-1-one **(2d)** (118 mg, 0.4 mmol) and *o*-xylene (0.1 ml) in 7 days in total yield of 118 mg (75%) with **6d/6da** ratio of 3 : 1. Pale yellow oil. Compound **6d**: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.82 s (1H), 7.60 dd (2H, J=8.6, 5.5 Hz), 7.26 s (1H), 7.19 t (2H, J=8.6 Hz), 6.53 d (1H, J=2.2 Hz), 4.59 d (1H, J=2.2 Hz), 2.38 s (3H), 2.34 s (3H). ^{13}C NMR

(CDCl3, 101 MHz) δ, ppm: 162.8 d (*J* = 247.5 Hz), 147.4, 142.4, 139.0, 137.1, 134.7, 130.9 d (*J* = 3.4 Hz), 129.5 d (*J* = 8.1 Hz), 129.1, 127.1, 122.0, 115.7 d (*J* = 21.6 Hz), 100.0, 67.3, 20.2, 20.2. ^{19}F NMR ($CDCl_3$, 376 MHz) δ, ppm: -104.6. Compound **6da**: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: (selected signals from spectrum of isomer mixture) 7.80 s (1H), 6.50 d (1H, J=2.2 Hz), 4.57 d (1H, J=2.2 Hz), 2.37 s (3H, Me), 2.30 s (3H, Me). For mixture of isomers: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: 7.82 s (1H), 7.64 d (2H, J =7.1Hz), 7.51 d (2H, J=7.1 Hz), 7.45 t (1H, J=7.1 Hz), 7.33 s (1H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 148.4, 142.5, 139.1, 136.7, 134.9, 134.5, 129.1, 128.7, 128.4, 127.8, 127.0, 122.2, 100.1, 67.3, 20.23, 20.18. MALDI, m/z: $[M+H]^+$ Calcd. for $C_{18}H_{15}Cl_3F$ 355.0218; Found 355.0215.

5,6-Dimethyl-3-(4-chlorophenyl)-1-(trichloromethyl)-1*H*-indene (6e) and 6,7-dimethyl-3-(4-chlorophenyl)-1-(trichloromethyl)-1*H*-indene (6ea). They were obtained from (*E*)-4,4,4-trichloro-1-(4-chlorophenyl)but-2-en-1-one **(2e)** (30 mg, 0.1 mmol) and *o*-xylene (0.1 ml) in 7 days in total yield of 16 mg (41%) with **6e/6ea** ratio of 2 : 1. Pale yellow oil. Compound **6e**: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: (selected signals from spectrum of isomer mixture) 7.81 s (1H), 7.56 d (2H, J=8.3 Hz), 7.47 d (2H, J=8.3 Hz), 7.26 s (1H), 6.55 d (1H, J=2.1 Hz), 4.58 d (1H, J=2.1 Hz), 2.38 s (3H), 2.34 s (3H). ^{13}C NMR (CDCl3, 101 MHz) δ, ppm: (selected signals from spectrum of isomer mixture) 20.23, 20.19. Compound **6ea**: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: (selected signals from spectrum of isomer mixture) 7.92 s (1H), 7.58 d (2H, J=8.3 Hz), 7.46 d (2H, J=8.3 Hz), 7.25 s (1H), 6.71 d (1H, J=2.1 Hz), 2.37 s (3H), 2.33 s (3H). ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: (selected signals from spectrum of isomer mixture) 20.30, 20.29. For mixture of isomers: ^{13}C NMR (CDCl3, 101 MHz) δ, ppm: 147.3, 144.4, 142.1, 140.3, 139.0, 138.3, 137.1, 136.9, 134.9, 134.8, 134.2, 133.4, 133.3, 132.8, 129.4, 129.1, 129.0, 128.9, 127.1, 125.9, 124.3, 122.6, 122.3, 122.0, 99.9, 67.3. MALDI, m/z: $[M+H]^+$ Calcd. for $C_{18}H_{15}Cl_4$ 370.9922; Found 370.9920.

4,5,7-Trimethyl-3-phenyl-1-(trichloromethyl)-1*H*-indene (6ab) and 4,6,7-trimethyl-3-phenyl-1-(trichloromethyl)-1*H*-indene (6aba). They were obtained from (*E*)-4,4,4-trichloro-1-phenylbut-2-en-1-one **(2a)** (30 mg, 0.1 mmol) and pseudocumene (0.1 ml) in 7 days in total yield of 10 mg (24%) with **6ab/6aba** ratio of 5 : 1. Pale yellow oil. Compound **6ab**: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: (selected signals from spectrum of isomer mixture) 7.40 dt (3H, J=8.9, 2.0 Hz), 7.29 – 7.34 m (2H), 6.96 s (1H), 6.40 d (1H, J=2.3 Hz), 4.63 d (1H, J=2.3 Hz), 2.58 s (3H, Me), 2.25 s (3H, Me), 1.85 s (3H, Me). Compound **6aba**: ^{1}H NMR ($CDCl_3$, 400 MHz) δ, ppm: (selected signals from spectrum of isomer mixture) 7.40 dt (3H, J=8.9, 2.0 Hz), 7.29 – 7.34 m (2H), 6.94 s (1H), 6.35 d (1H, J=2.3 Hz), 4.70 d (1H, J=2.3 Hz), 2.58 s (3H, Me), 2.25 s (3H, Me), 1.91 s (3H, Me). For mixture of isomers: ^{13}C NMR ($CDCl_3$, 101 MHz) δ, ppm: 150.2, 143.4, 138.8, 137.4, 137.0, 133.9, 133.6, 132.5, 131.2, 129.7, 129.6, 128.43, 128.39, 128.3, 101.6, 65.7, 22.5, 20.1, 15.9. MALDI, m/z: $[M+H]^+$ Calcd. for $C_{19}H_{18}Cl_3$ 351.0469; Found 351.0473.

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2. Copies of ^{1}H, $^{13}C\{^{1}H\}$, $^{19}F\{^{1}H\}$ NMR spectra of compounds 3-6

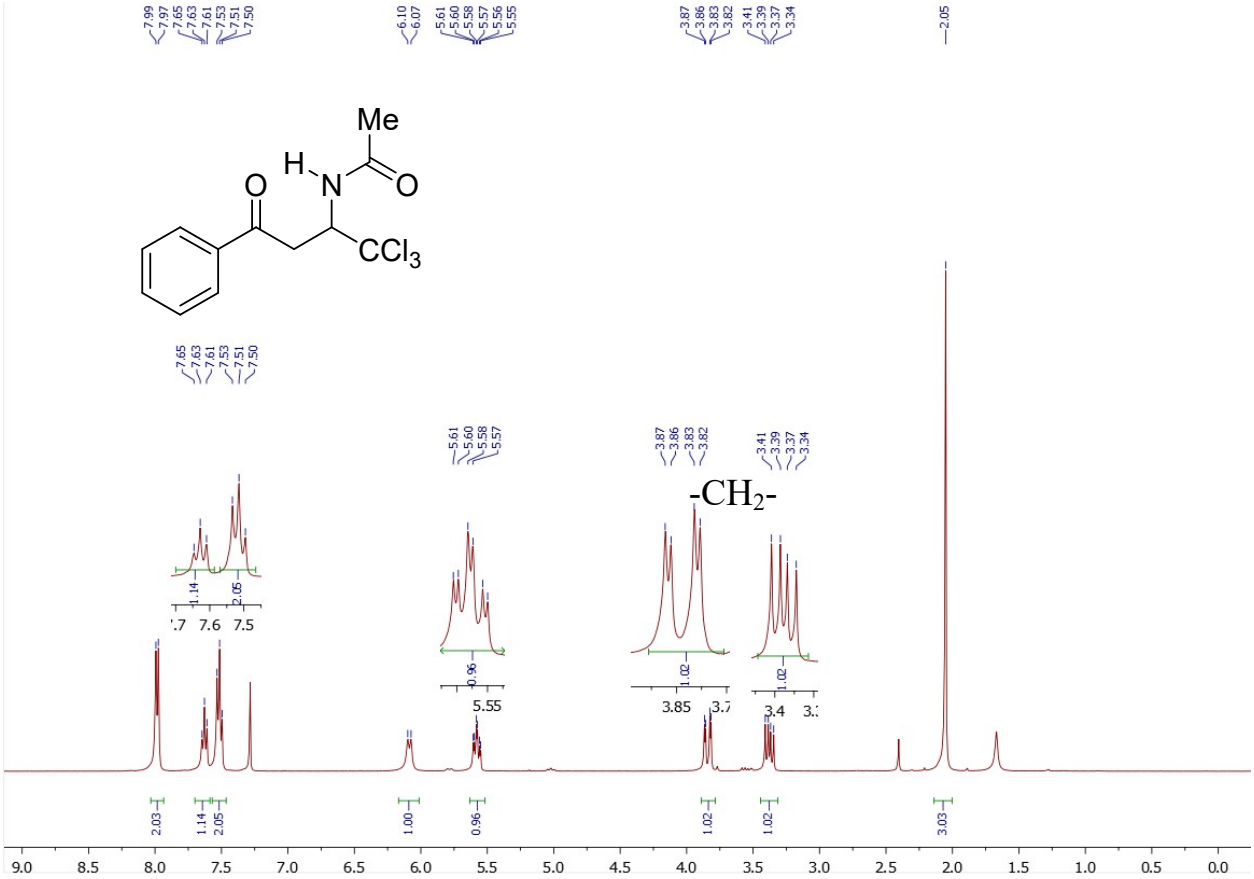


Fig.S1. ^{1}H NMR spectrum of the compound **3a** ($CDCl_3$, 400 MHz).

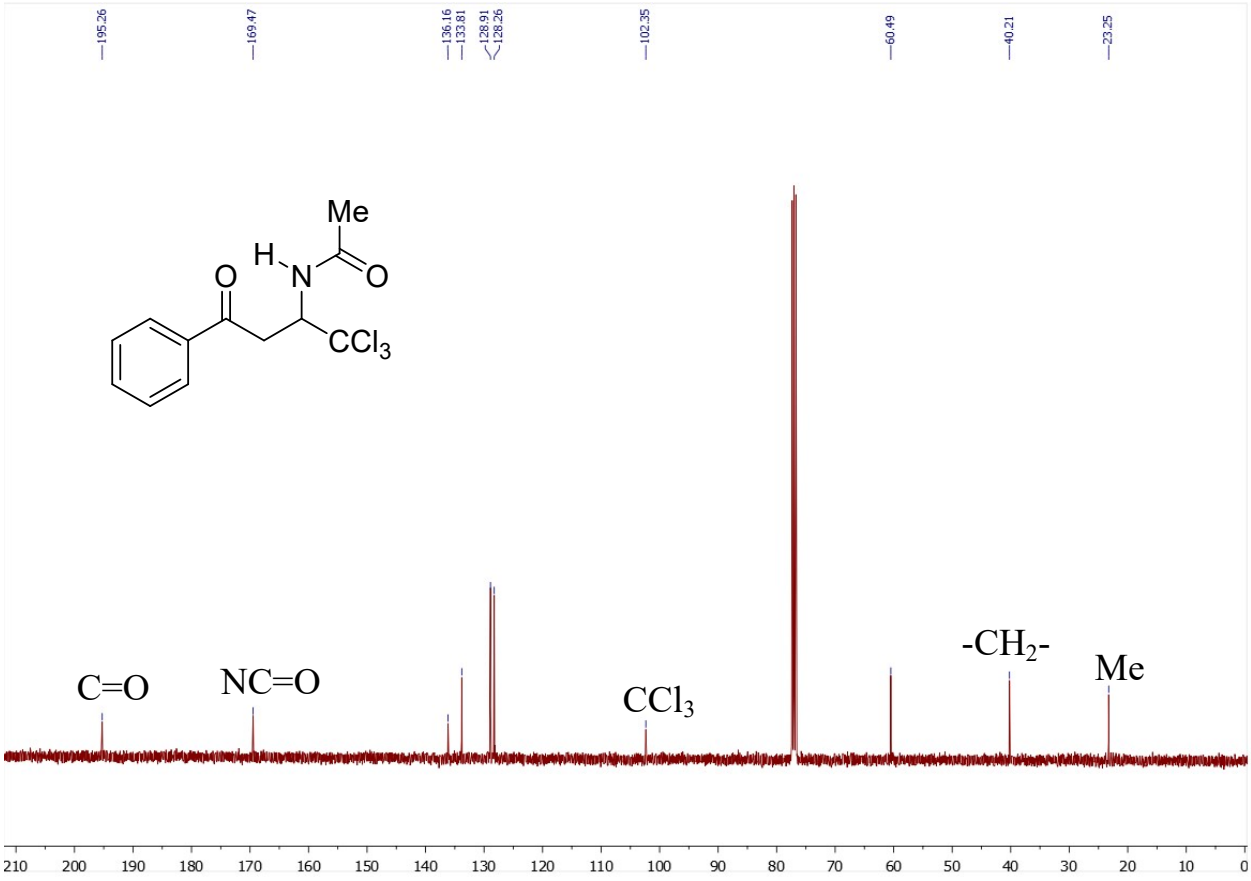


Fig. S2. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3a** ($CDCl_3$, 101 MHz).

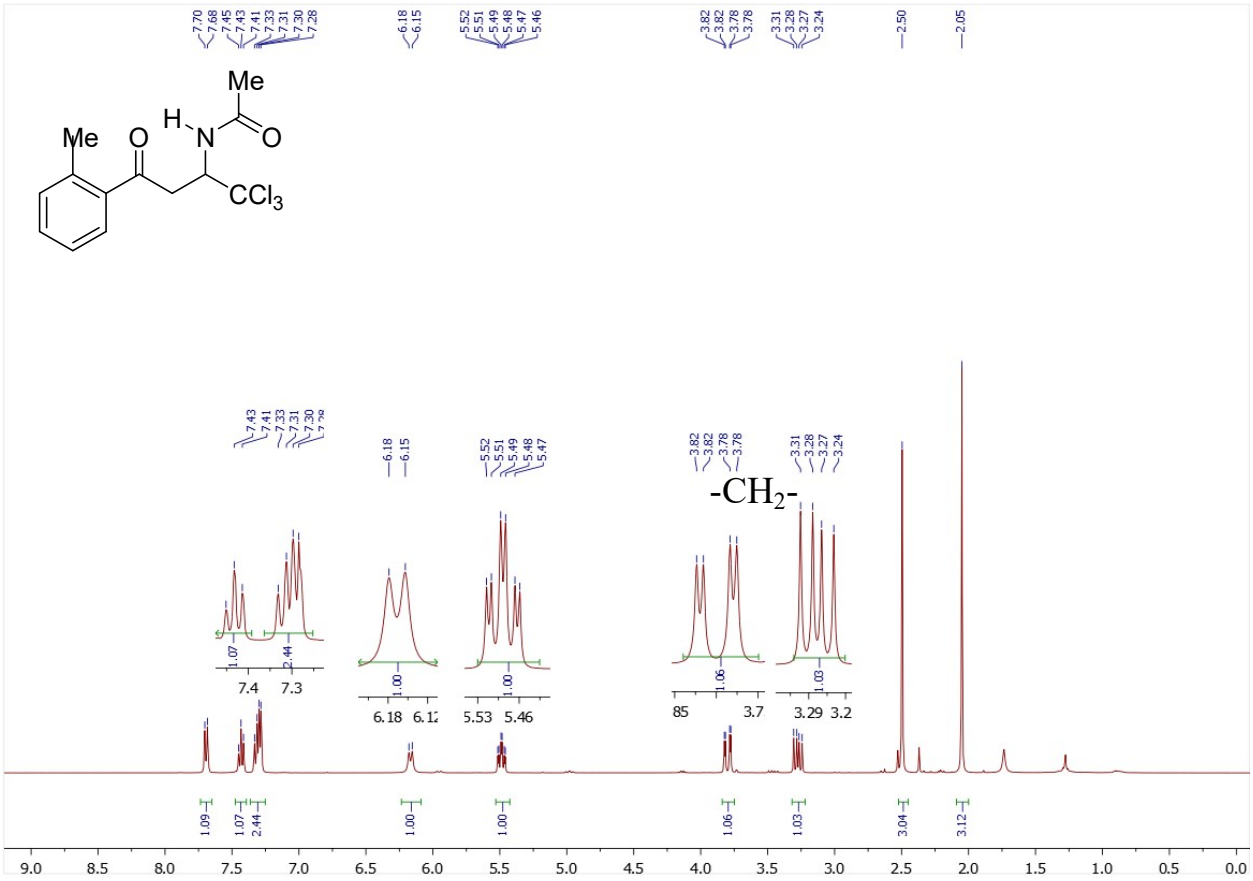


Fig.S3. ^{1}H NMR spectrum of the compound **3b** ($CDCl_3$, 400 MHz).

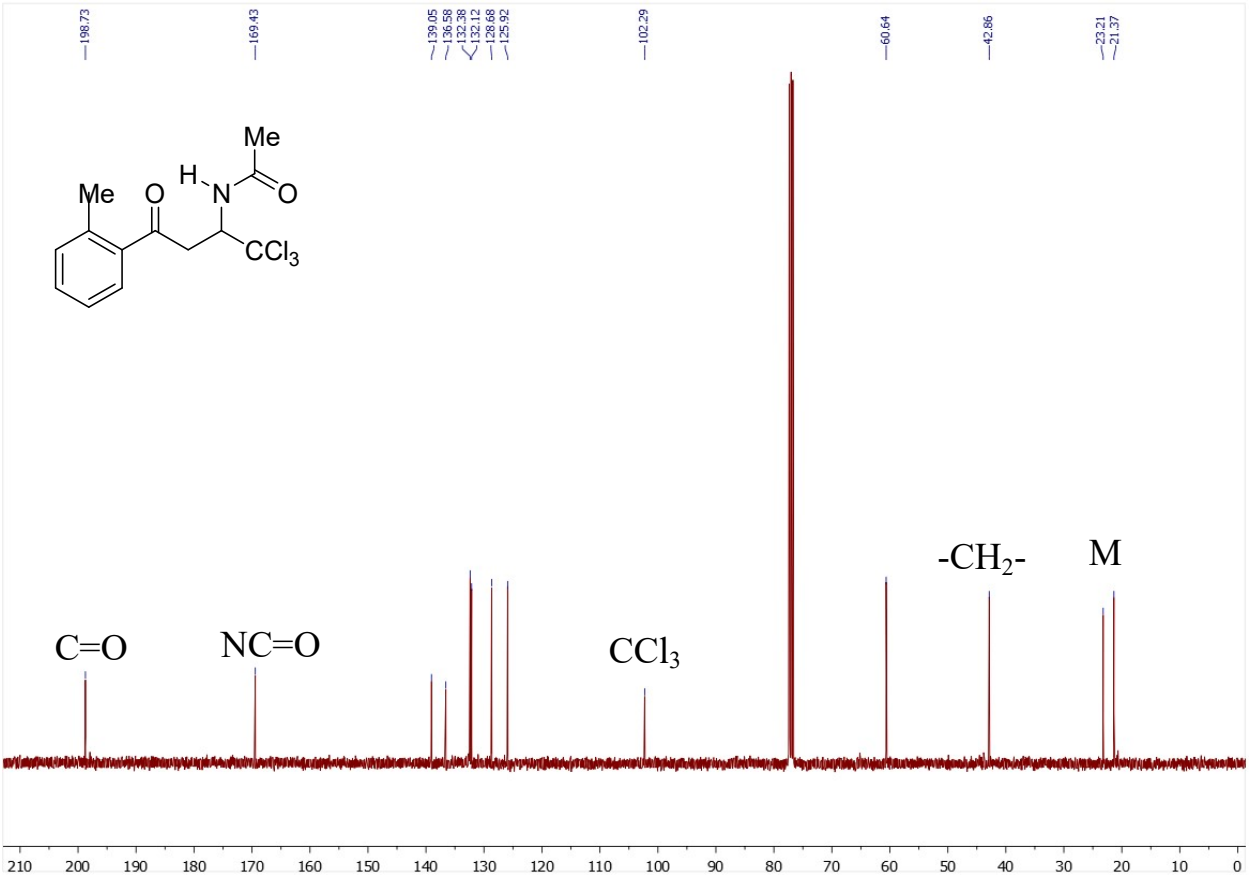


Fig. S4. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3b** ($CDCl_3$, 101 MHz).

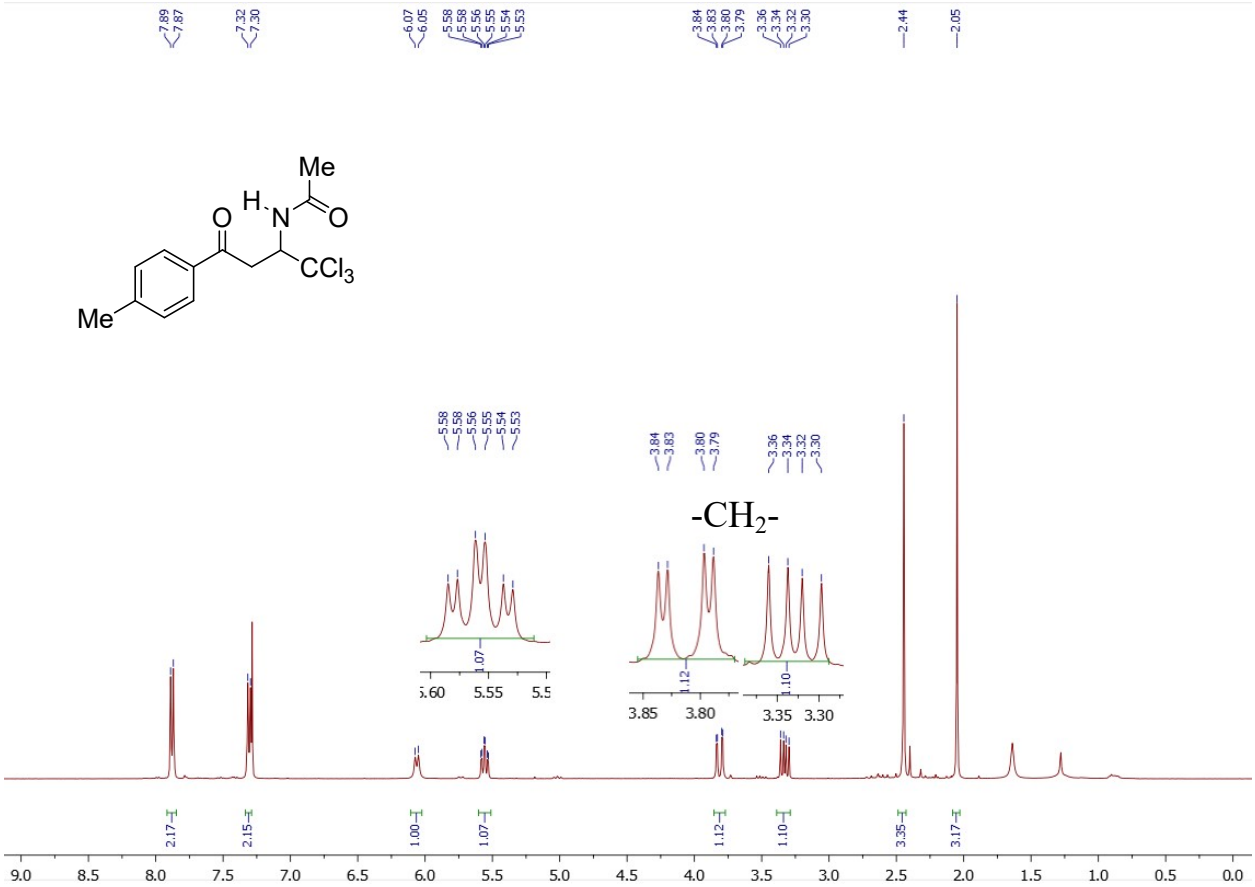


Fig.S5. ^{1}H NMR spectrum of the compound**3c** ($CDCl_3$, 400 MHz).

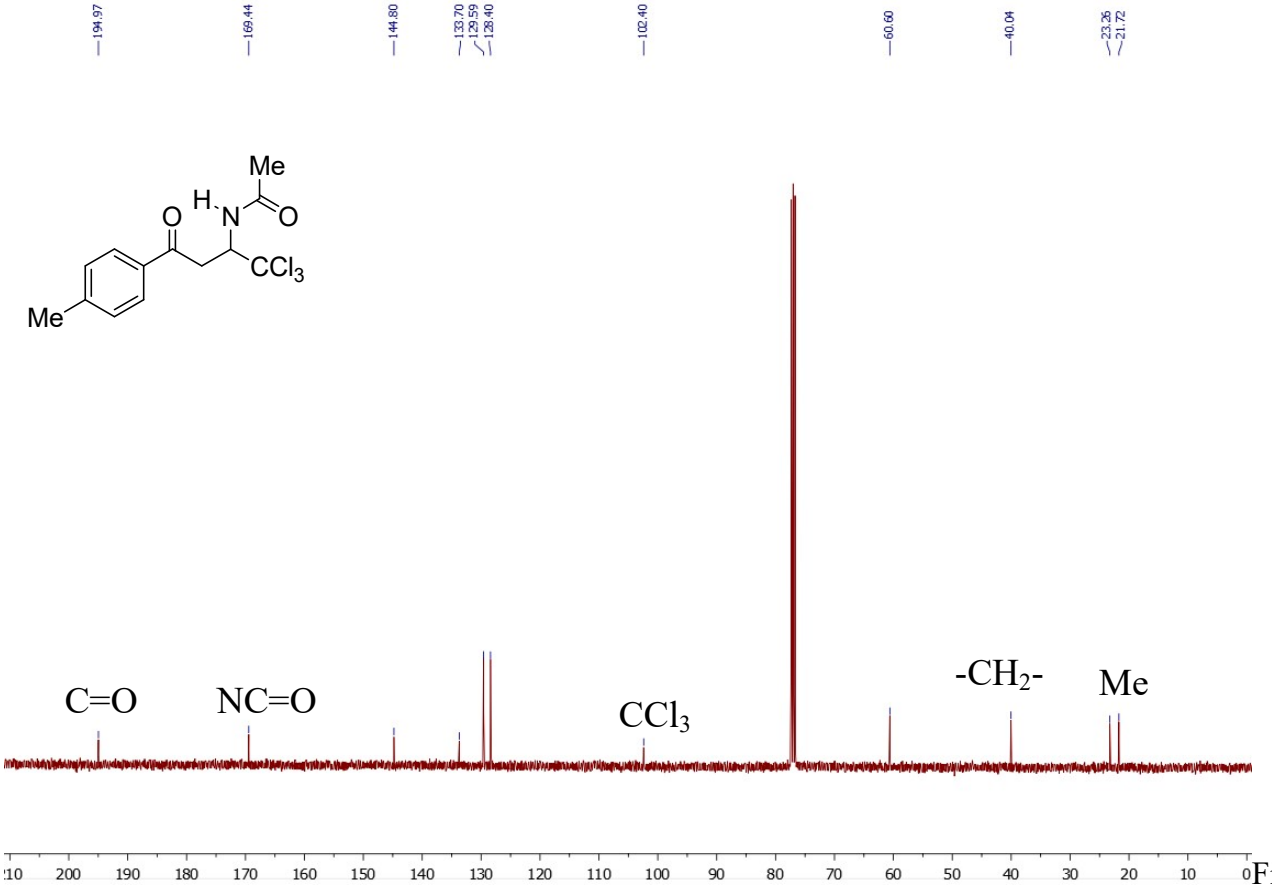


Fig. S6. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3c** ($CDCl_3$, 101 MHz).

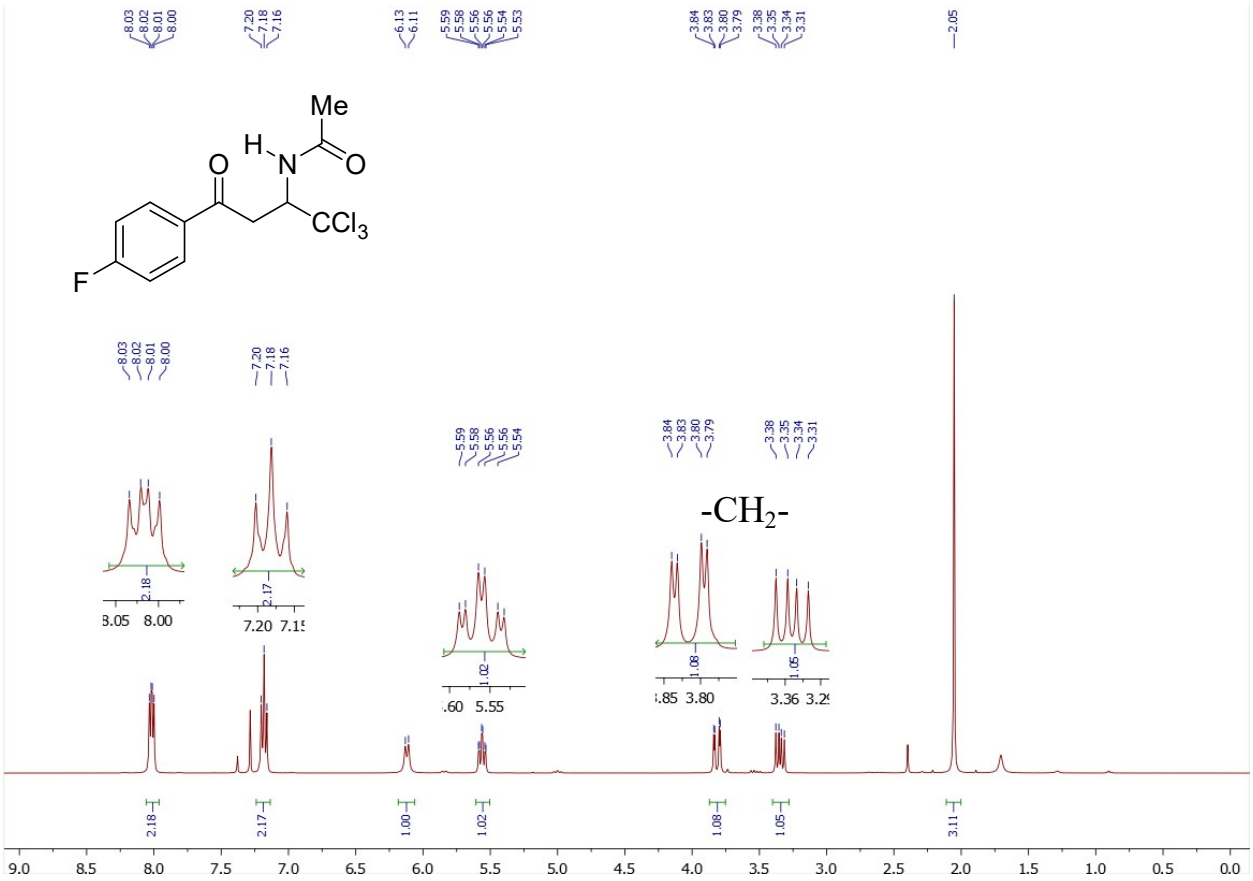


Fig.S7. ^{1}H NMR spectrum of the compound **3d** ($CDCl_3$, 400 MHz).

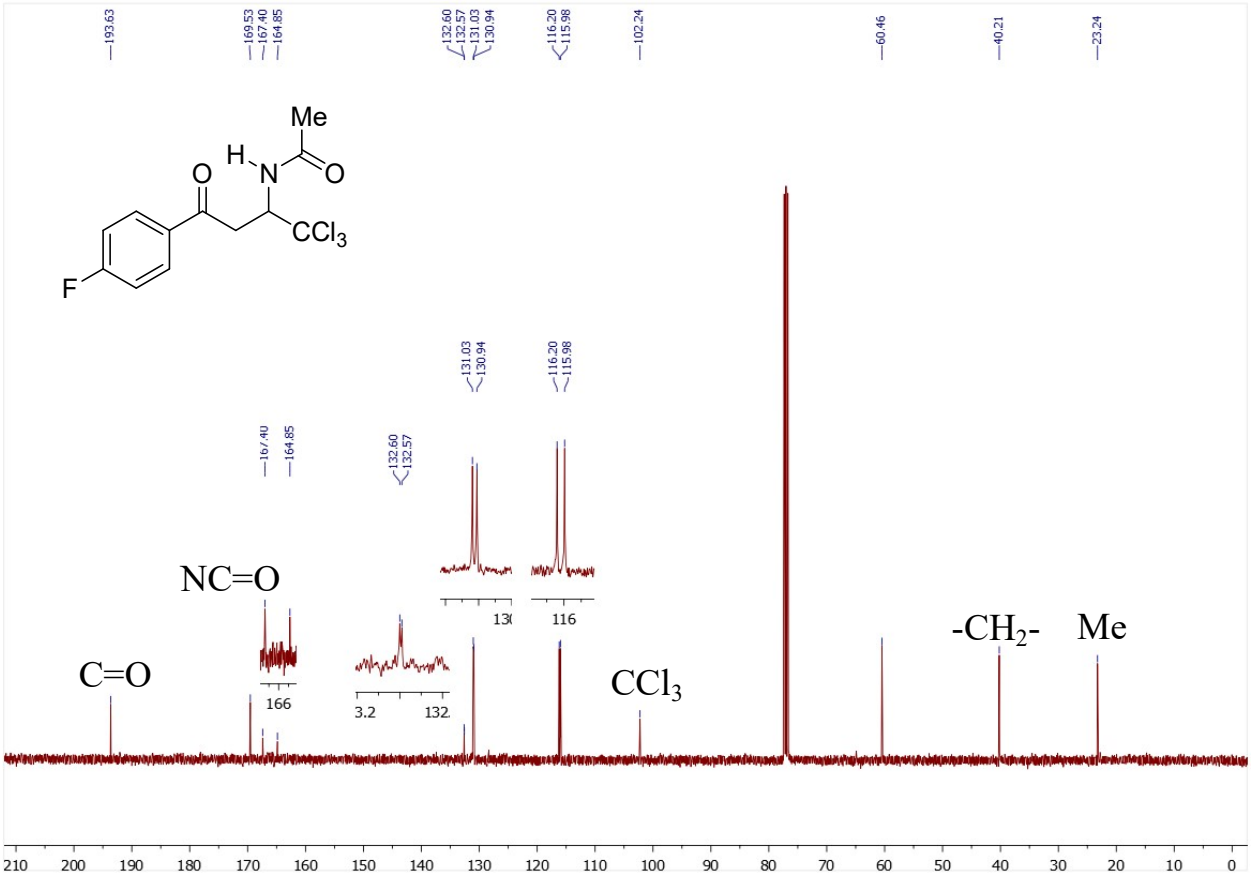


Fig. S8. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3d** ($CDCl_3$, 101 MHz).

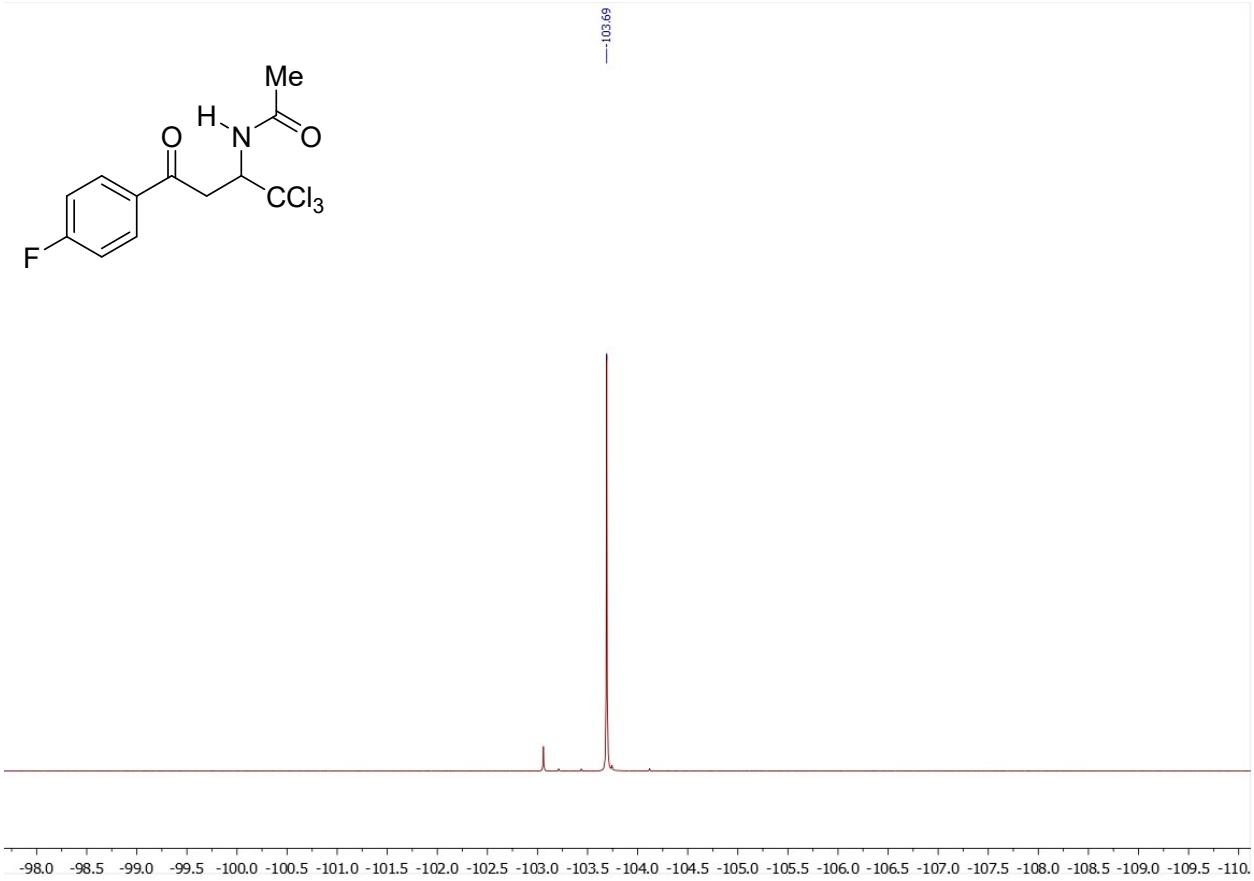


Fig. S9. $^{19}F\{^{1}H\}$ NMR spectrum of the compound **3d** ($CDCl_3$, 376 MHz).

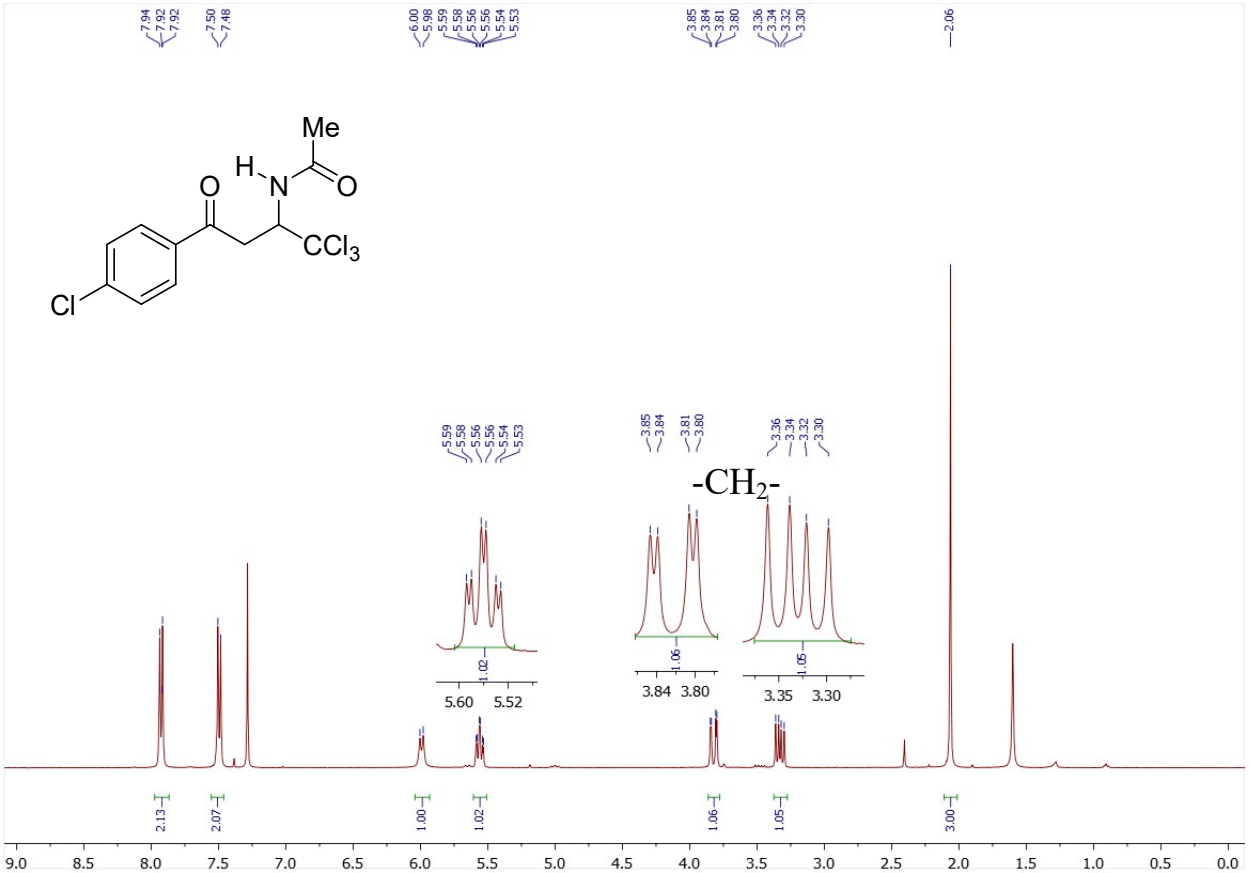


Fig.S10. ^{1}H NMR spectrum of the compound **3e** ($CDCl_3$, 400 MHz).

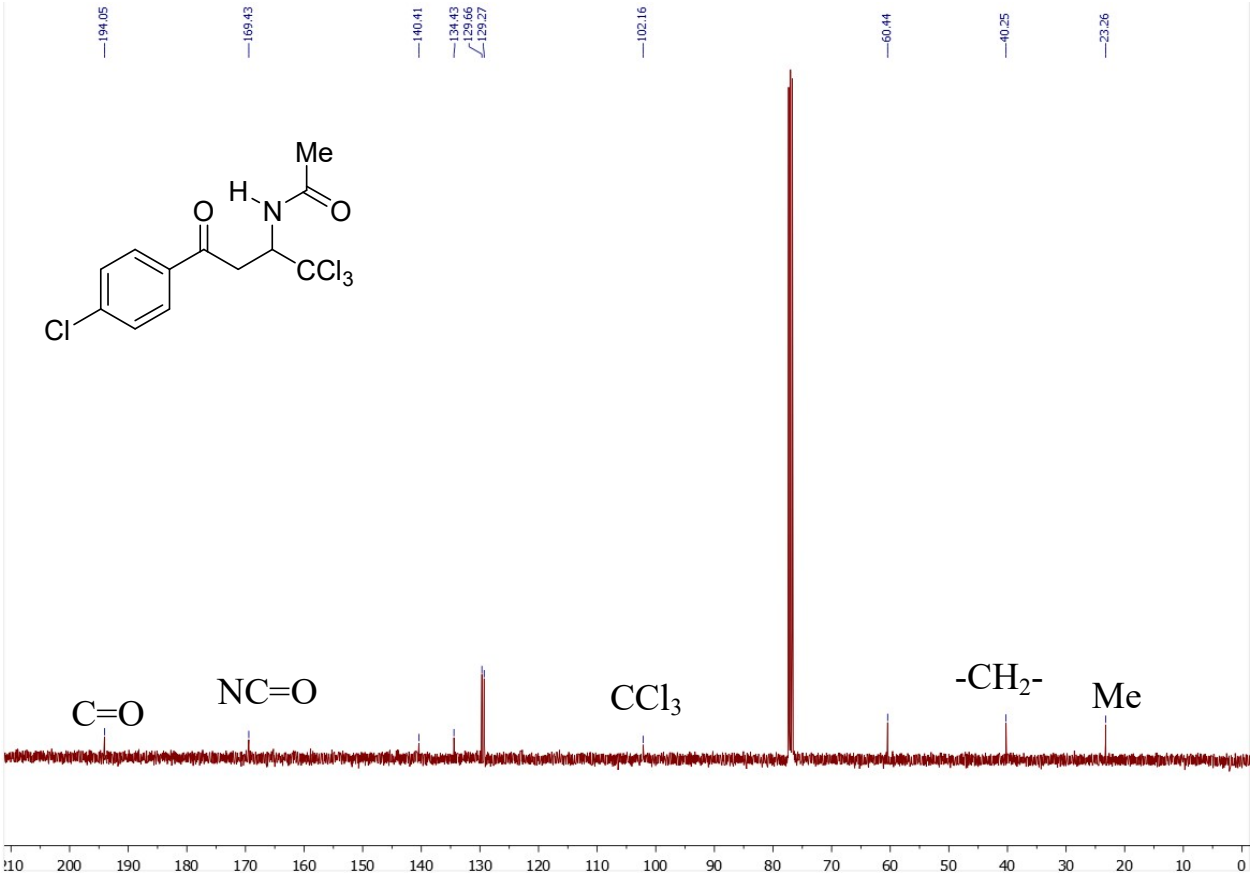


Fig. S11. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3e** ($CDCl_3$, 101 MHz).

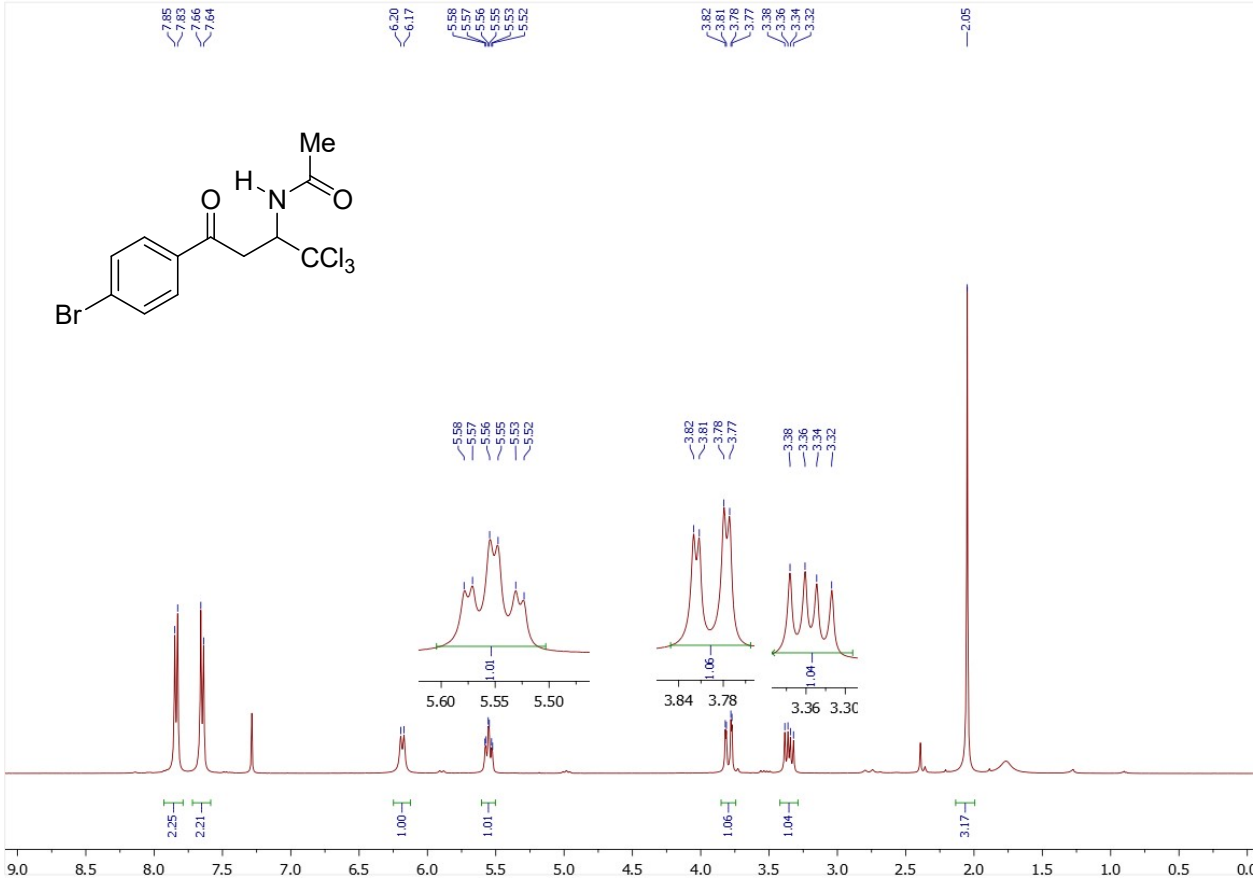


Fig.S12. ^{1}H NMR spectrum of the compound **3f** ($CDCl_3$, 400 MHz).

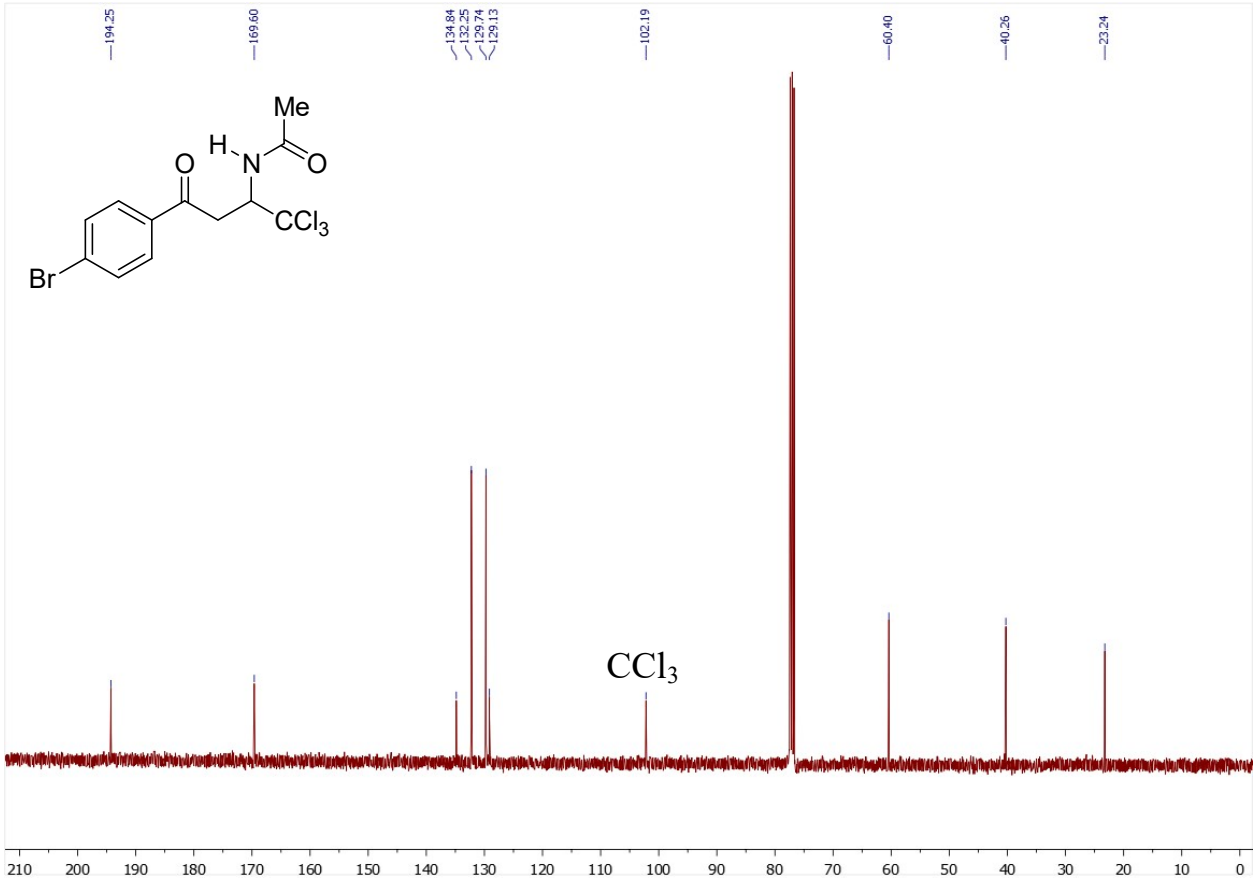


Fig. S13. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3f** ($CDCl_3$, 101 MHz).

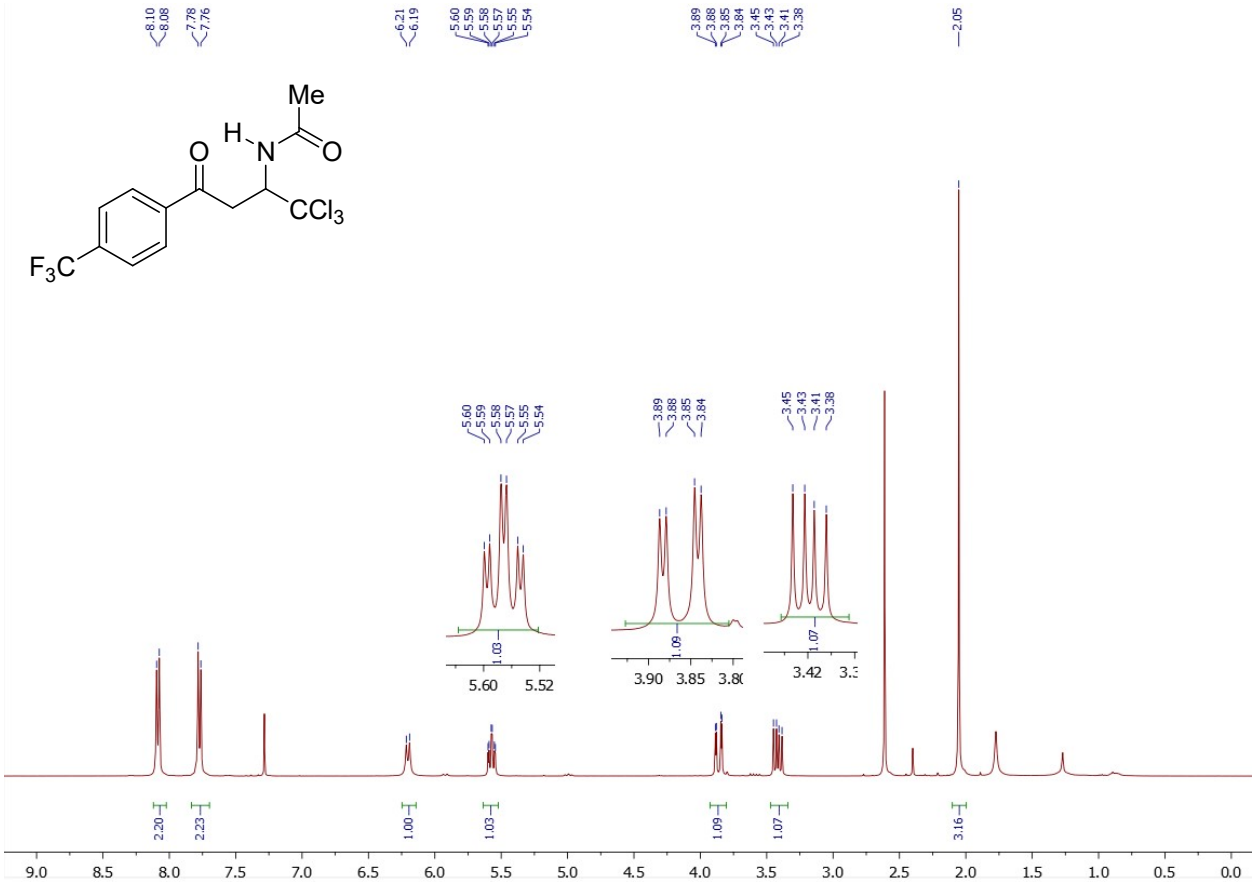


Fig.S14. ^{1}H NMR spectrum of the compound **3g** ($CDCl_3$, 400 MHz).

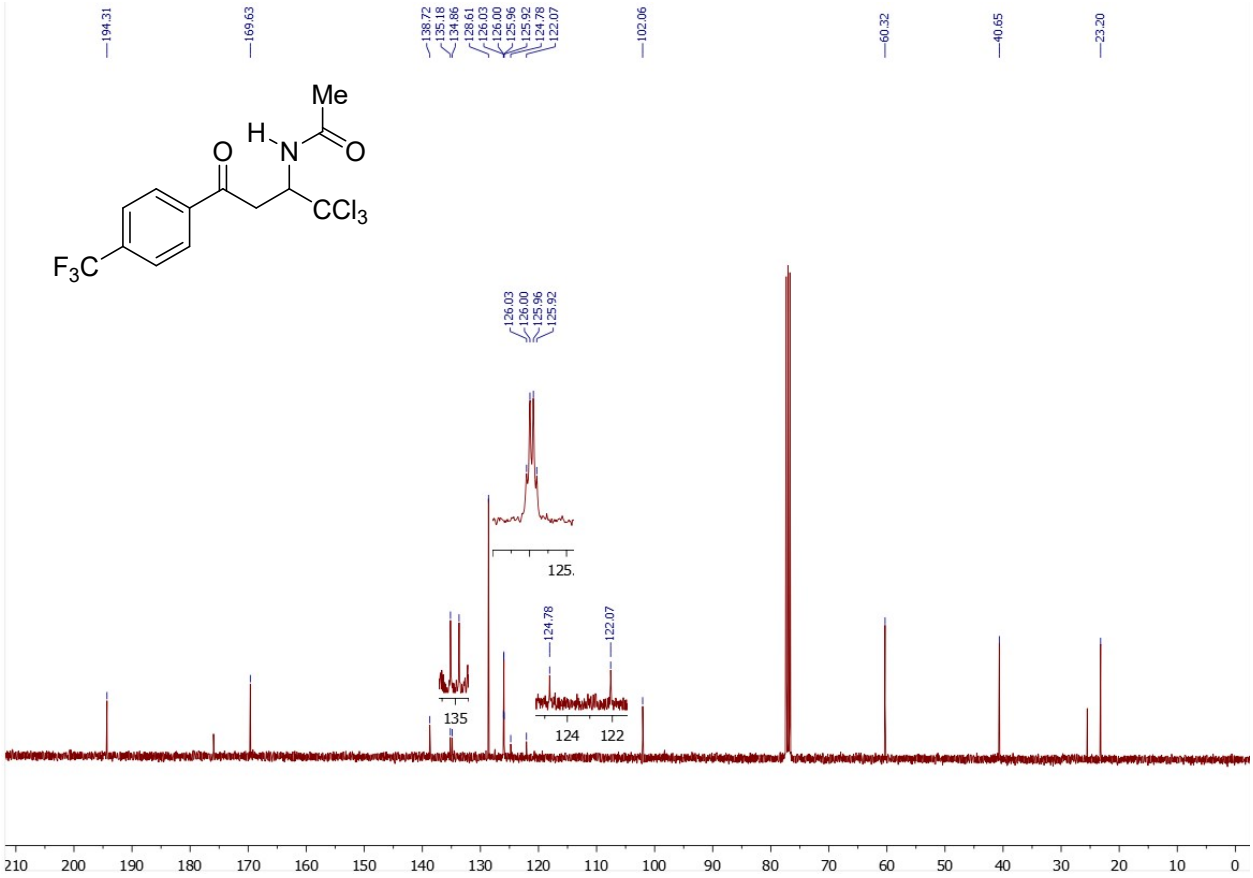


Fig. S15. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3g** ($CDCl_3$, 101 MHz).

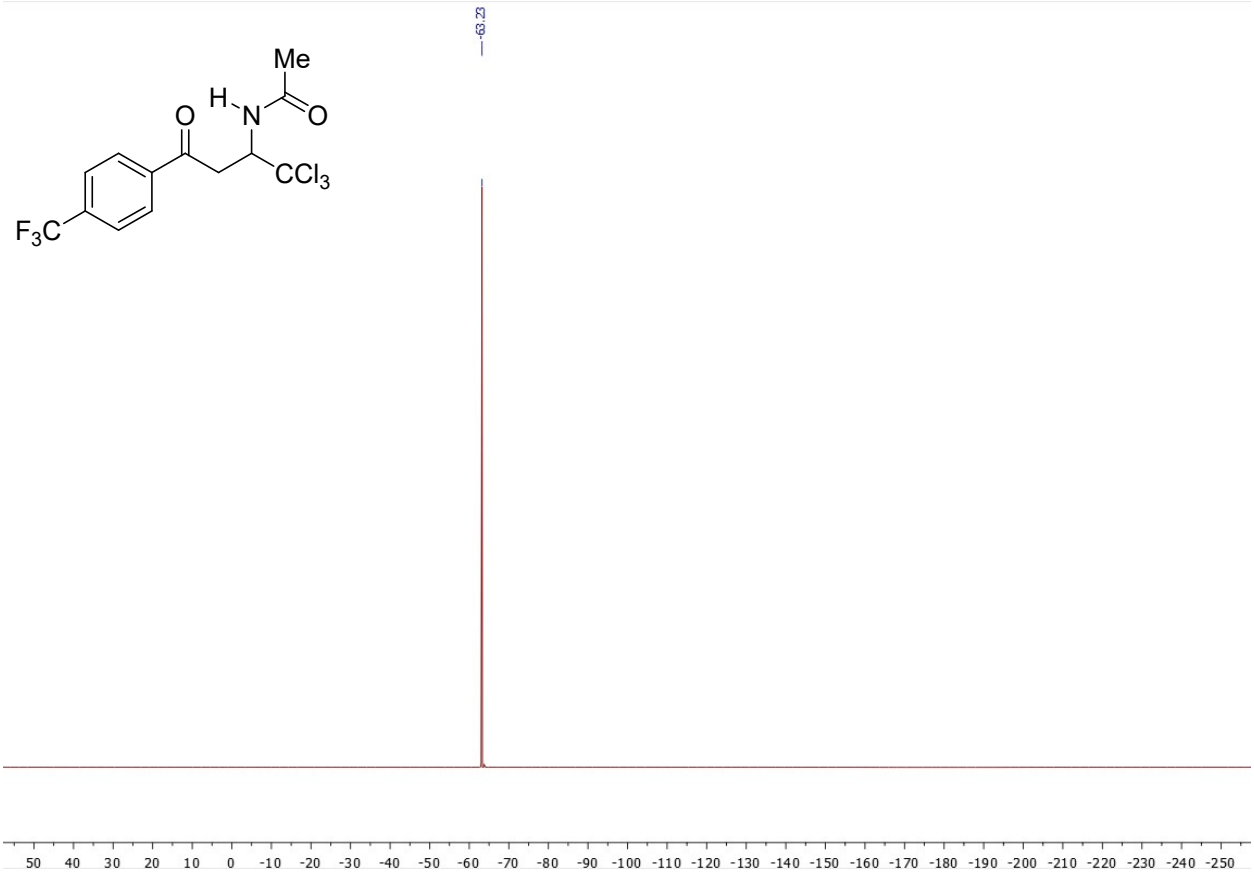


Fig. S16. $^{19}F\{^{1}H\}$ NMR spectrum of the compound **3d** ($CDCl_3$, 376 MHz).

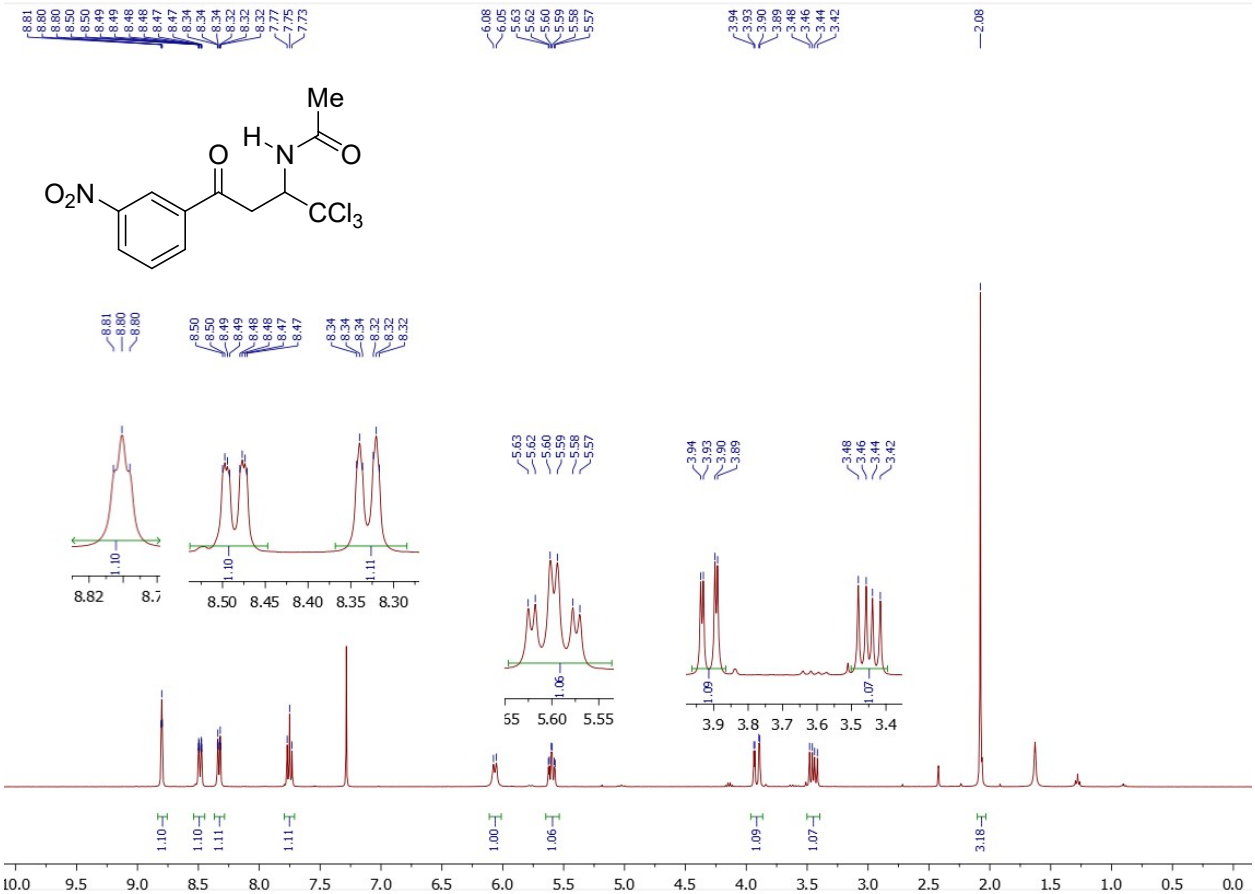


Fig.S17. ^{1}H NMR spectrum of the compound **3h** ($CDCl_3$, 400 MHz).

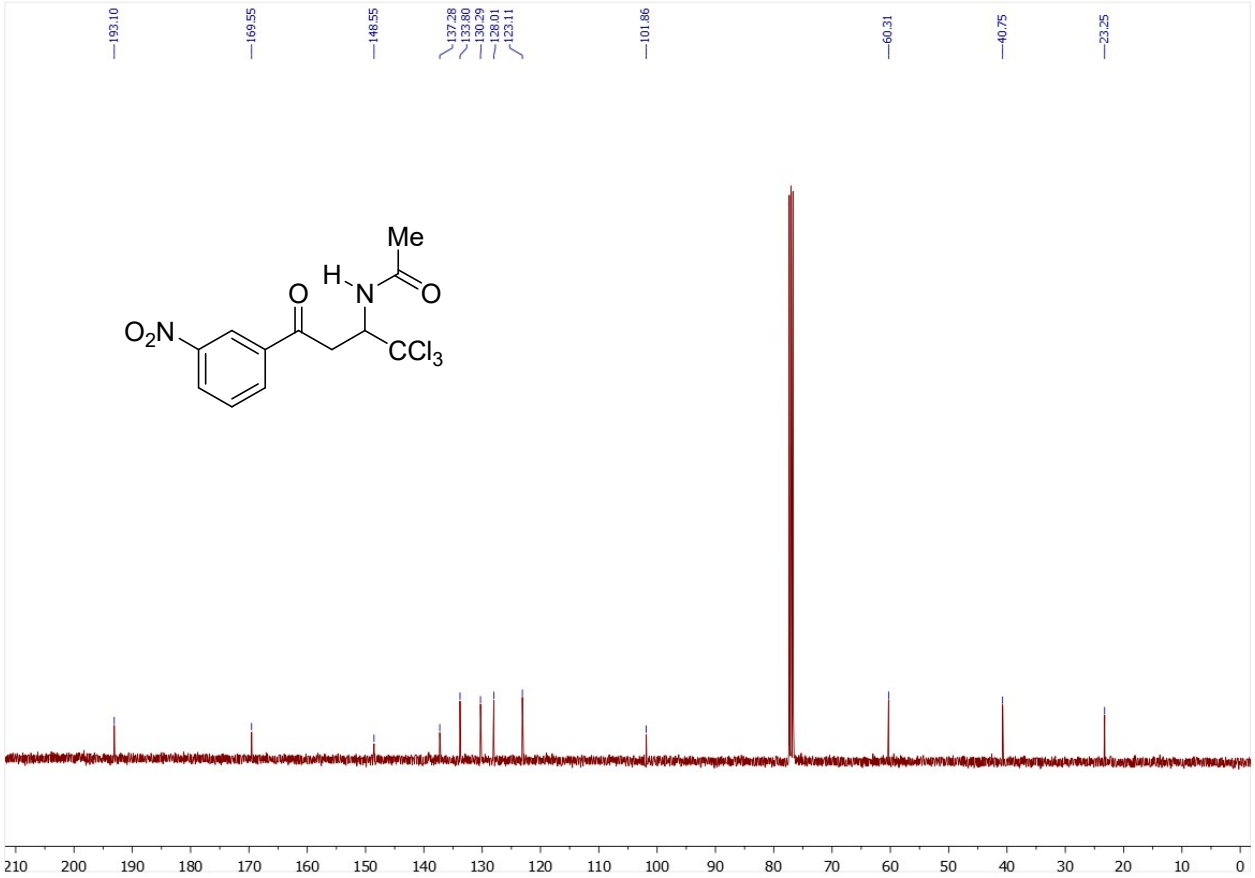


Fig. S18. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3h** ($CDCl_3$, 101 MHz).

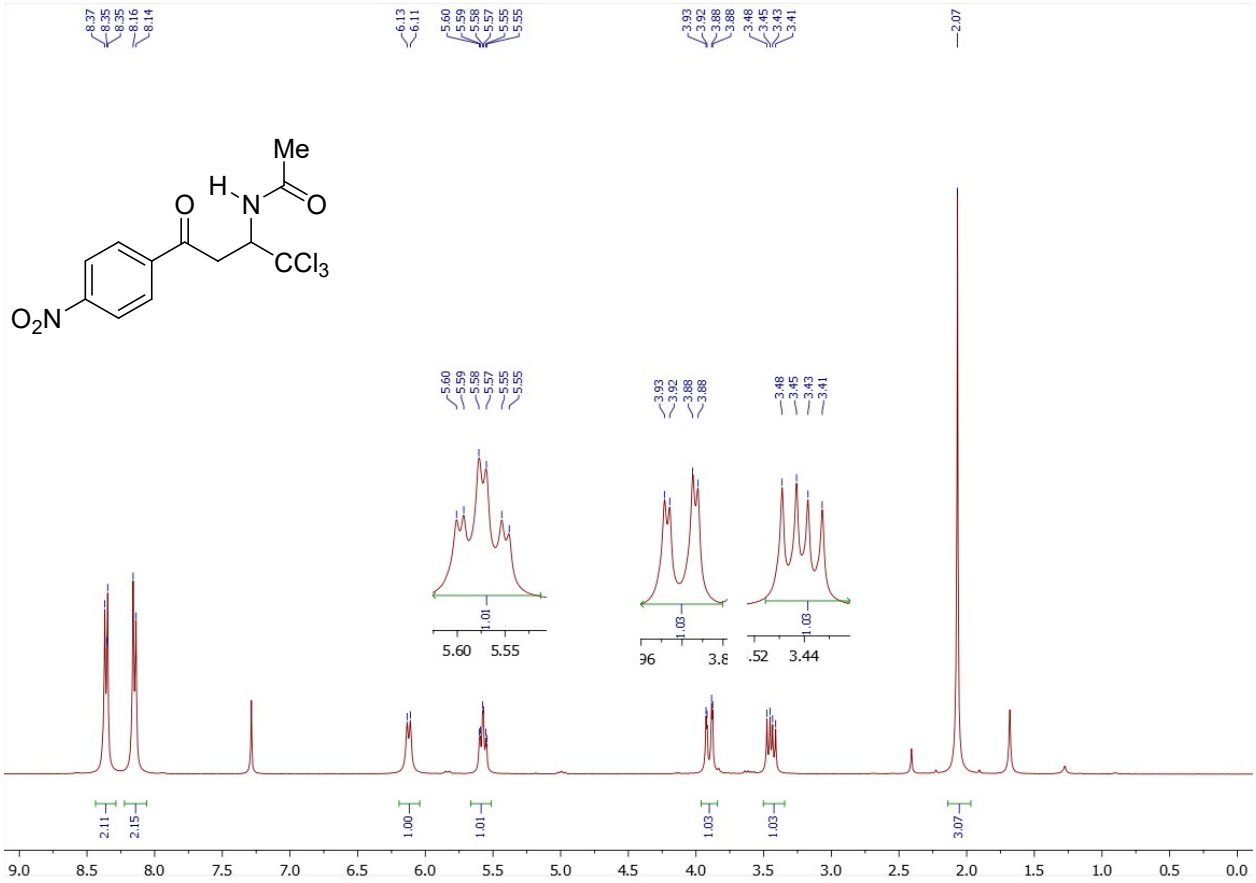


Fig.S19. ^{1}H NMR spectrum of the compound **3i** ($CDCl_3$, 400 MHz).

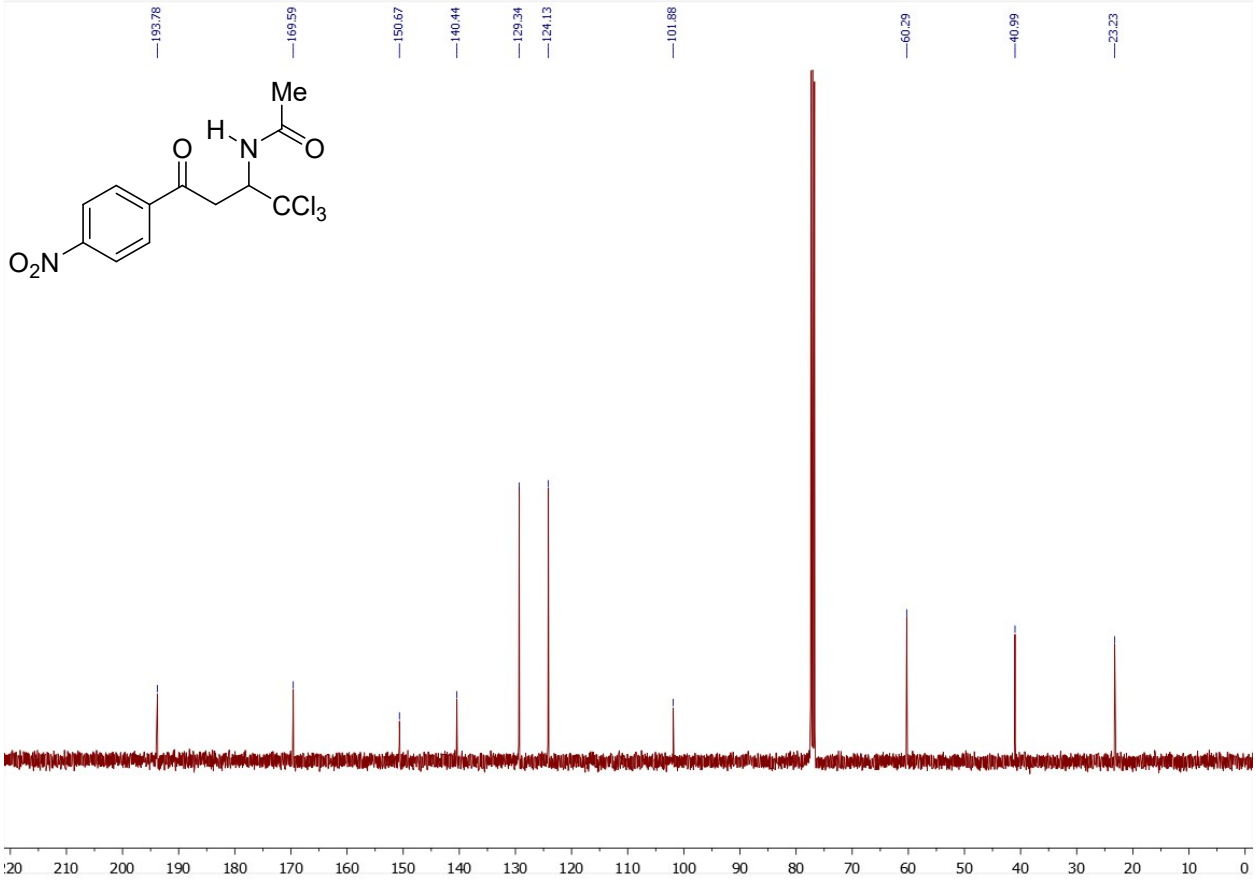


Fig. S20. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3i** ($CDCl_3$, 101 MHz).

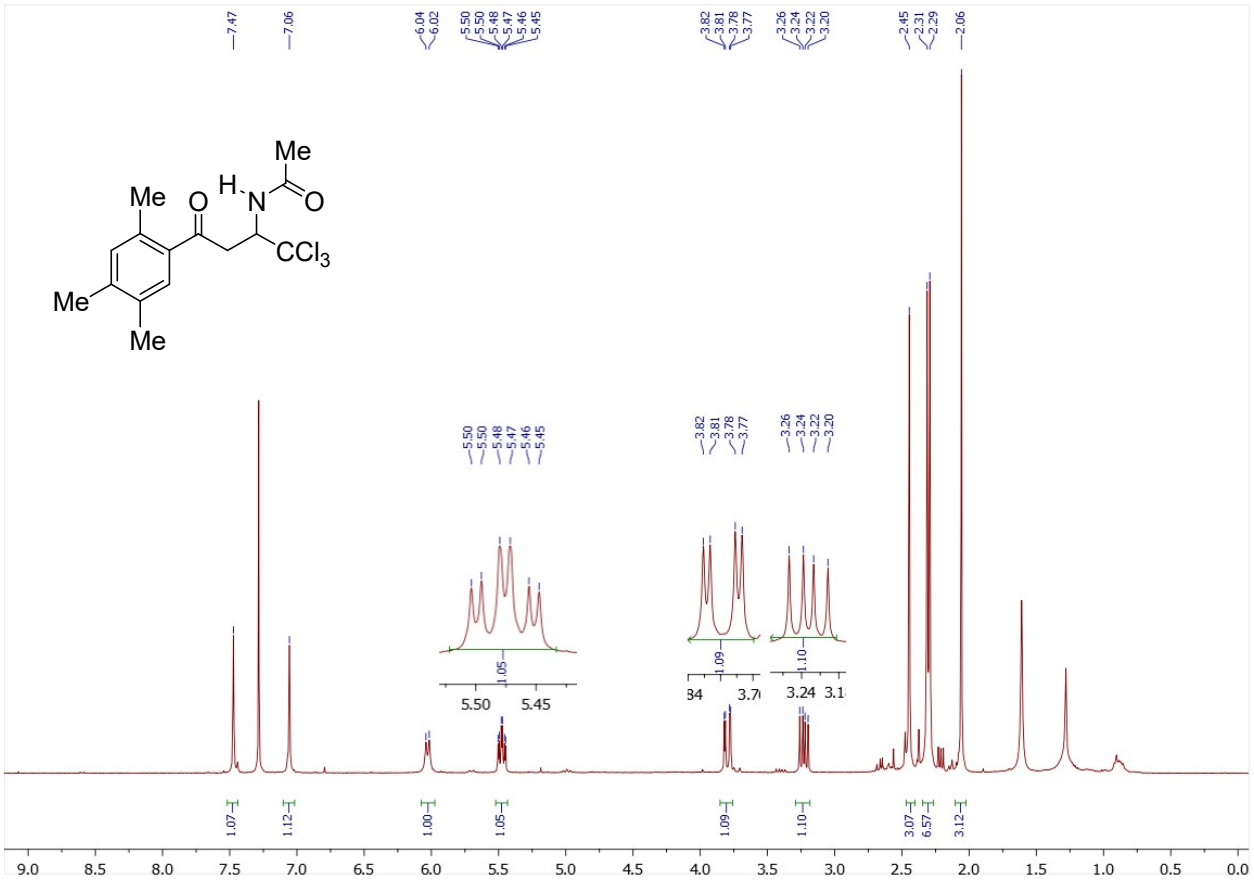


Fig.S21. ^{1}H NMR spectrum of the compound **3j** ($CDCl_3$, 400 MHz).

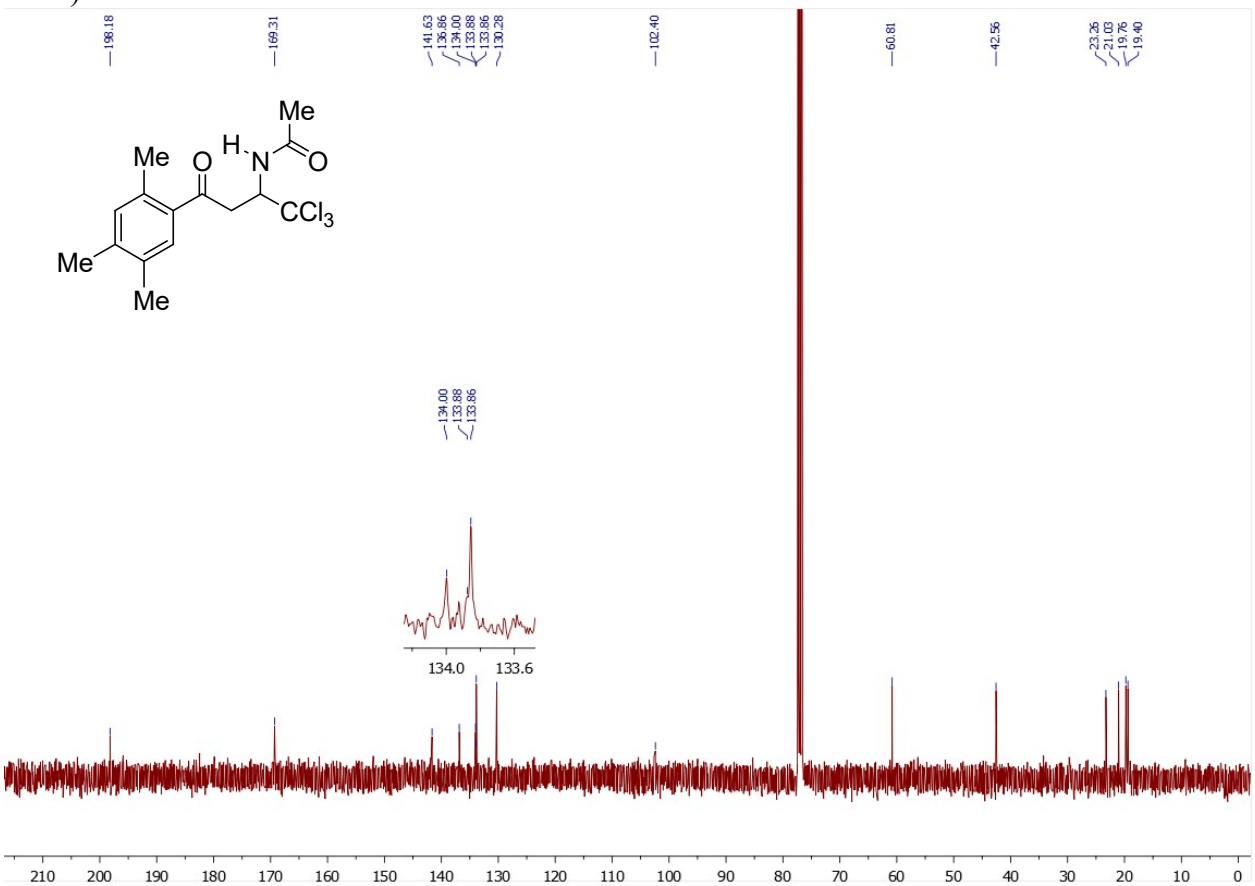


Fig. S22. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3j** ($CDCl_3$, 101 MHz).

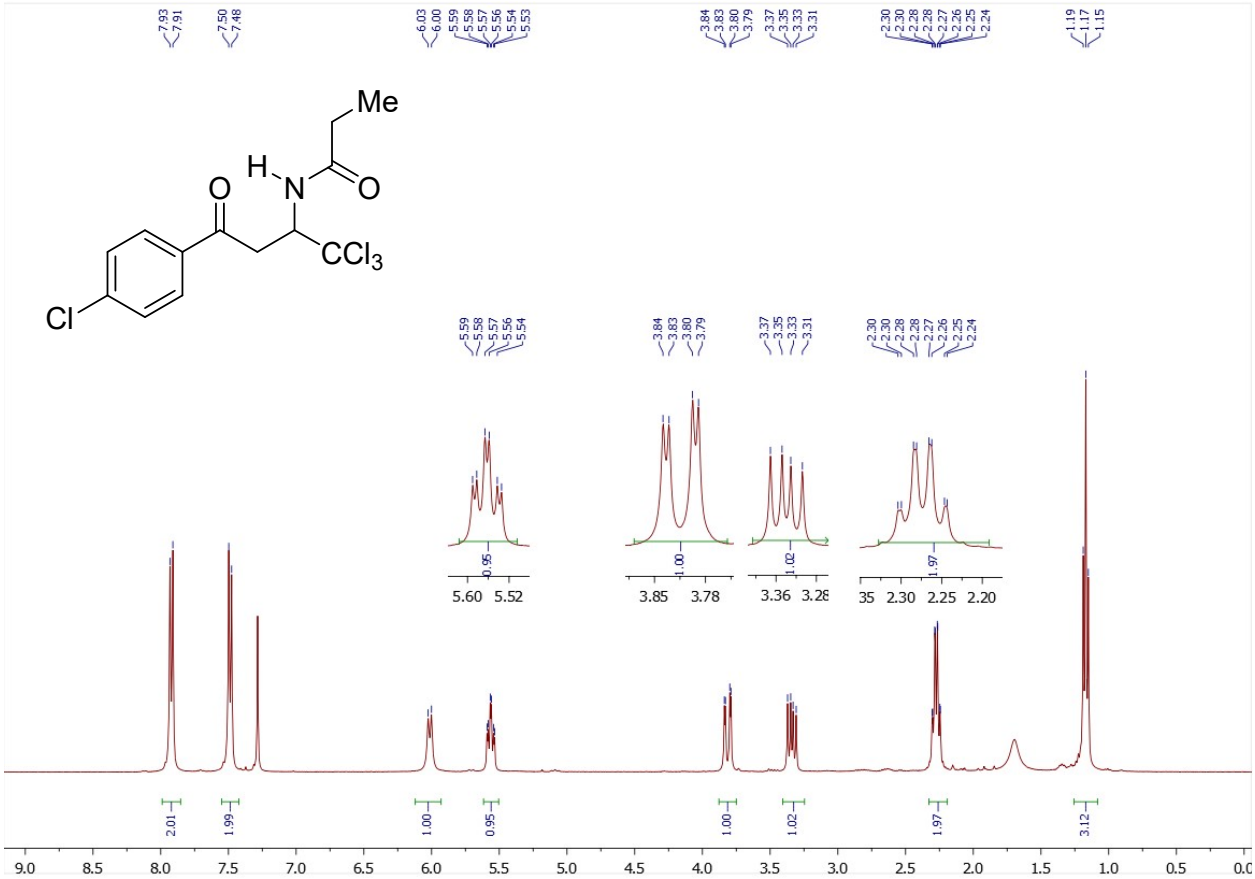


Fig.S23. ^{1}H NMR spectrum of the compound **3ea** ($CDCl_3$, 400 MHz).

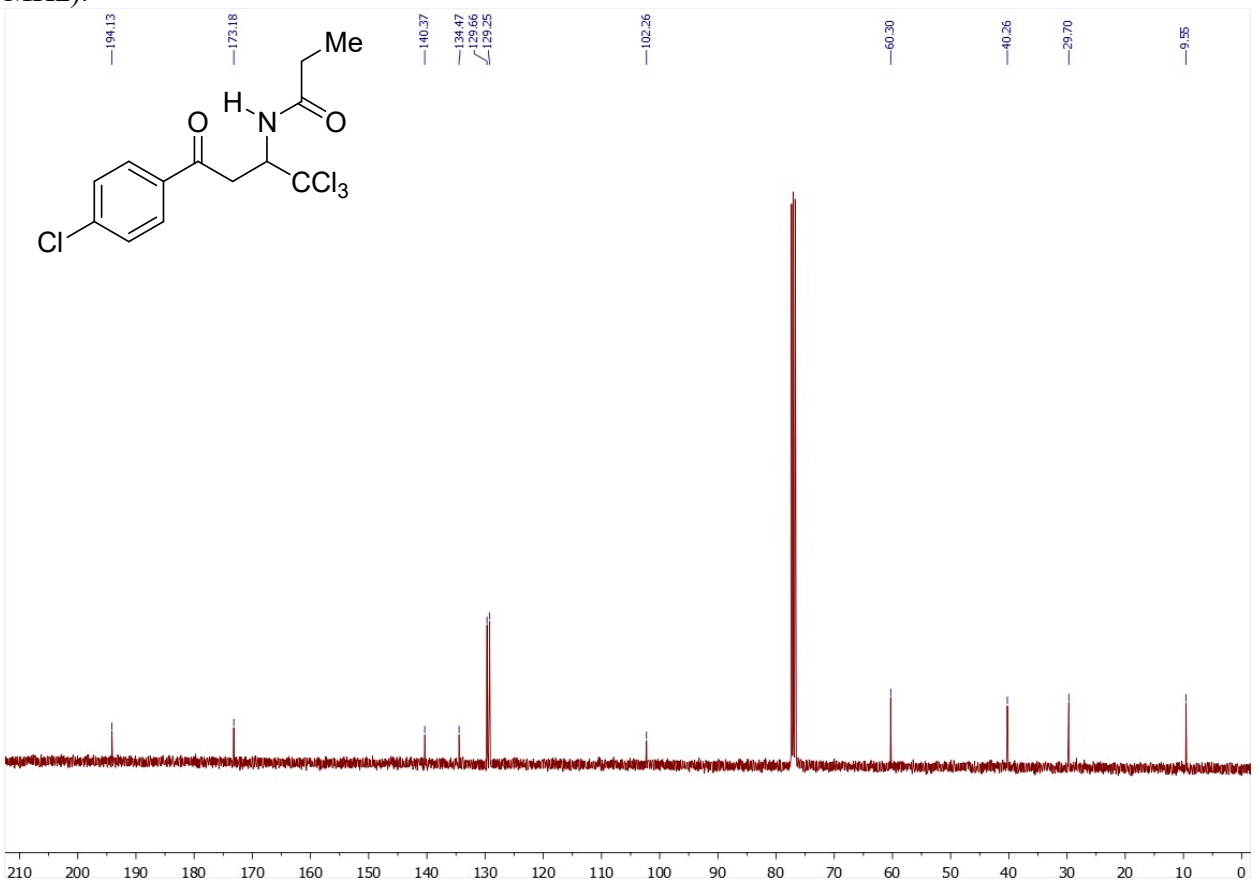


Fig. S24. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3ea** ($CDCl_3$, 101 MHz).

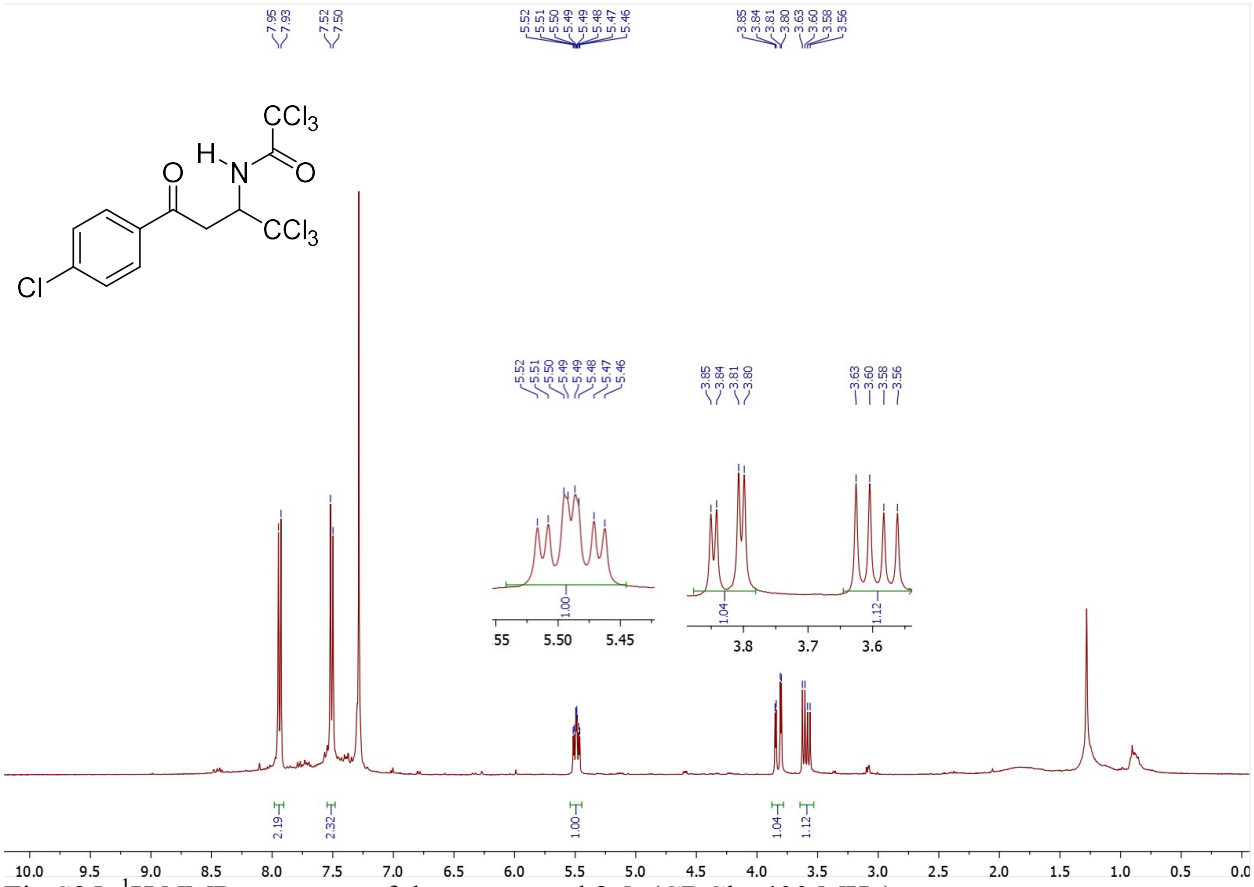


Fig.S25. ^{1}H NMR spectrum of the compound **3eb** ($CDCl_3$, 400 MHz).

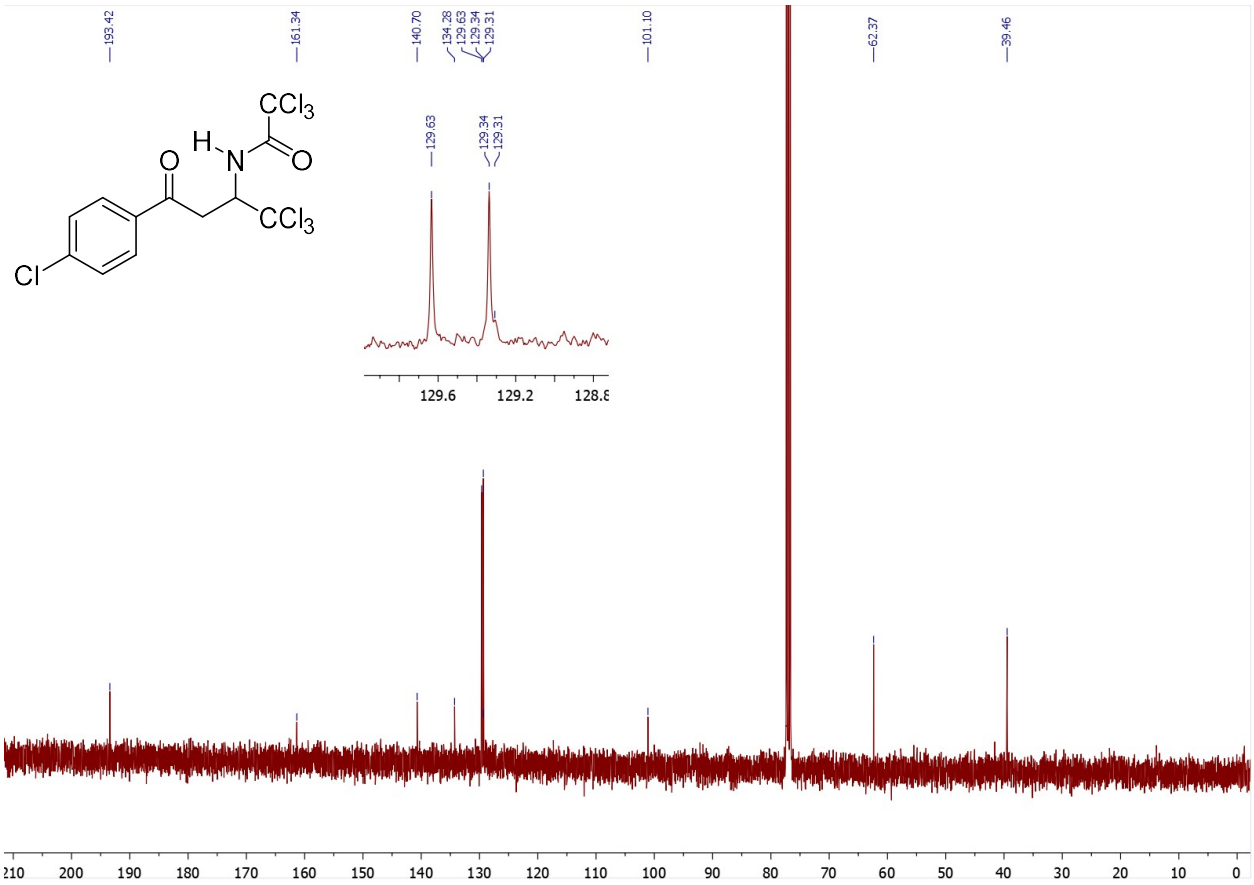


Fig. S26. ^{13}C{^{1}H} NMR spectrum of the compound **3eb** ($CDCl_3$, 101 MHz).

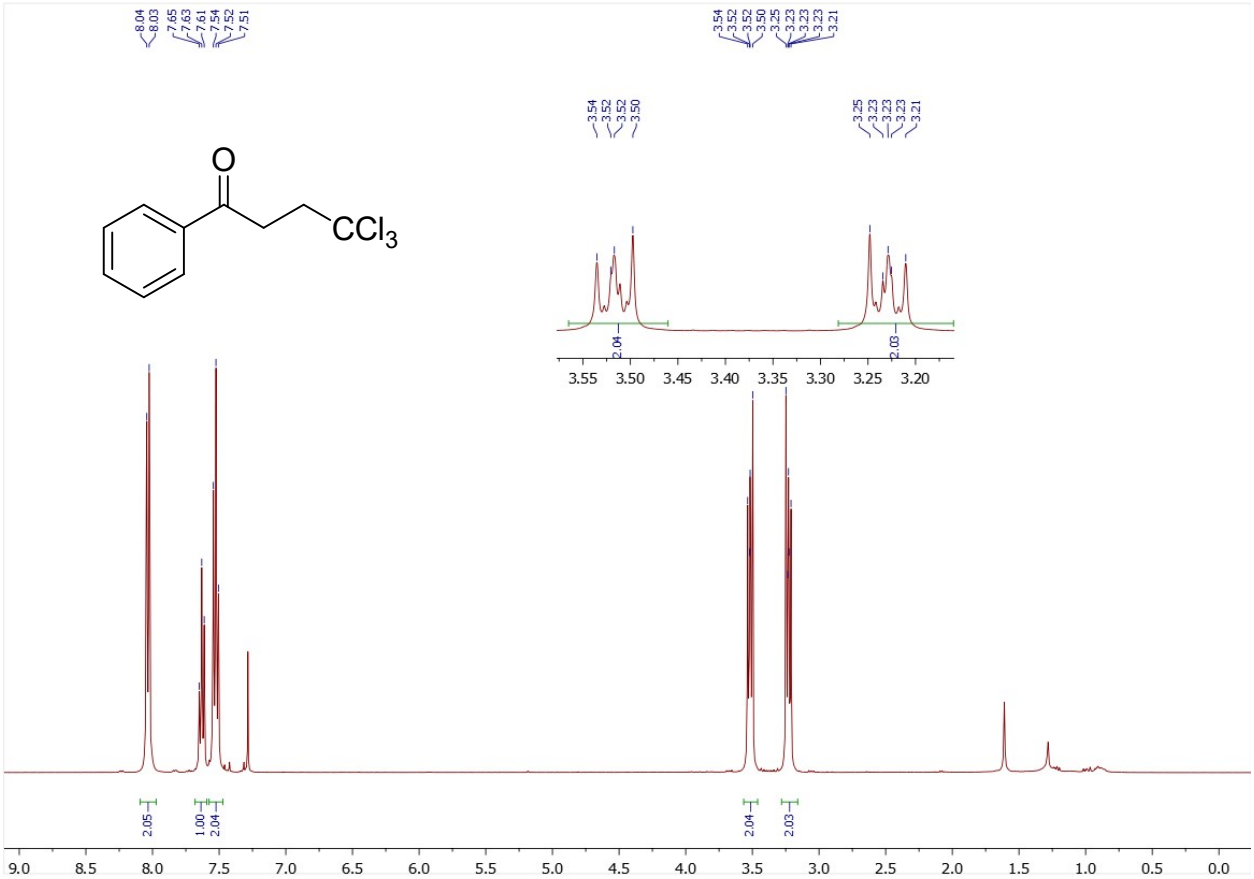


Fig.S27. ^{1}H NMR spectrum of the compound **4a** ($CDCl_3$, 400 MHz).

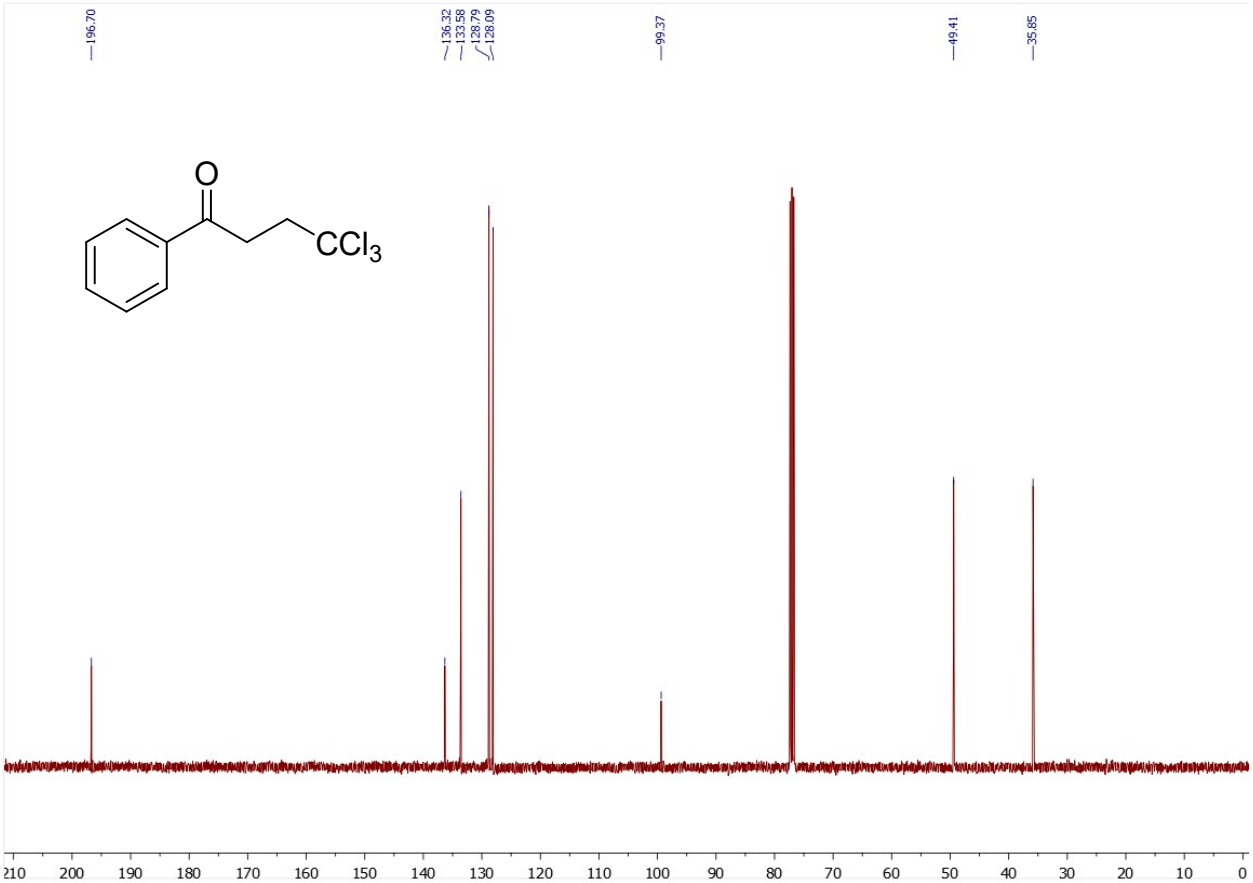


Fig. S28. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **4a** ($CDCl_3$, 101 MHz).

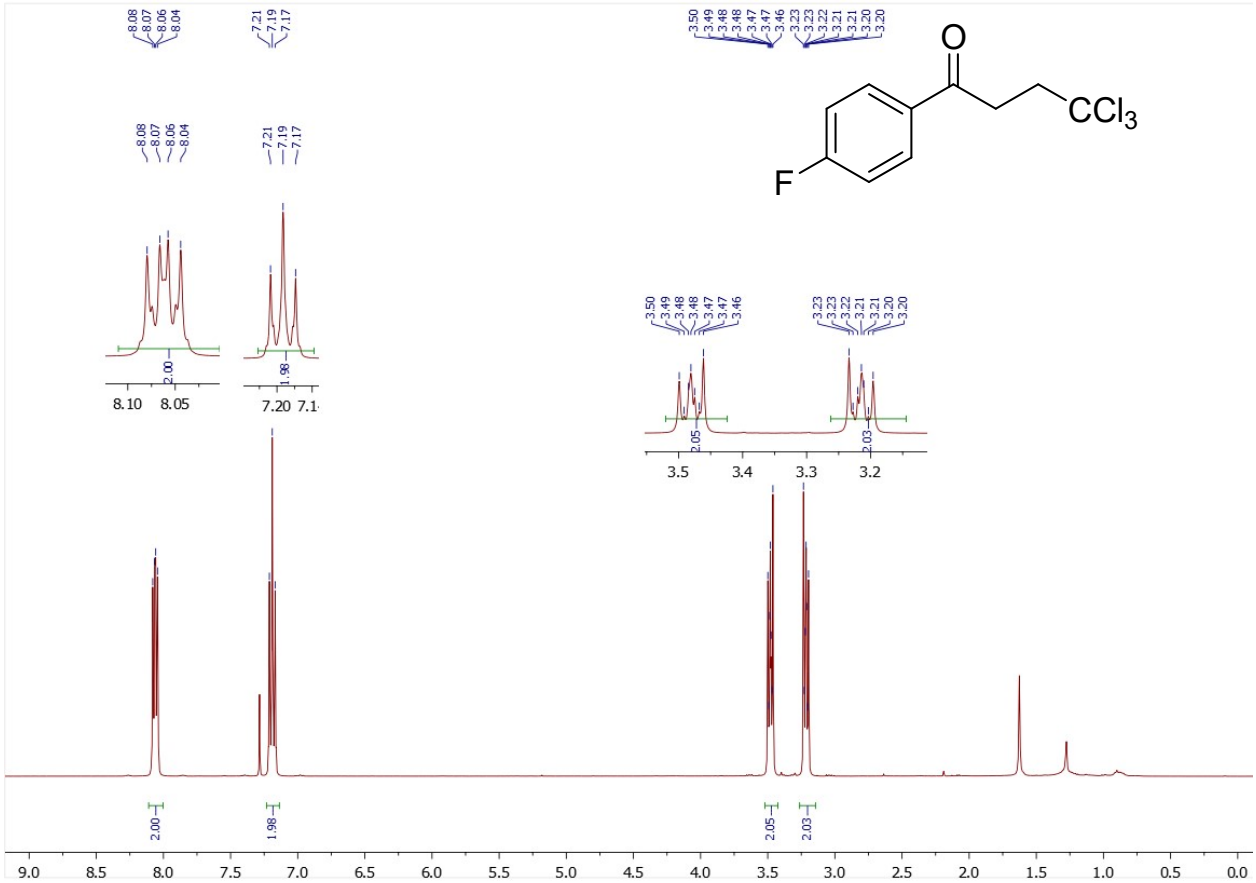


Fig.S28. ^{1}H NMR spectrum of the compound **4d** ($CDCl_3$, 400 MHz).

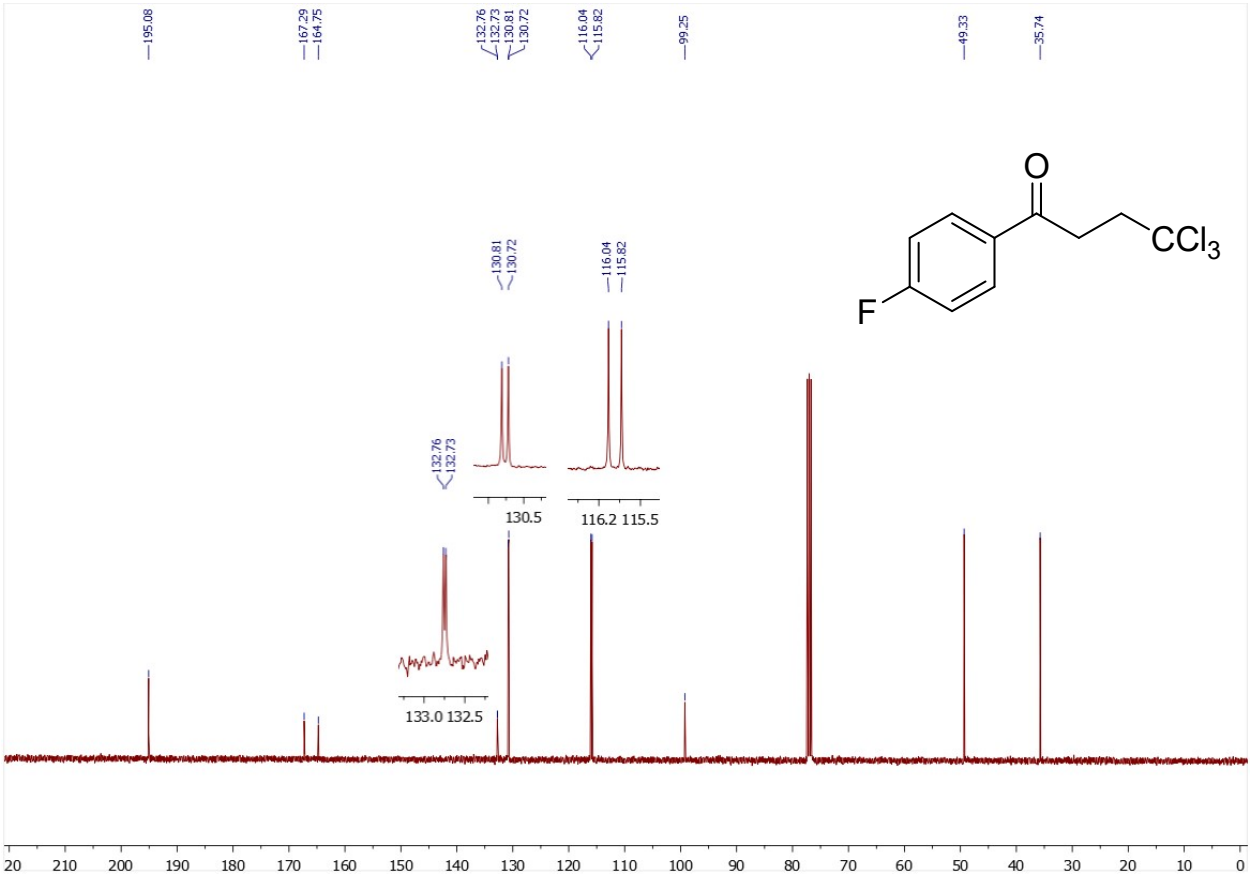


Fig. S29. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **4d** ($CDCl_3$, 101 MHz).

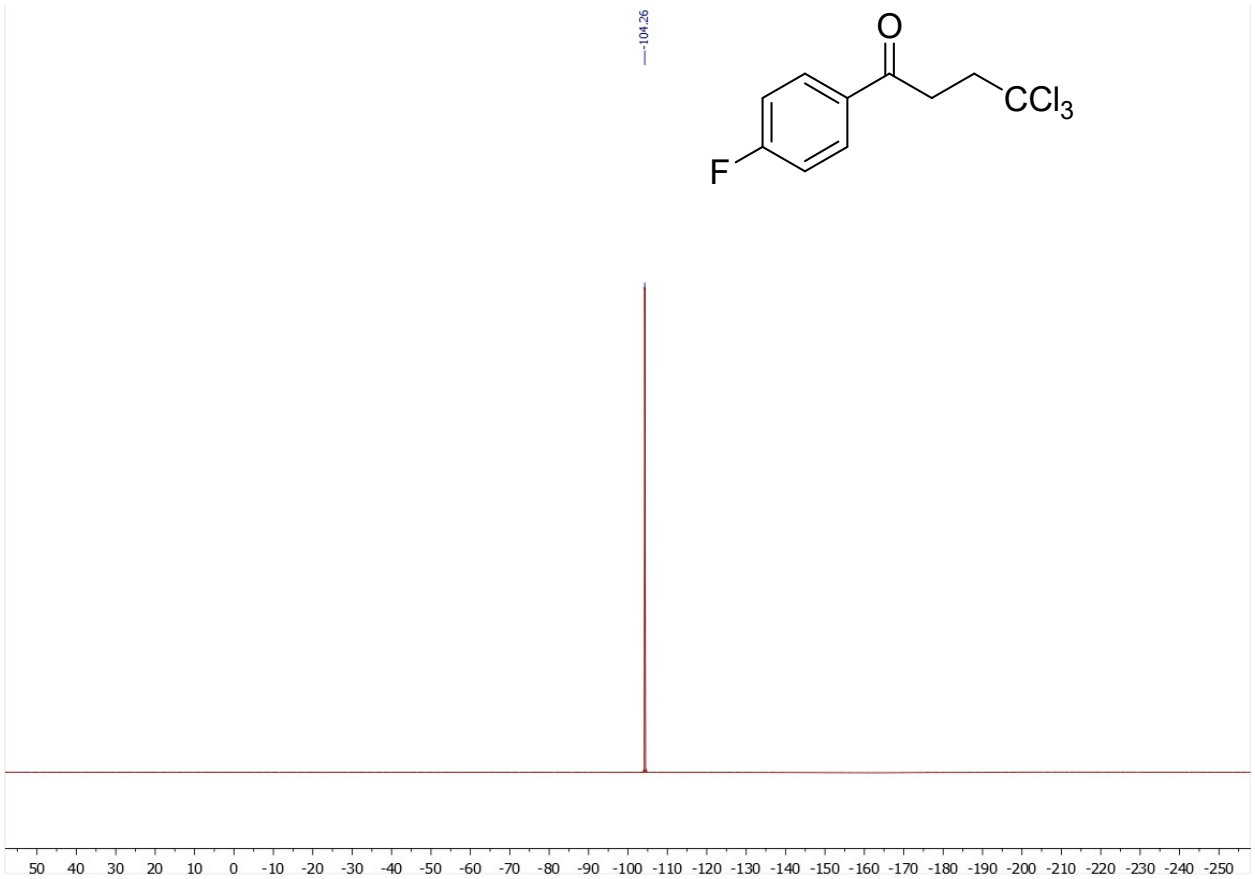


Fig. S30. $^{19}F\{^{1}H\}$ NMR spectrum of the compound **4d** ($CDCl_3$, 376 MHz).

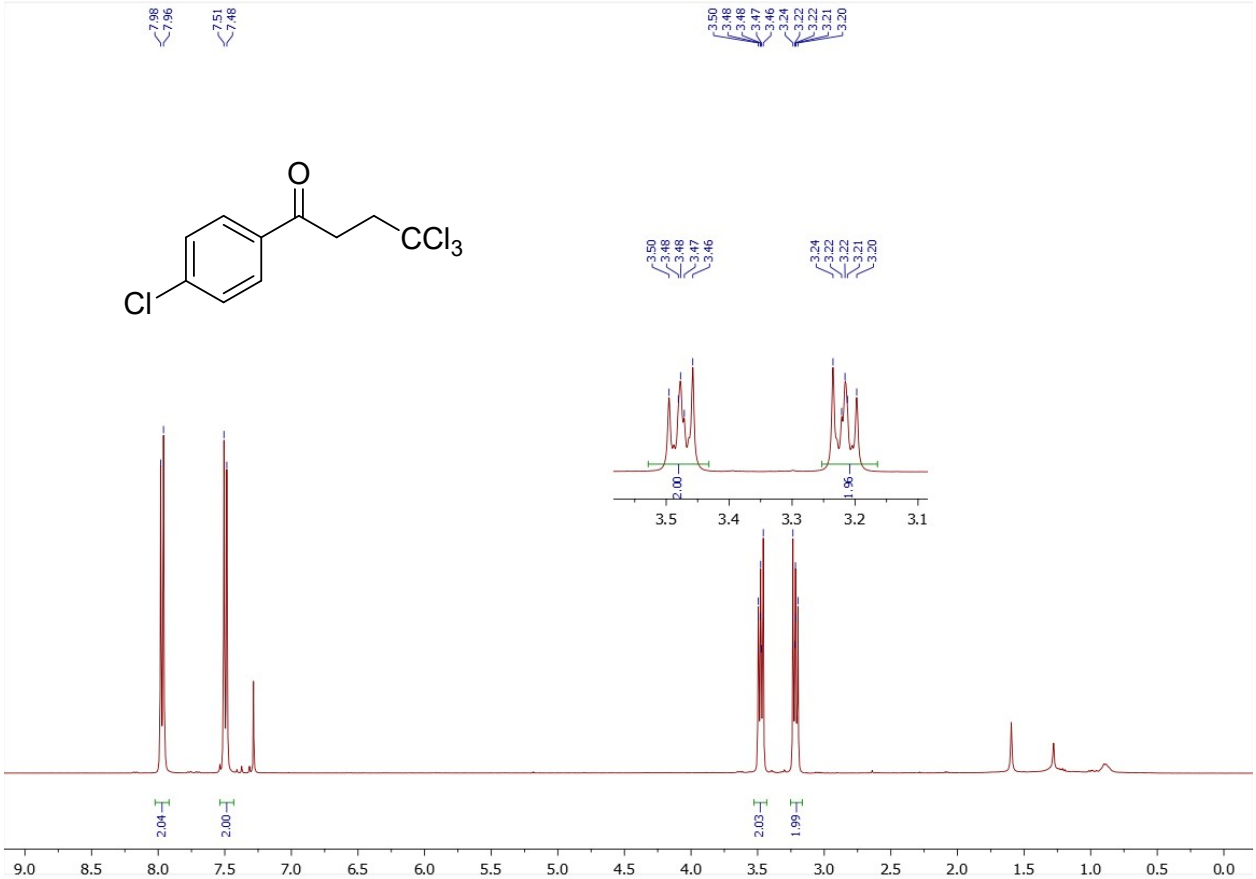


Fig.S31. ^{1}H NMR spectrum of the compound**4e** ($CDCl_3$, 400 MHz).

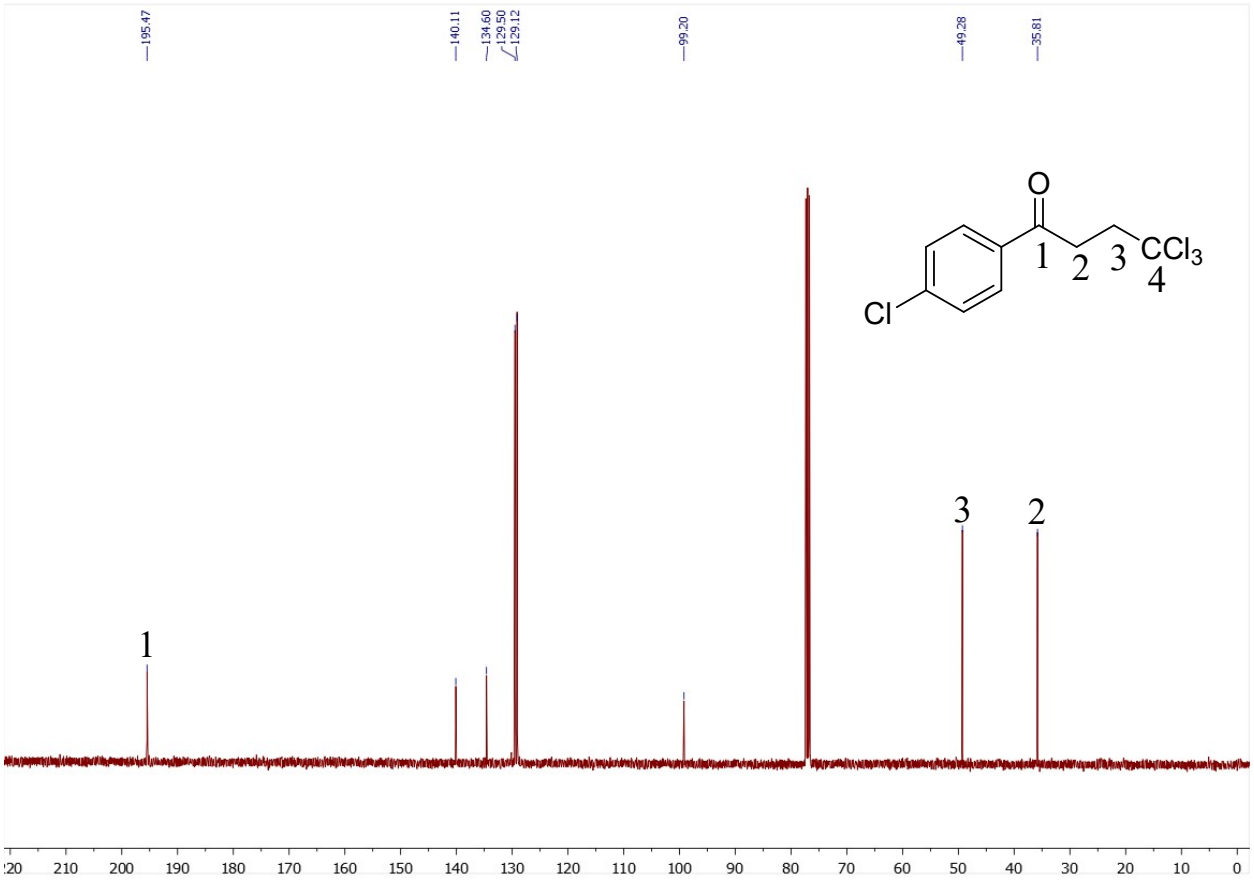


Fig. S32. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **4e** ($CDCl_3$, 101 MHz).

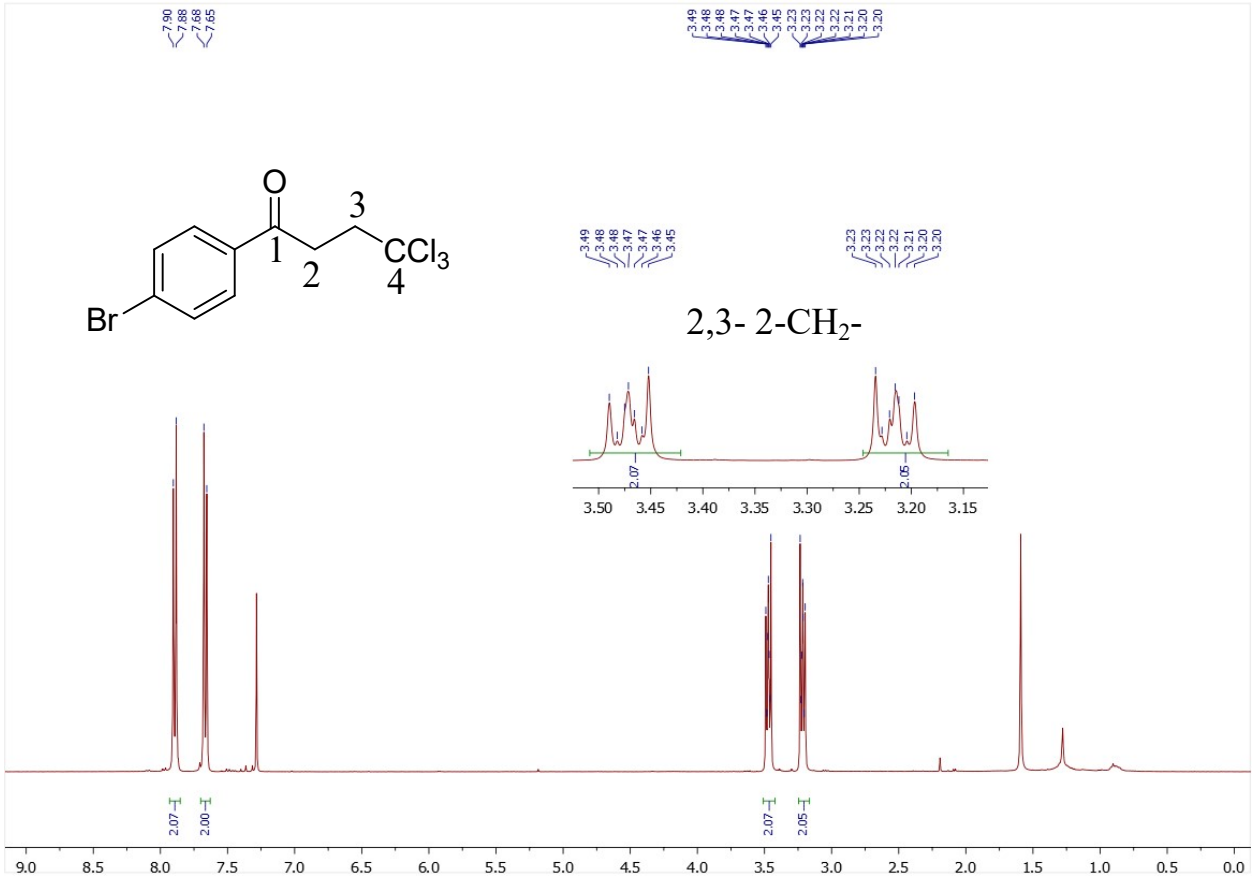


Fig.S33. ^{1}H NMR spectrum of the compound **4f** ($CDCl_3$, 400 MHz).

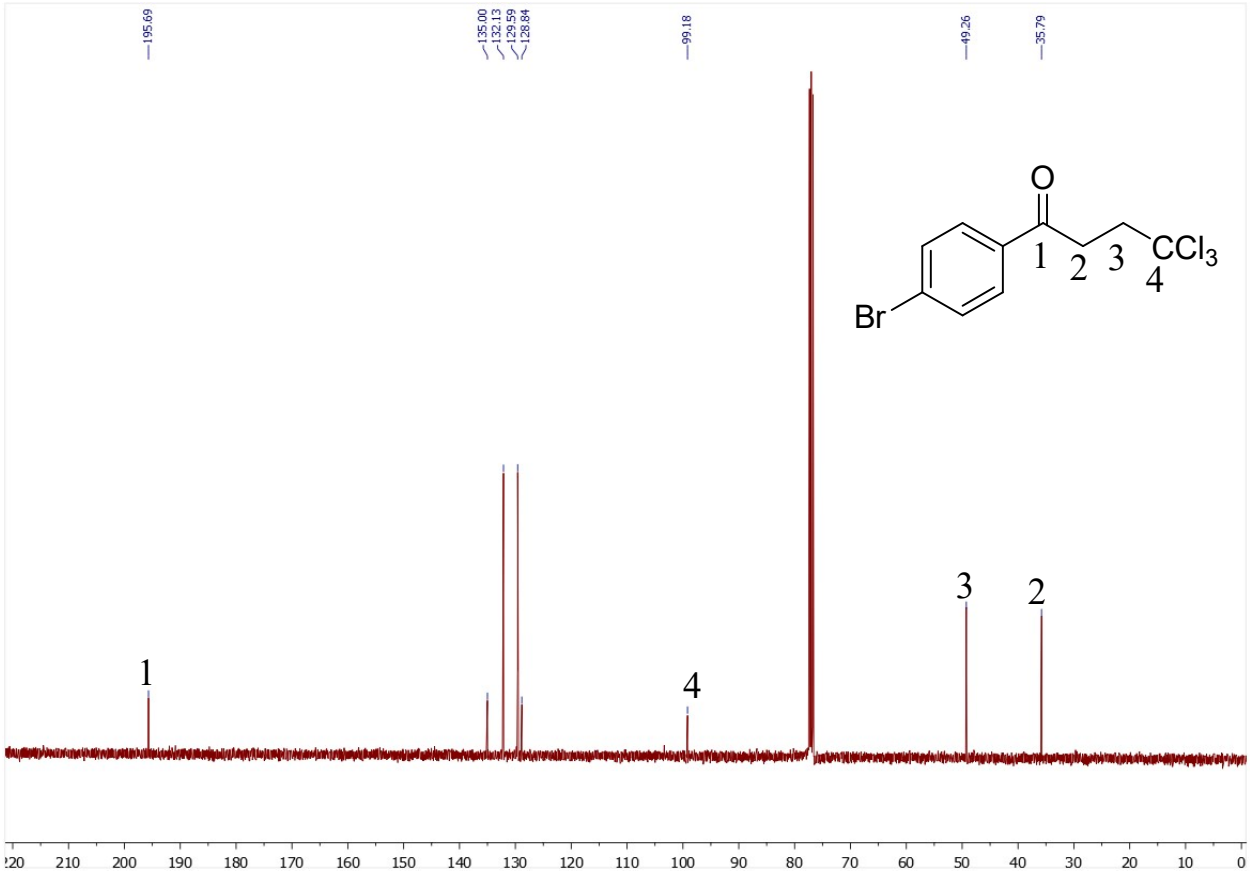


Fig. S34. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **4f** ($CDCl_3$, 101 MHz).

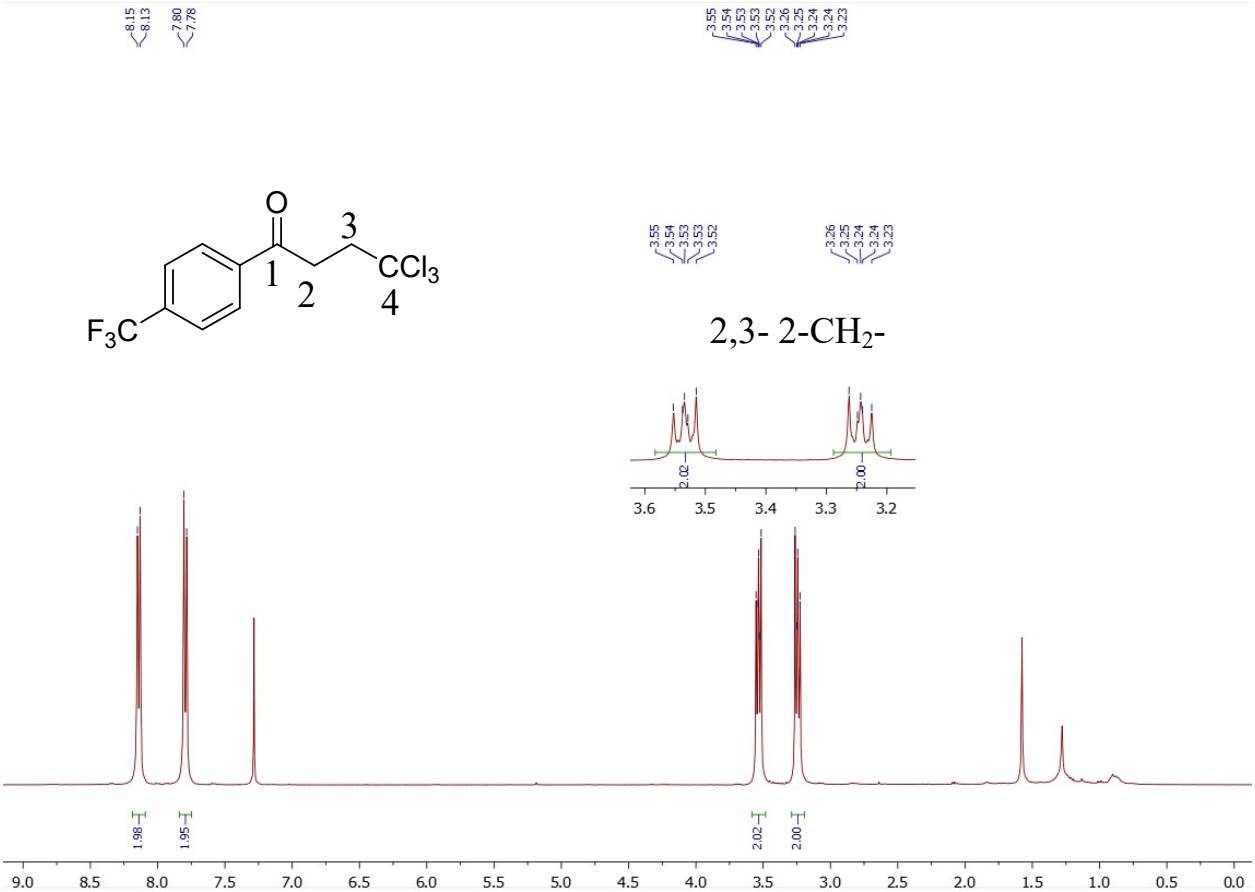


Fig.S35. ^{1}H NMR spectrum of the compound **4g** ($CDCl_3$, 400 MHz).

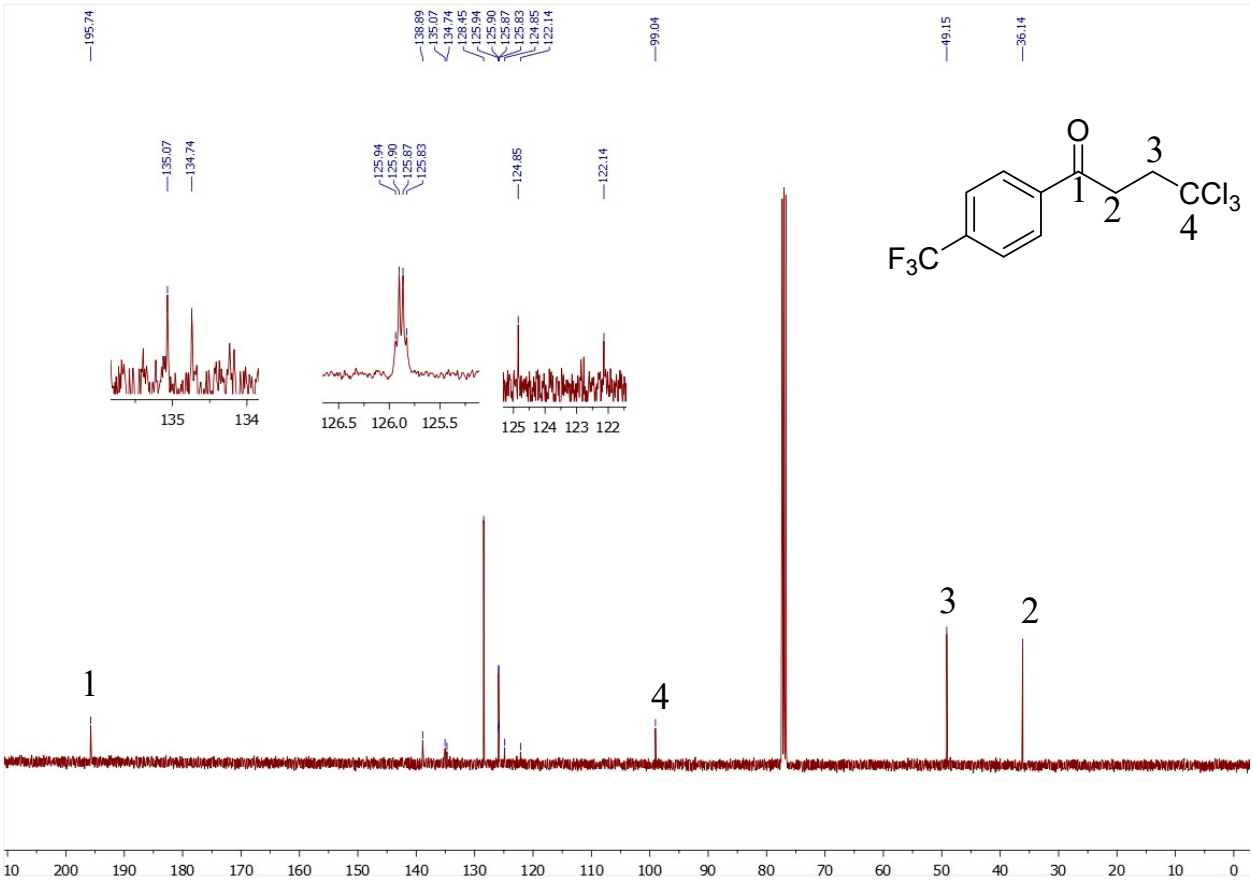


Fig. S36. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **4g** ($CDCl_3$, 101 MHz).

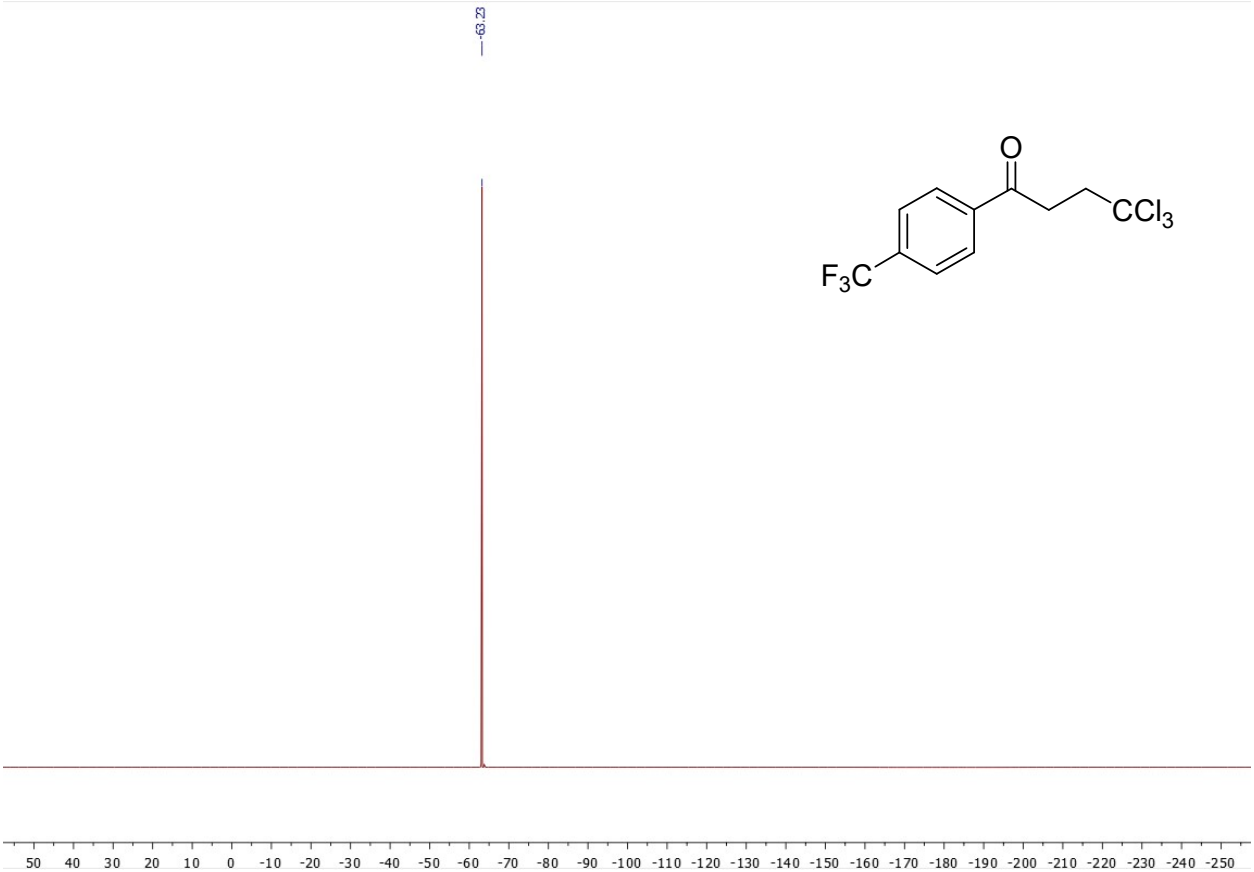


Fig. S37. $^{19}F\{^{1}H\}$ NMR spectrum of the compound **4g** ($CDCl_3$, 376 MHz).

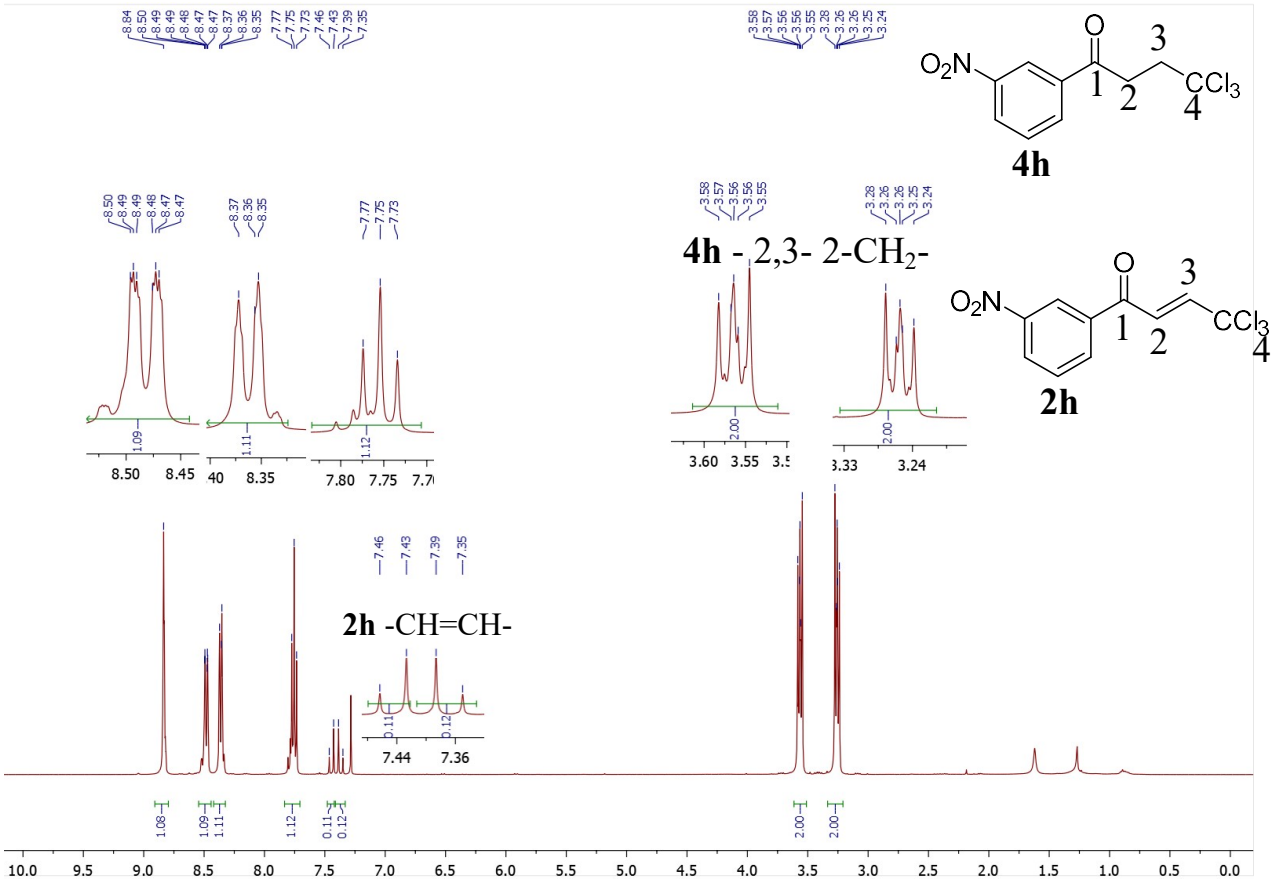


Fig.S38. ^{1}H NMR spectrum of the compound **4h** ($CDCl_3$, 400 MHz).

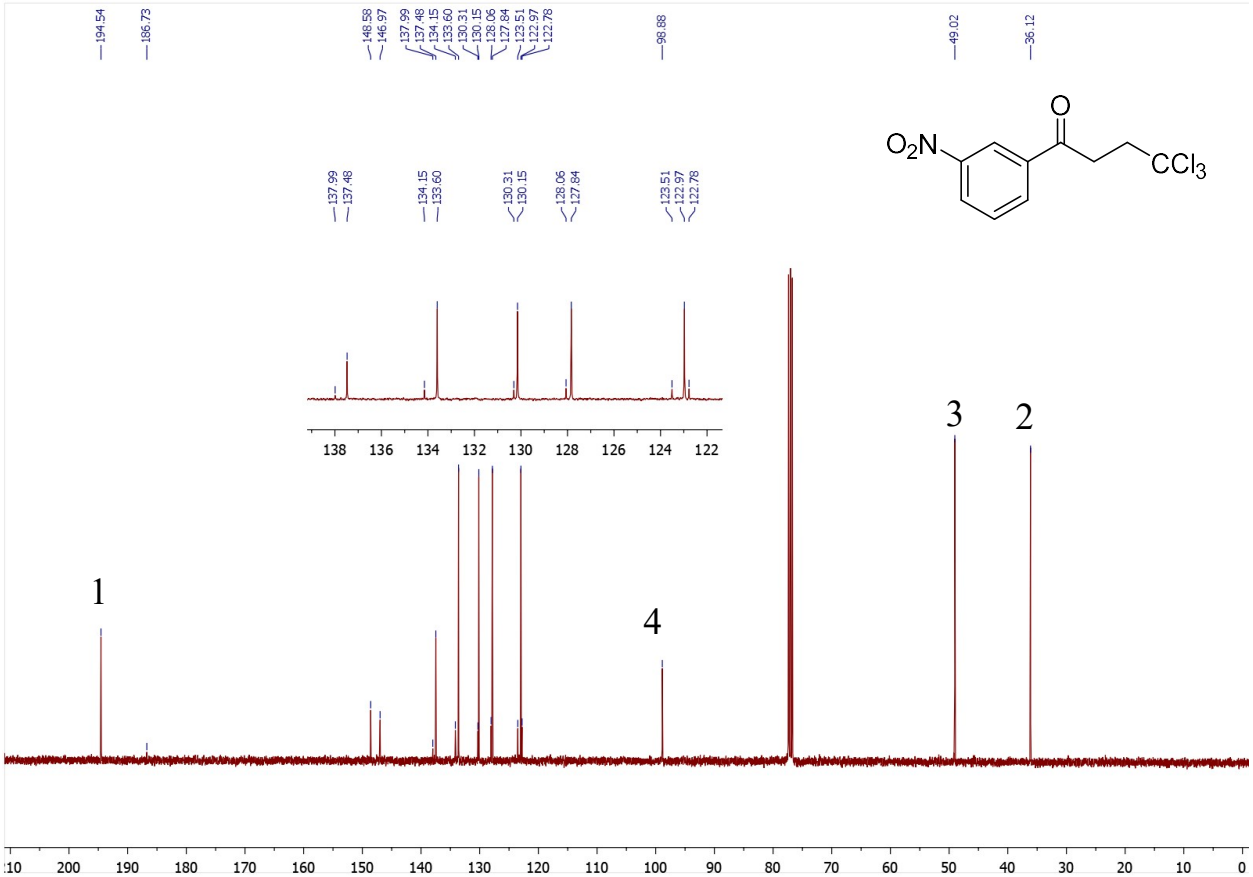


Fig. S39. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **4h** ($CDCl_3$, 101 MHz).

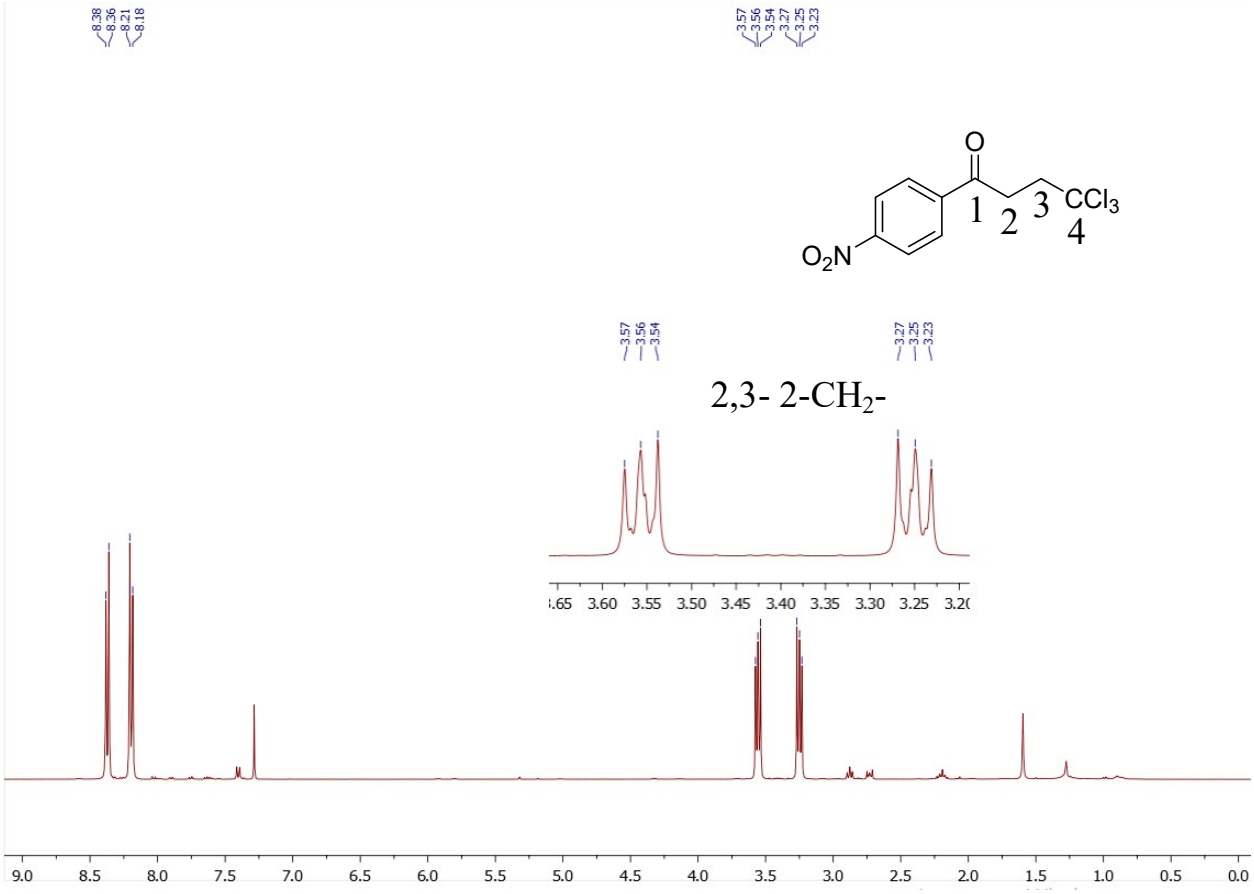


Fig.S40. ^{1}H NMR spectrum of the compound **4i** ($CDCl_3$, 400 MHz).

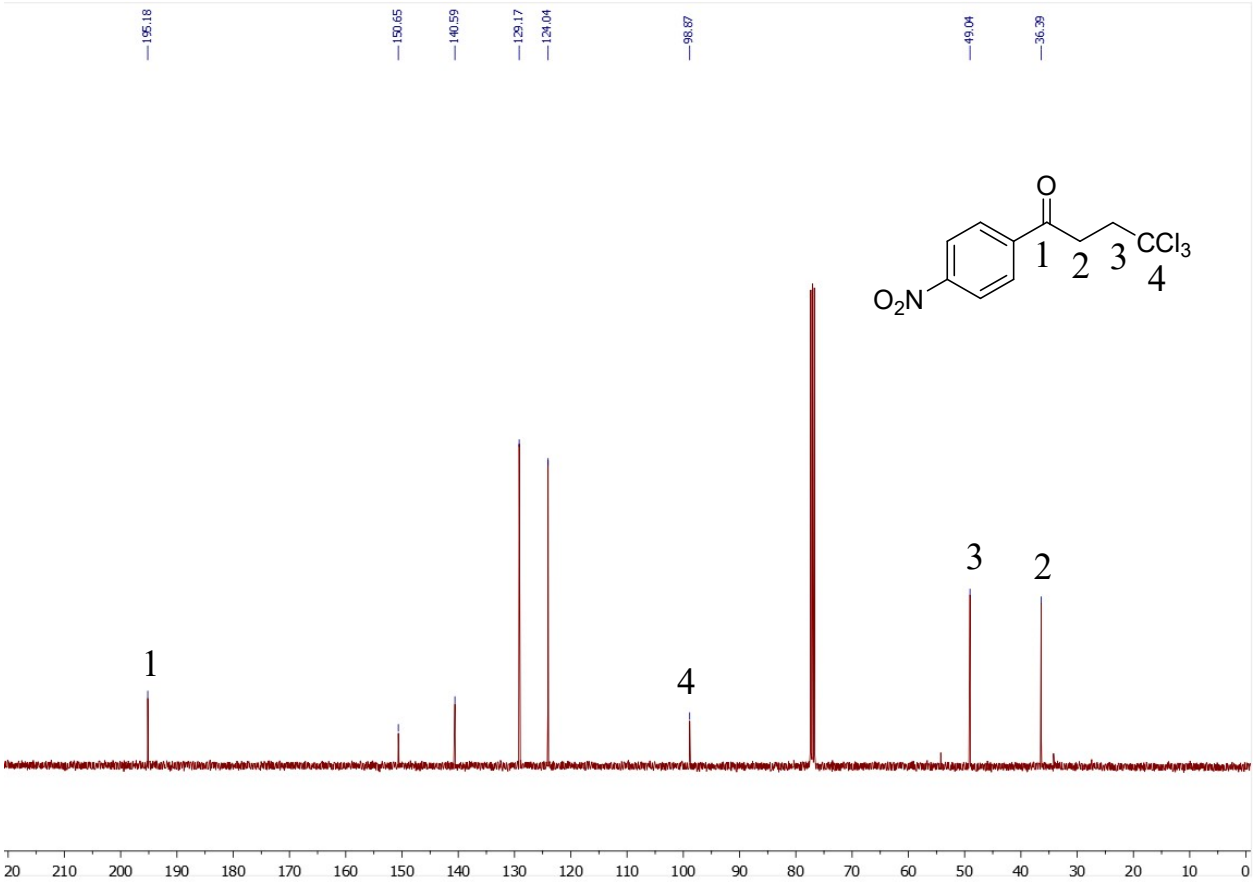


Fig. S41. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **4i** ($CDCl_3$, 101 MHz).

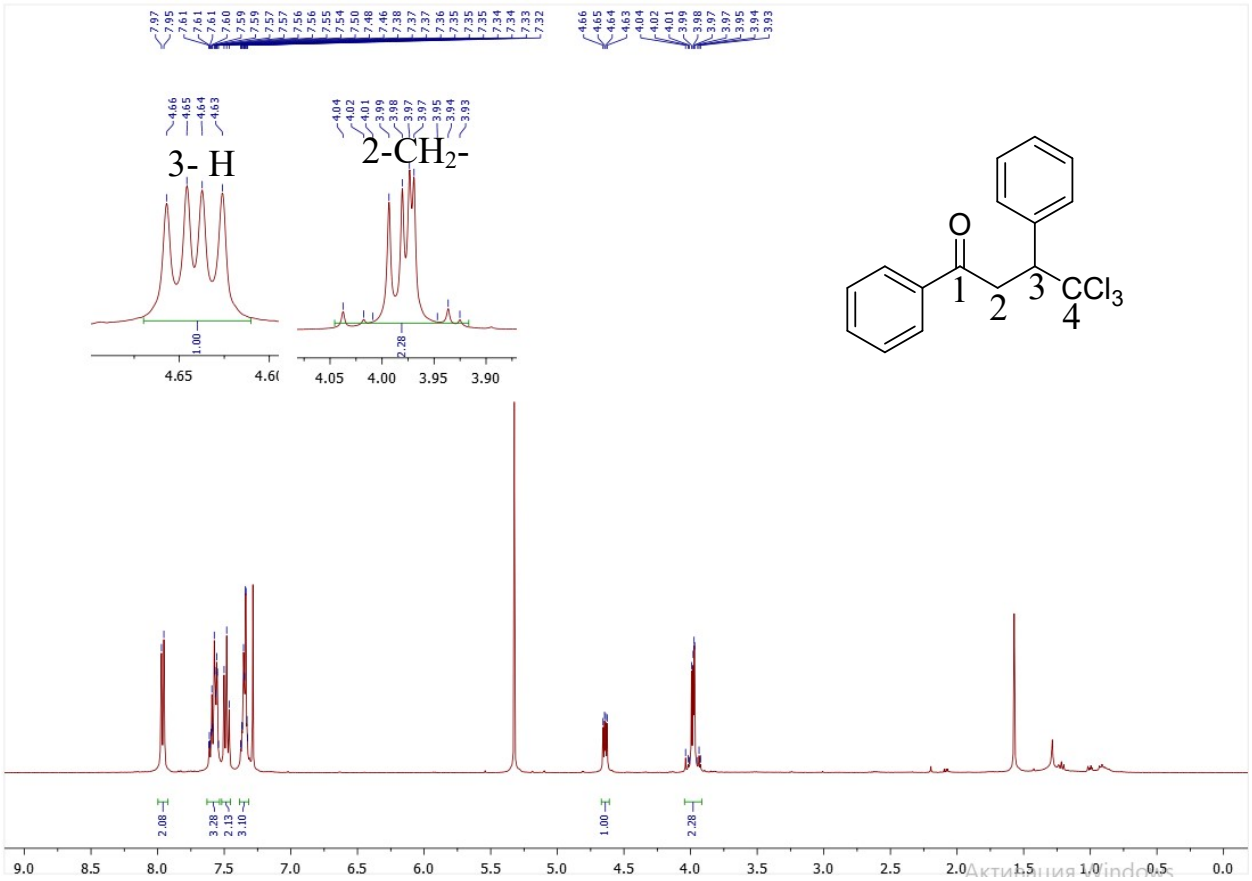


Fig.S42. ^{1}H NMR spectrum of the compound **5a** ($CDCl_3$, 400 MHz).

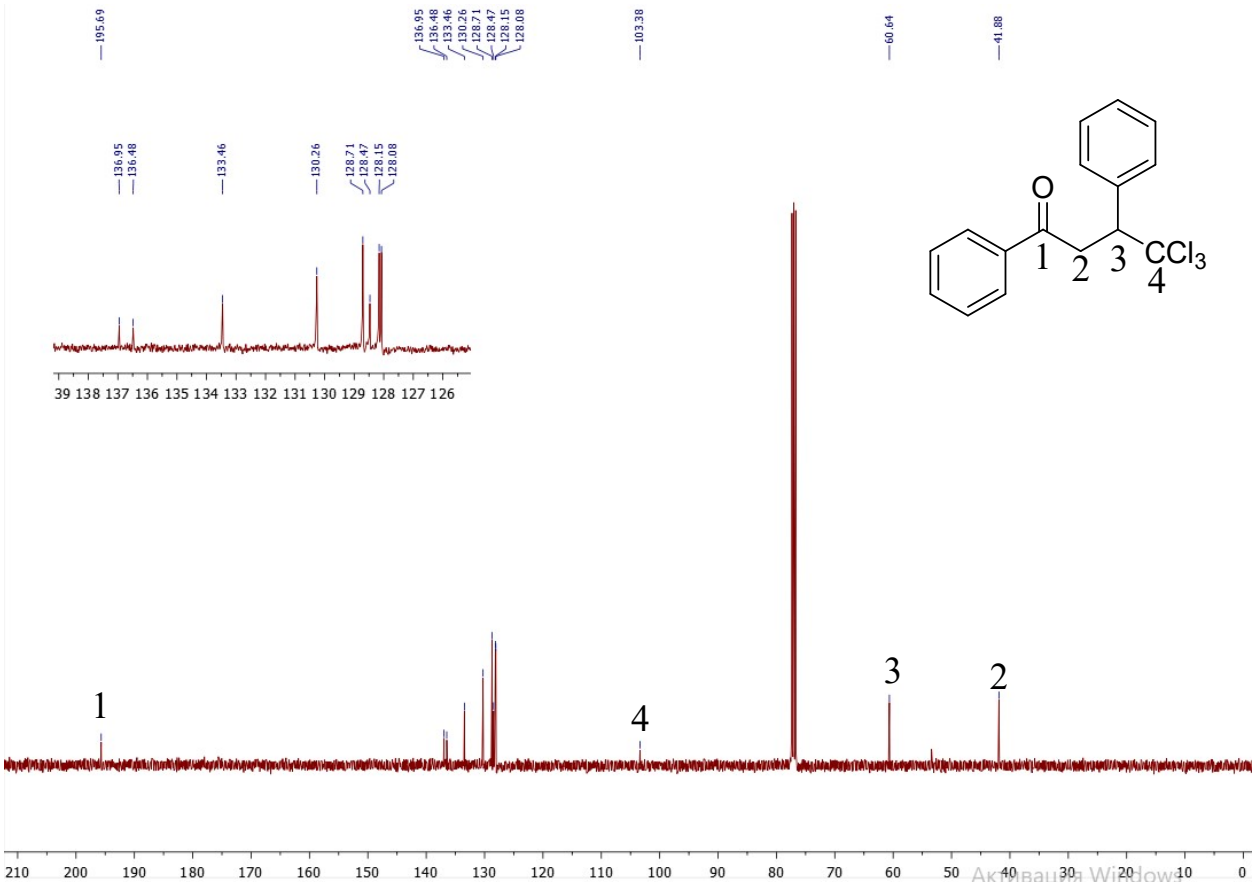


Fig. S43. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5a** ($CDCl_3$, 101 MHz).

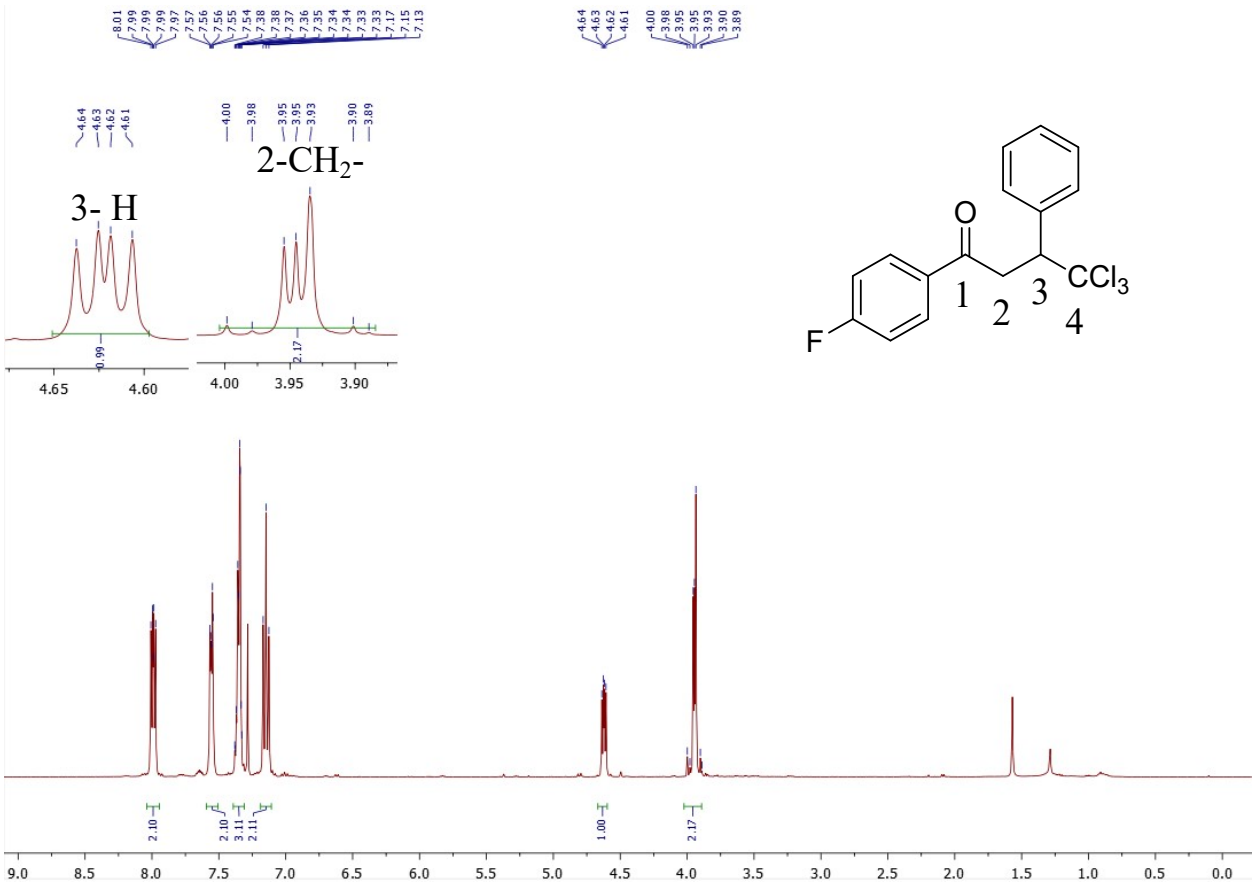


Fig.S44. ^{1}H NMR spectrum of the compound **5d** ($CDCl_3$, 400 MHz).

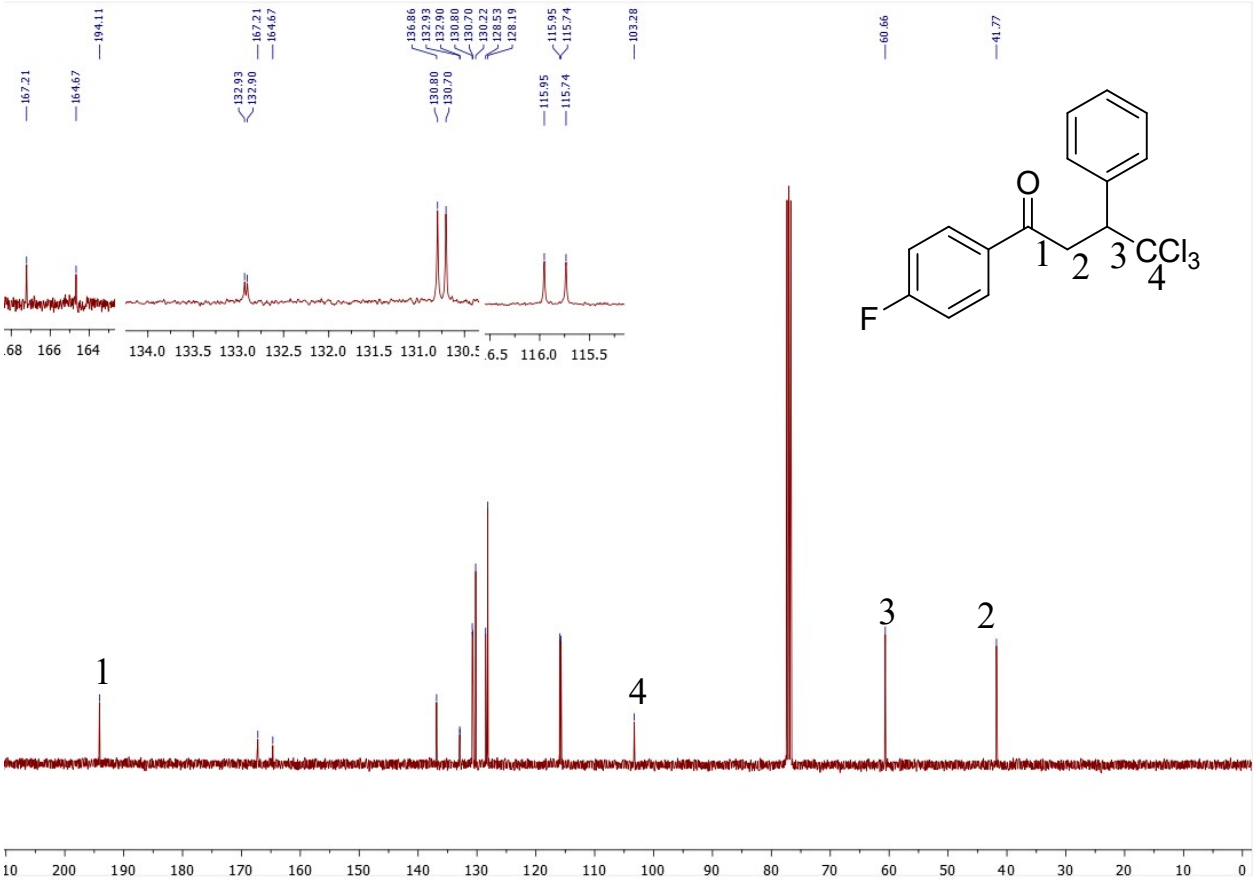


Fig. S45. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5d** ($CDCl_3$, 101 MHz).

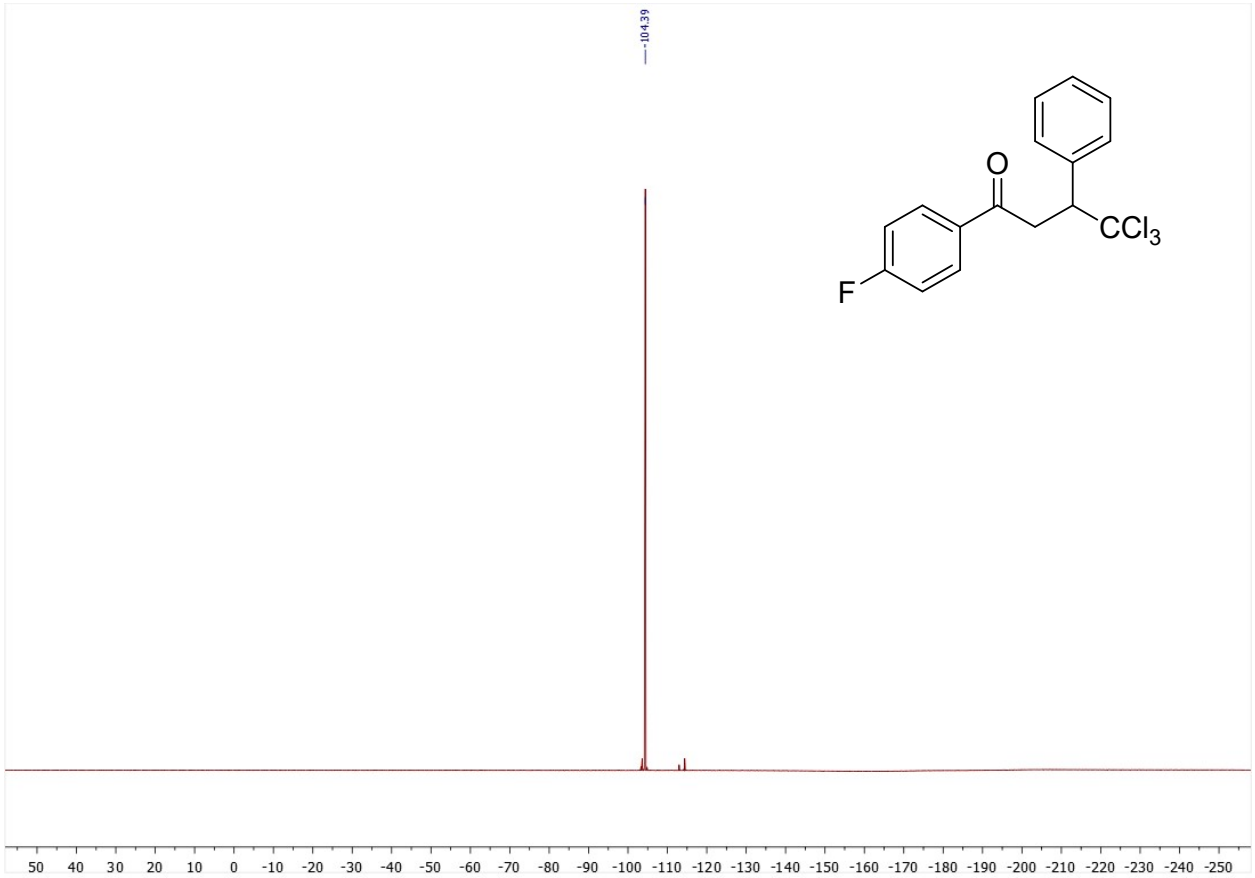


Fig. S46. $^{19}F\{^{1}H\}$ NMR spectrum of the compound **5d** ($CDCl_3$, 376 MHz).

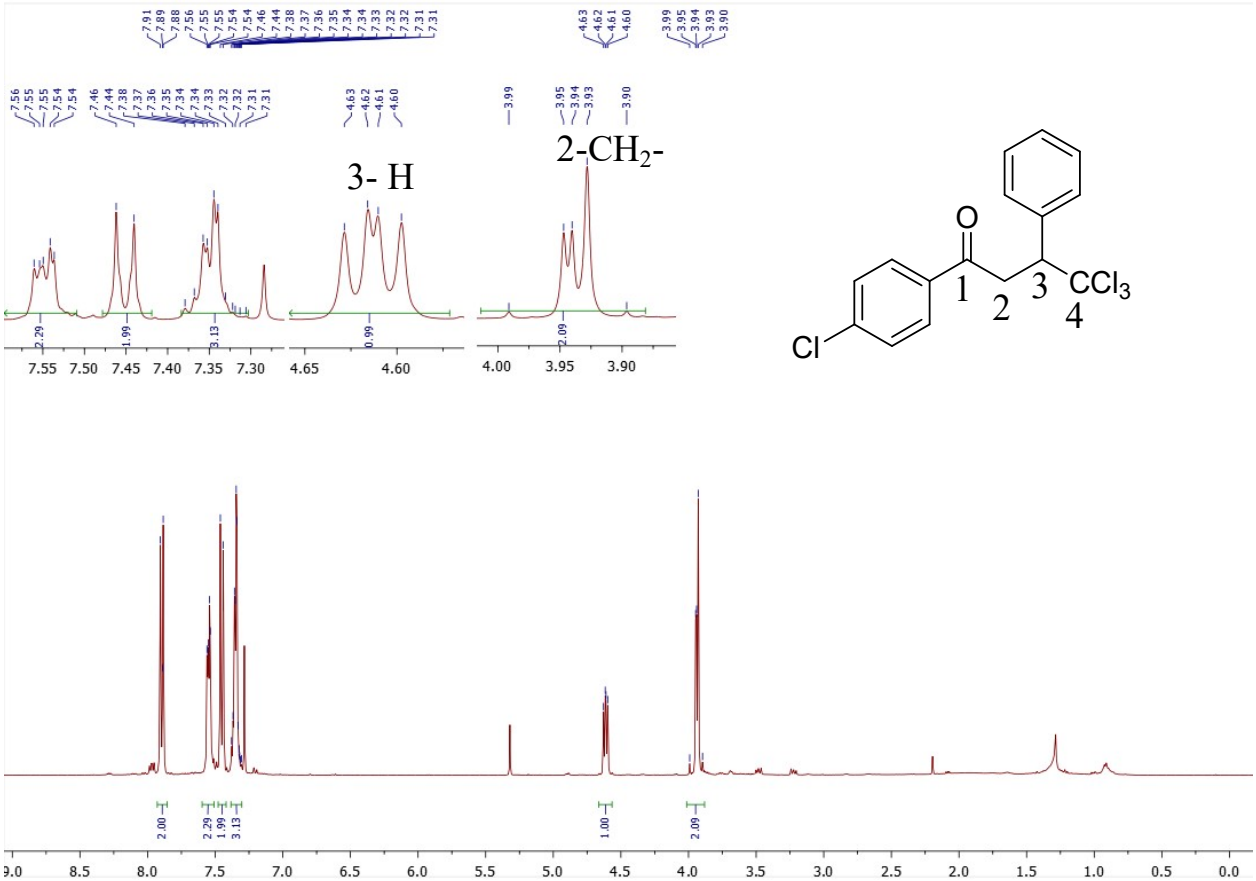


Fig.S47. ^{1}H NMR spectrum of the compound **5e** ($CDCl_3$, 400 MHz).

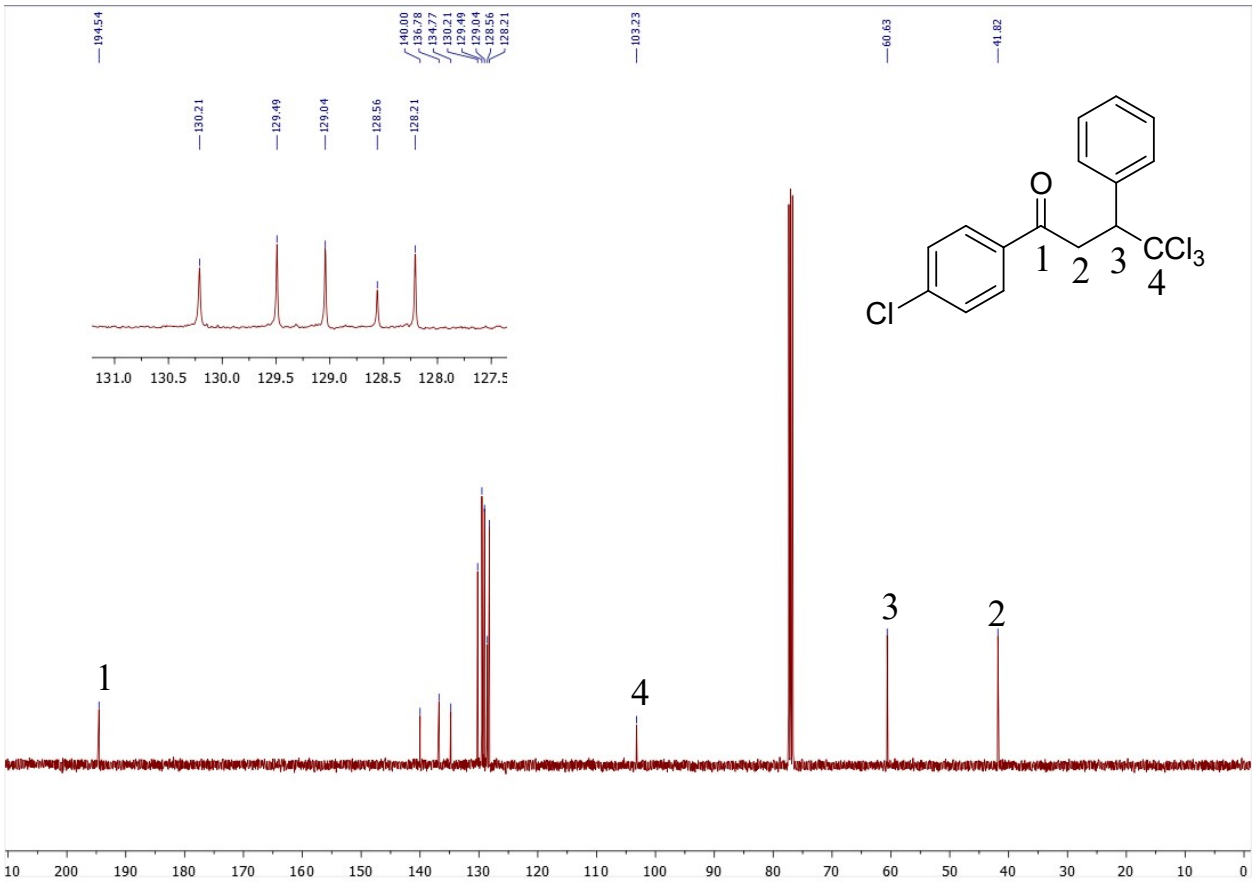


Fig. S48. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5e** ($CDCl_3$, 101 MHz).

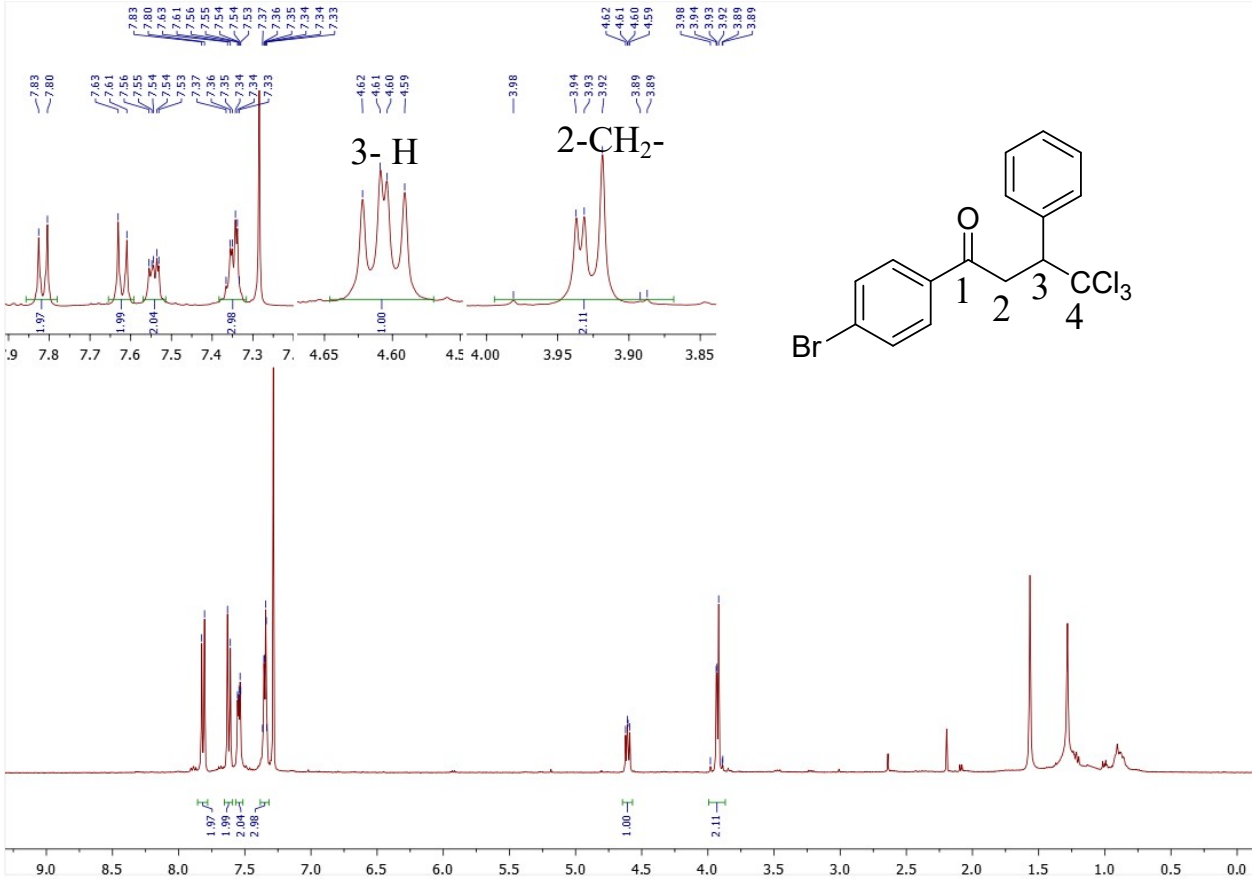


Fig.S49. ^{1}H NMR spectrum of the compound **5f** ($CDCl_3$, 400 MHz).

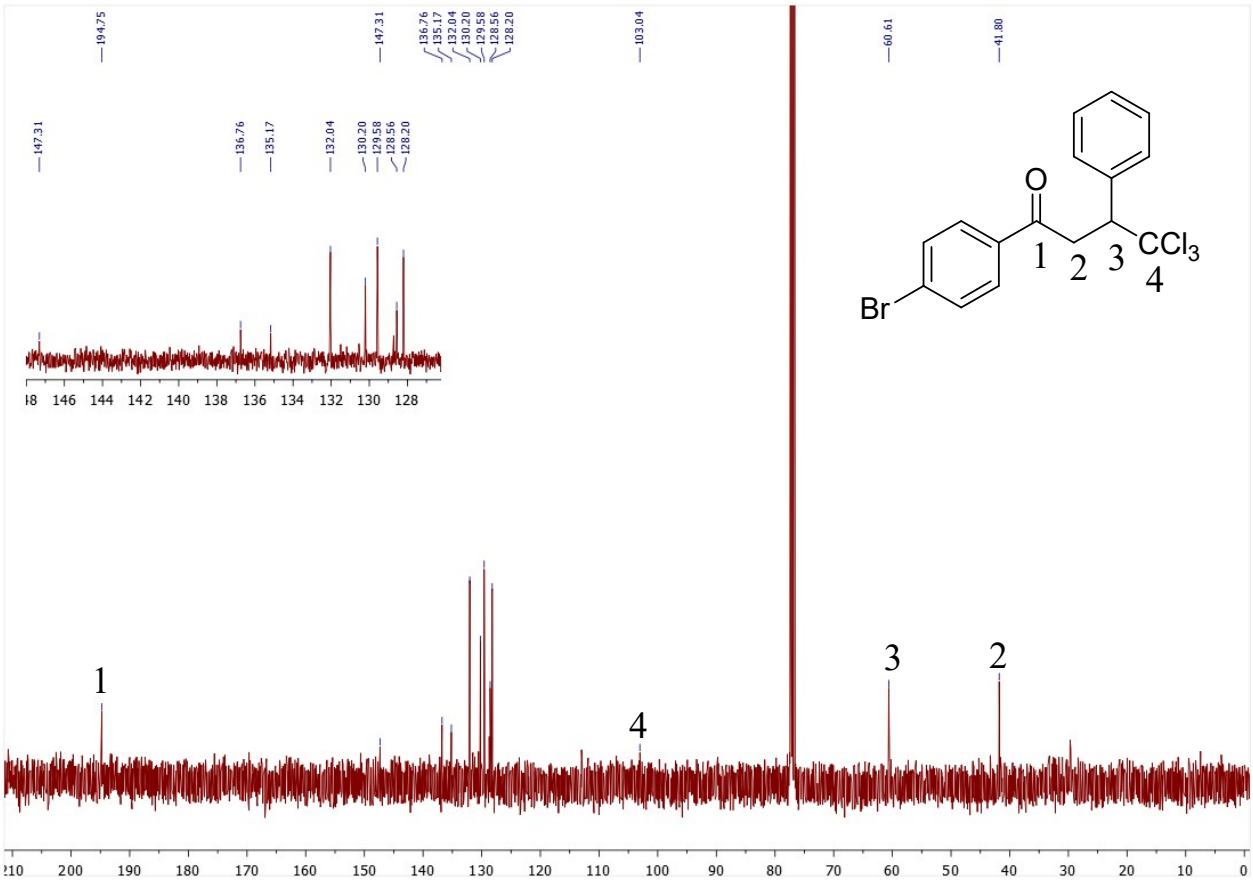


Fig. S50. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5f** ($CDCl_3$, 101 MHz).

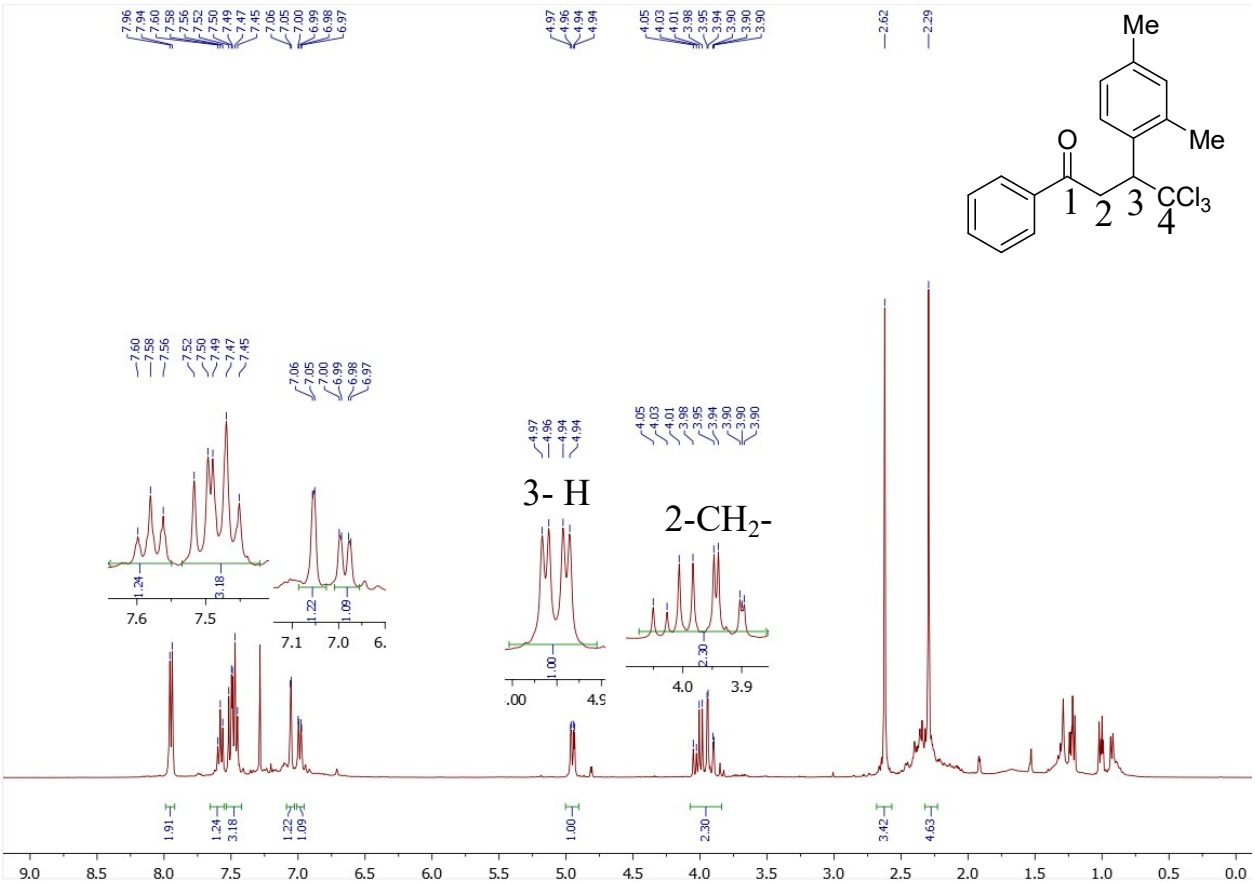


Fig.S51. ^{1}H NMR spectrum of the compound **5aa** ($CDCl_3$, 400 MHz).

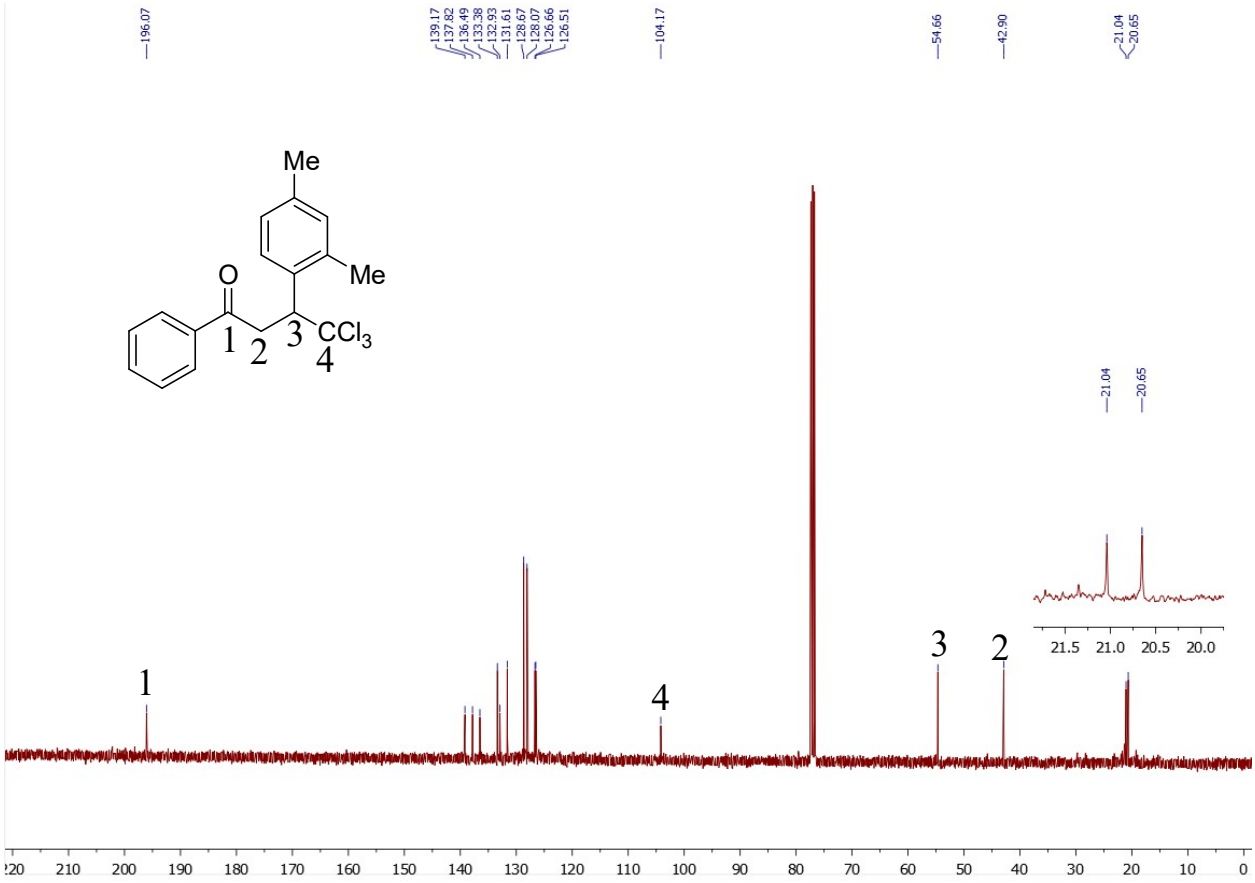


Fig. S52. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5aa** ($CDCl_3$, 101 MHz).

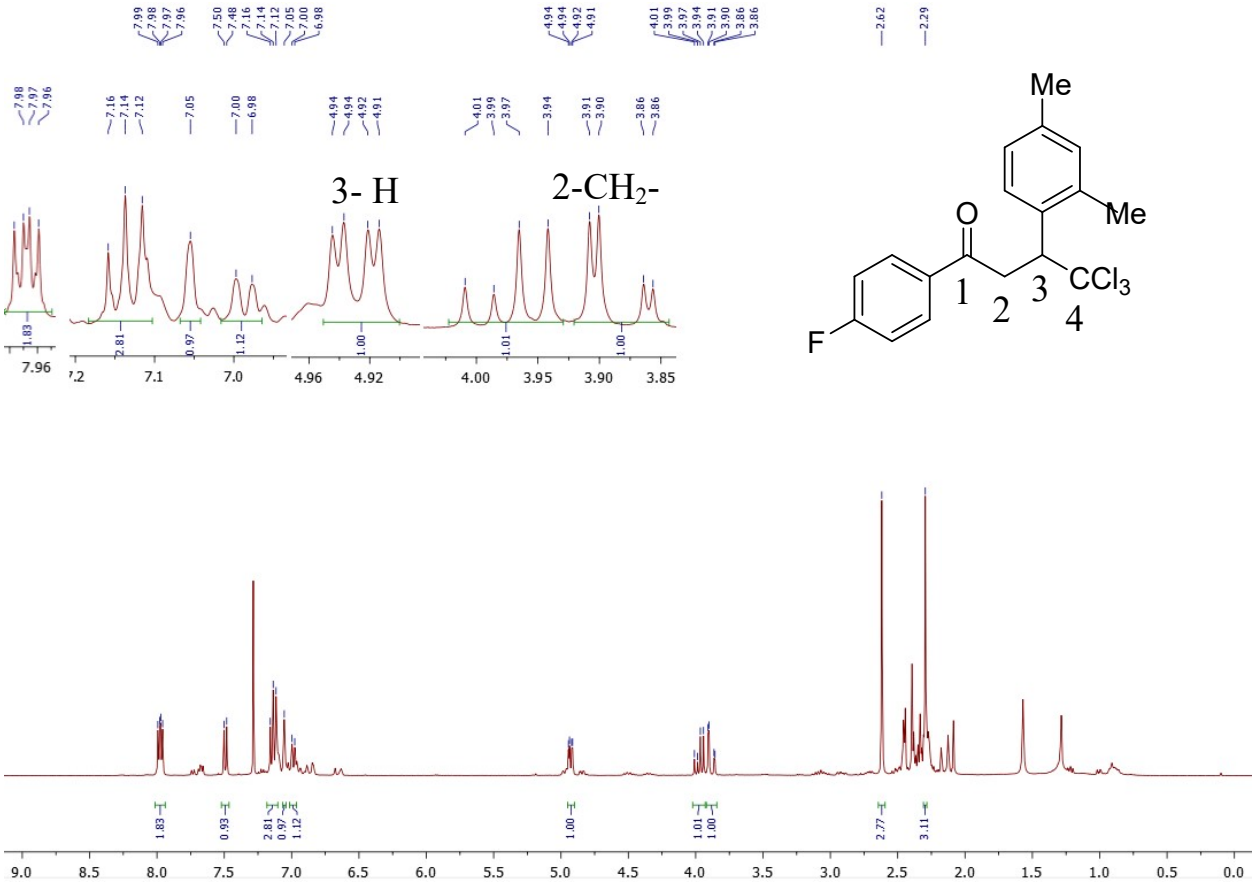


Fig.S53. ^{1}H NMR spectrum of the compound **5da** ($CDCl_3$, 400 MHz).

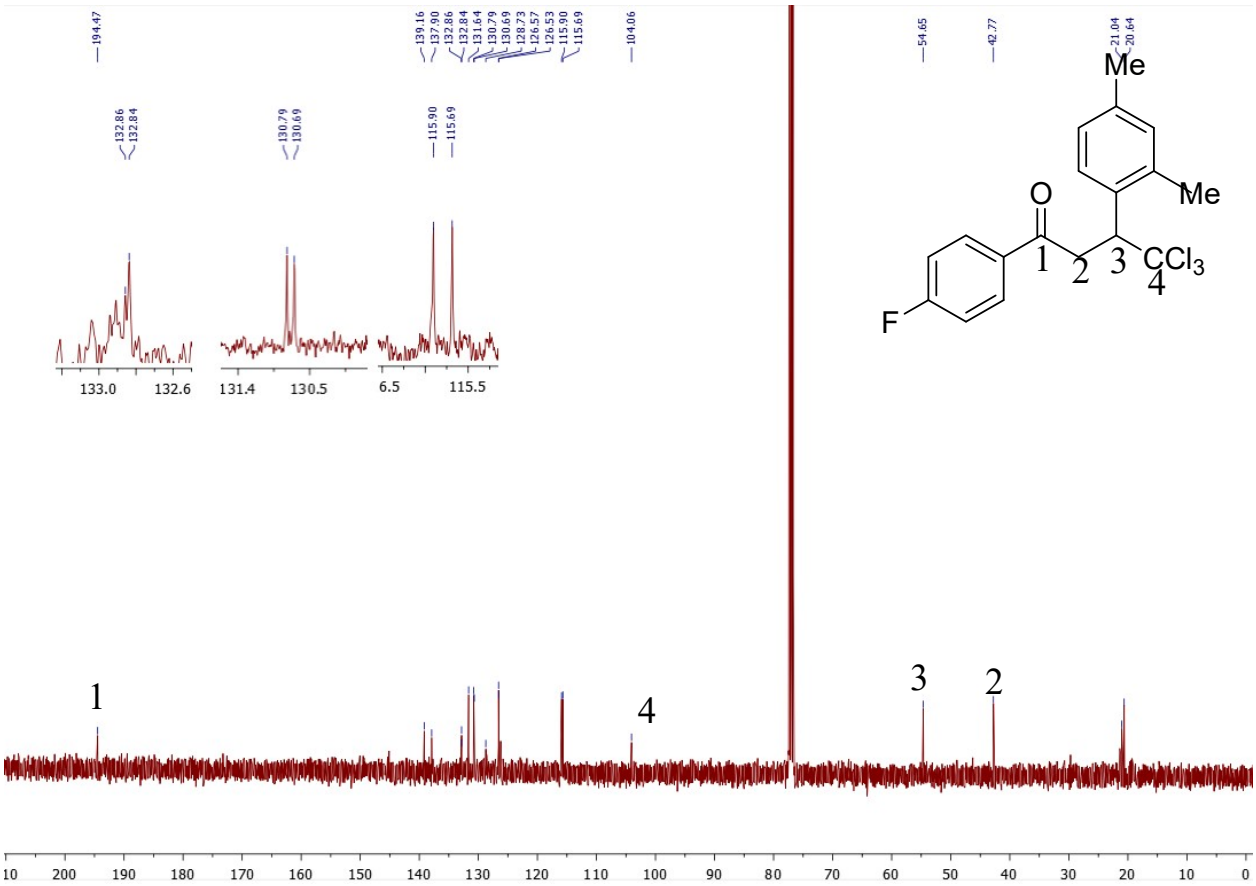


Fig. S54. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5da** ($CDCl_3$, 101 MHz).

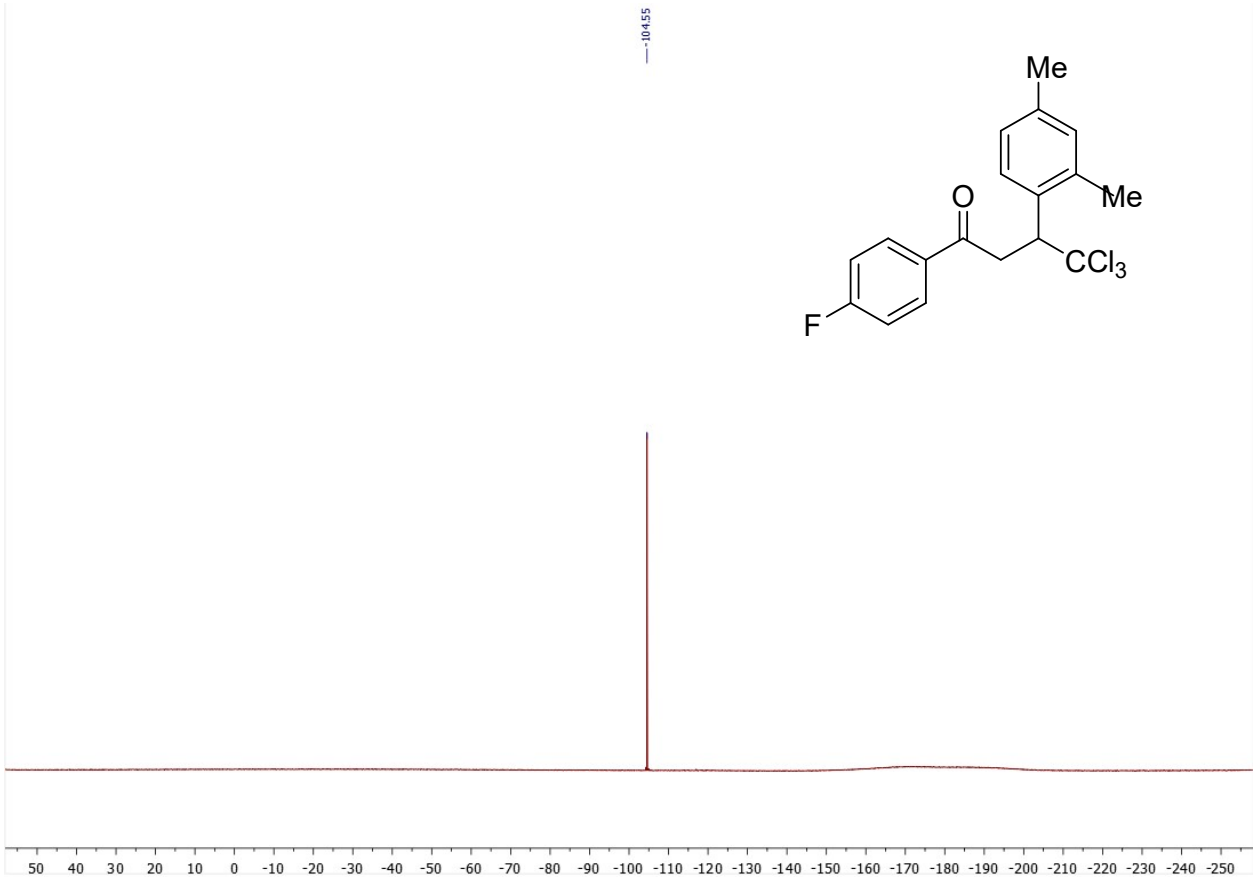


Fig. S55. $^{19}F\{^{1}H\}$ NMR spectrum of the compound **5da** ($CDCl_3$, 376 MHz).

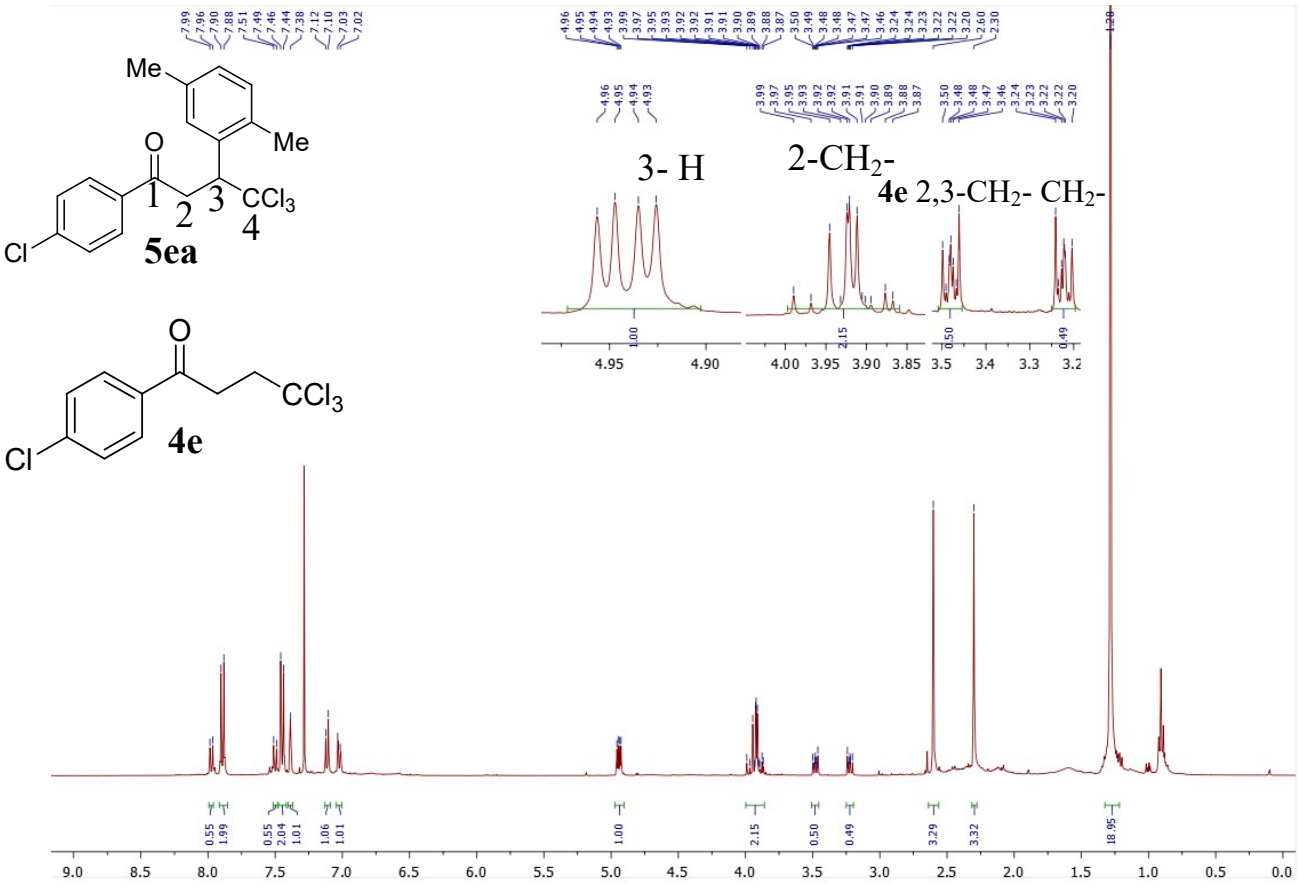


Fig.S56. ^{1}H NMR spectrum of the compound **5ea** ($CDCl_3$, 400 MHz).

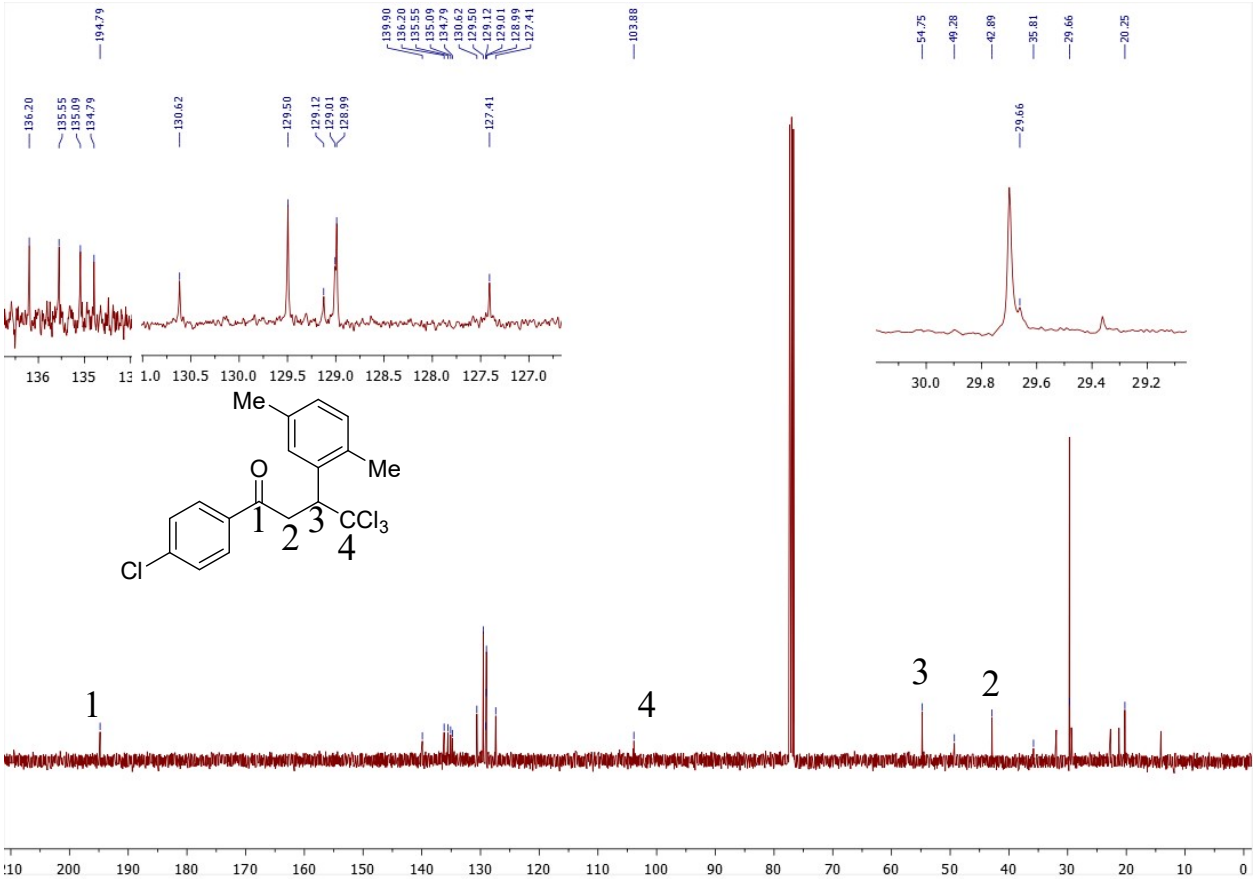


Fig. S57. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5ea** ($CDCl_3$, 101 MHz).

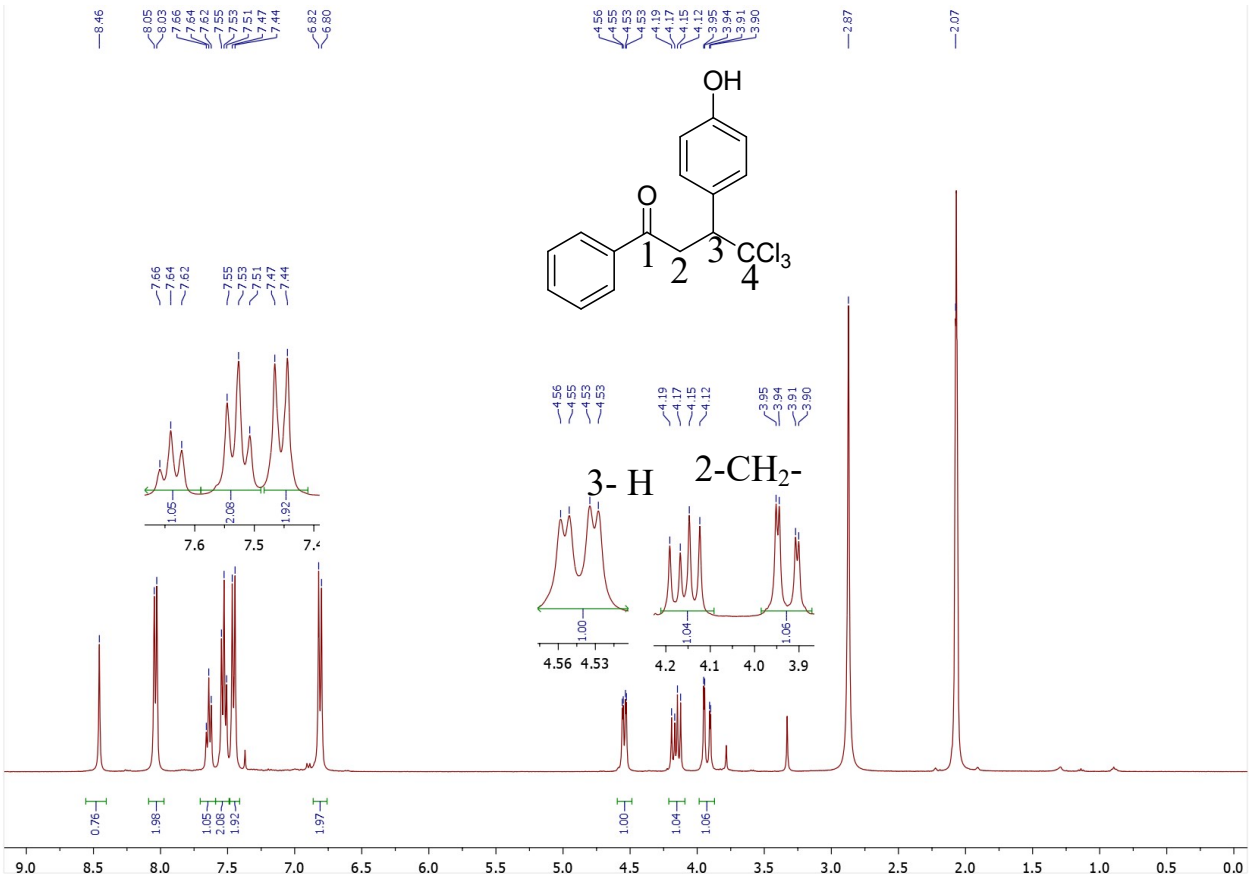


Fig.S58. ^{1}H NMR spectrum of the compound **5ab** ($(CD_3)_2CO$, 400 MHz).

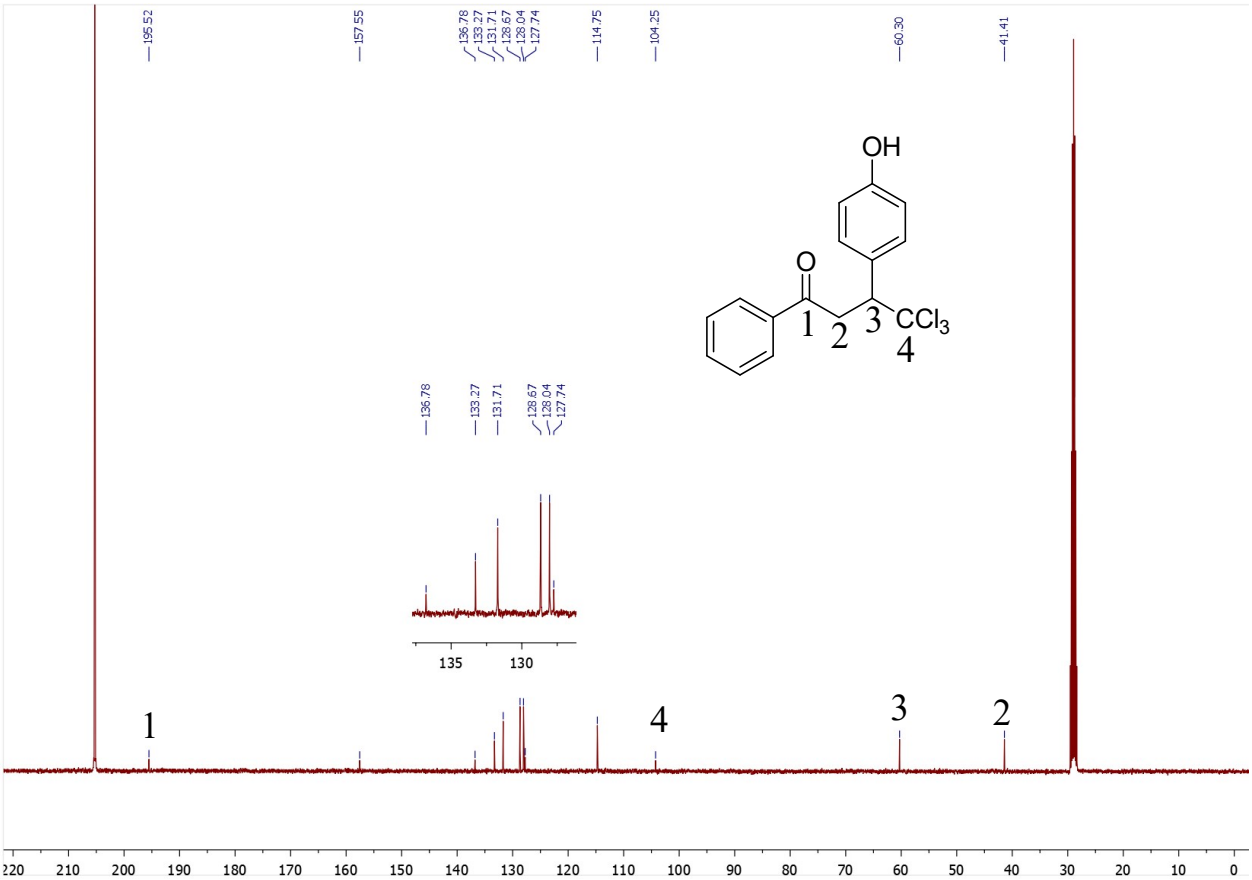


Fig. S59. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5ab** ($(CD_3)_2CO$, 101 MHz).

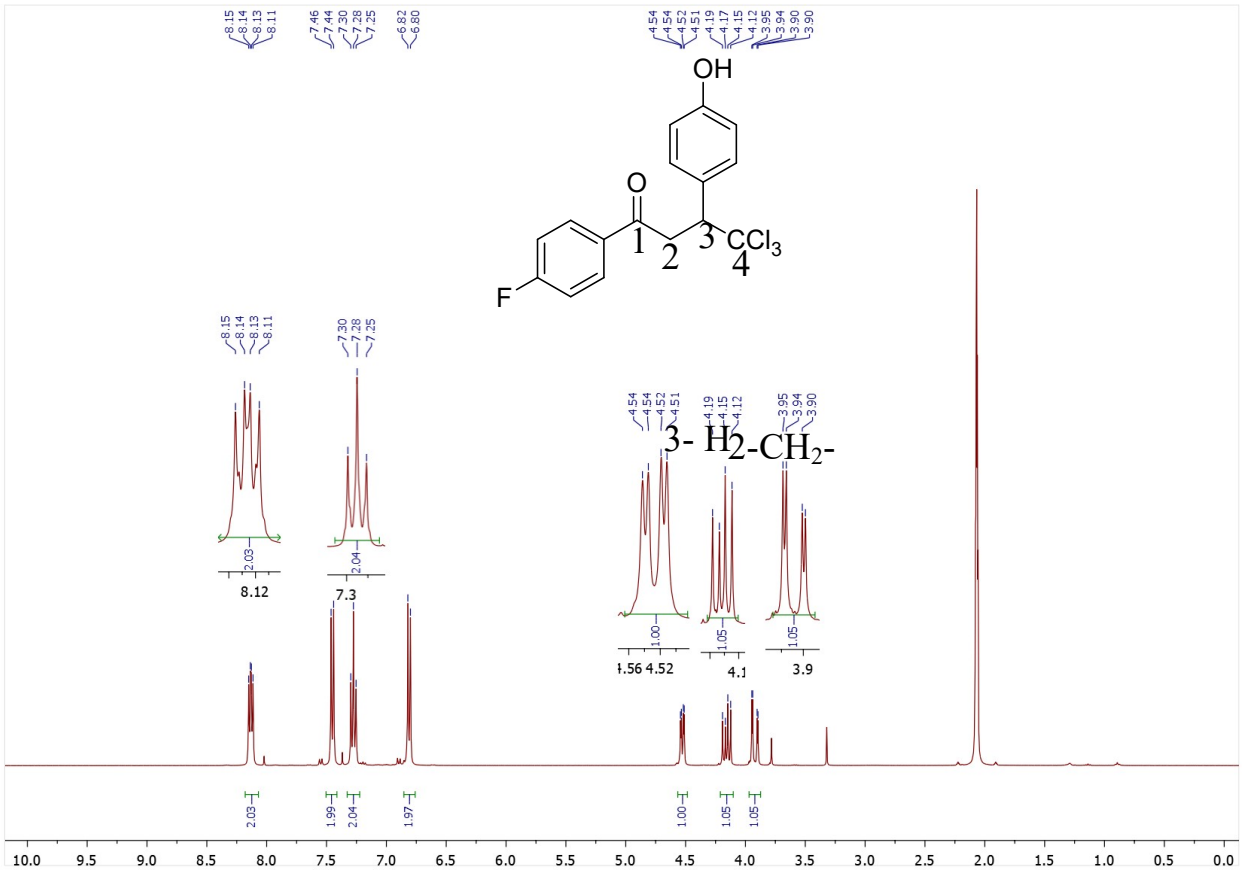


Fig.S60. ^{1}H NMR spectrum of the compound **5db** ($(CD_3)_2CO$, 400 MHz).

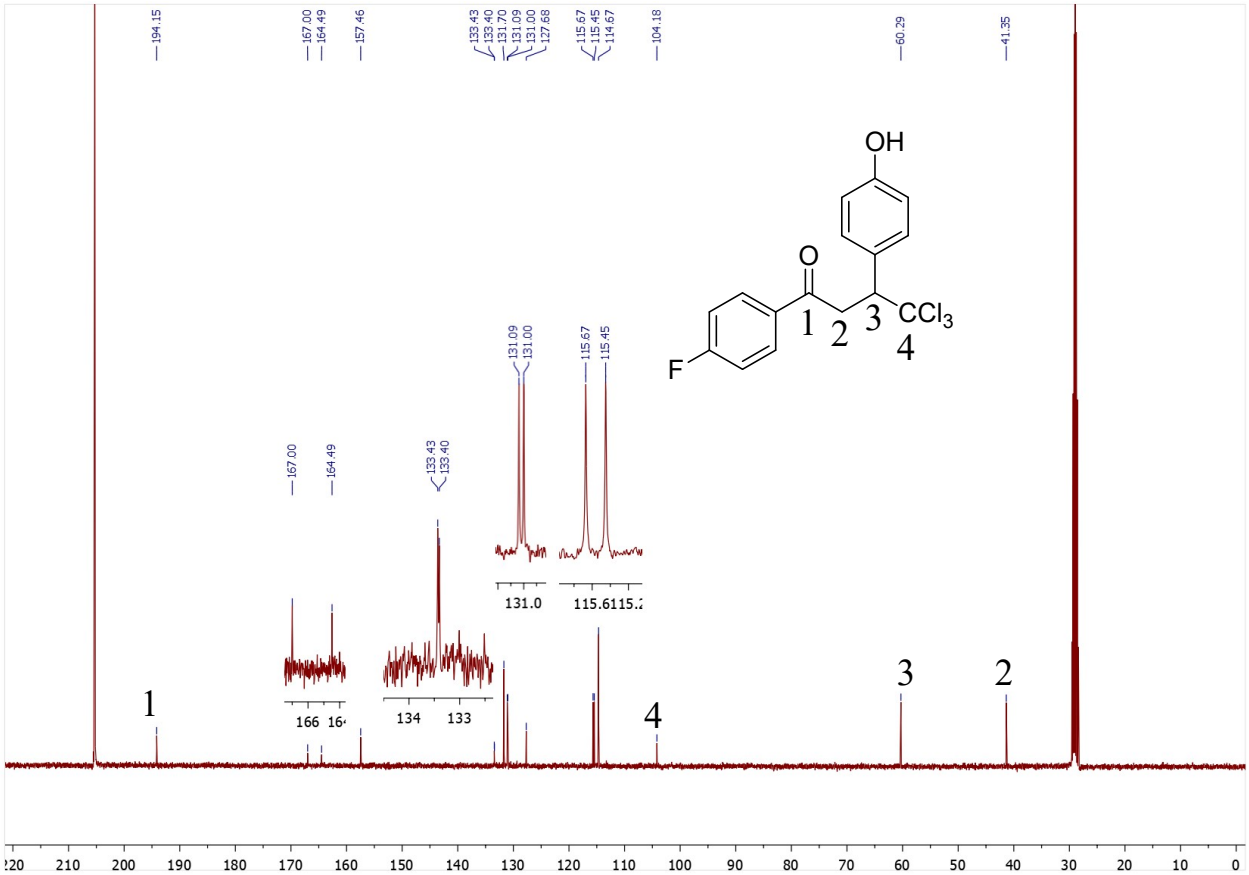


Fig. S61. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5db** ($(CD_3)_2CO$, 101 MHz).

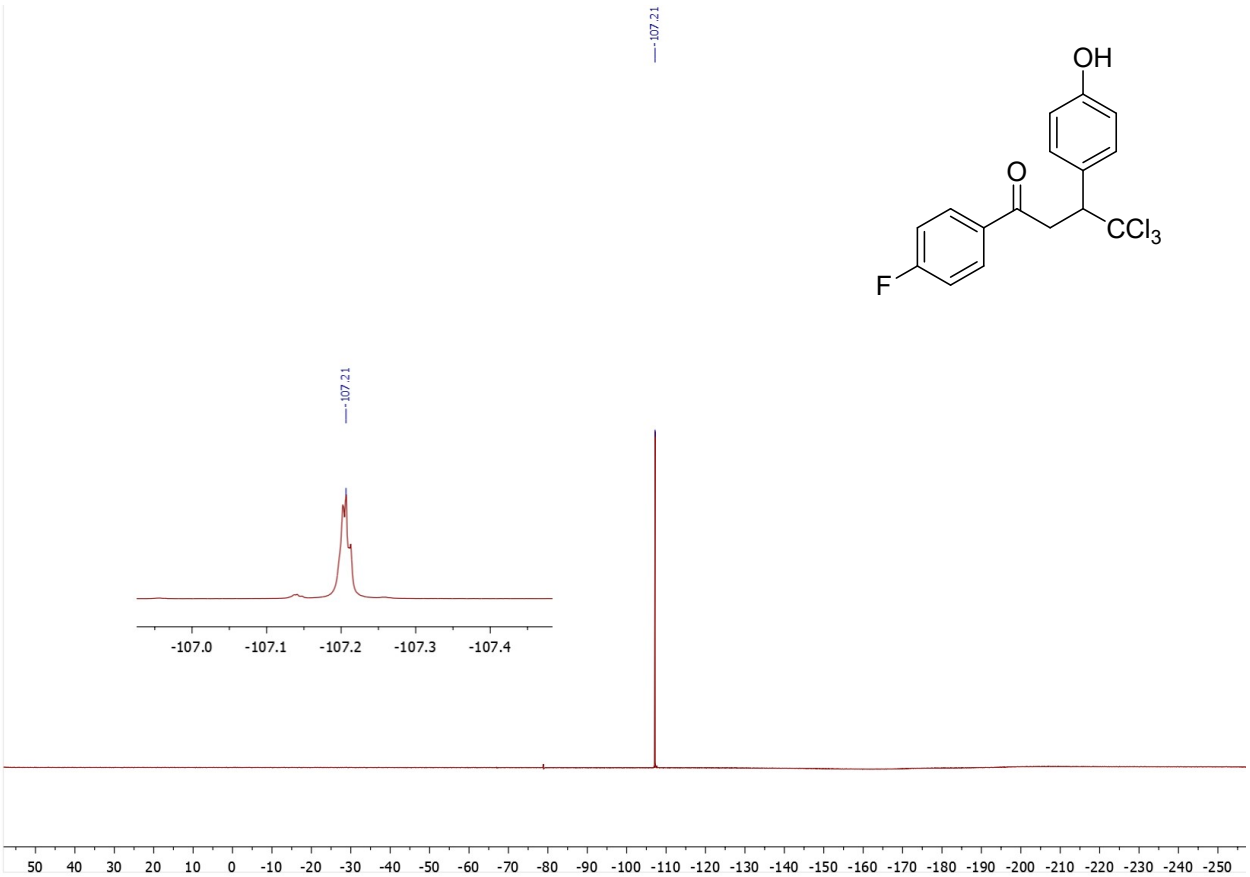


Fig. S62. $^{19}F\{^{1}H\}$ NMR spectrum of the compound **5db** ($CDCl_3$, 376 MHz).

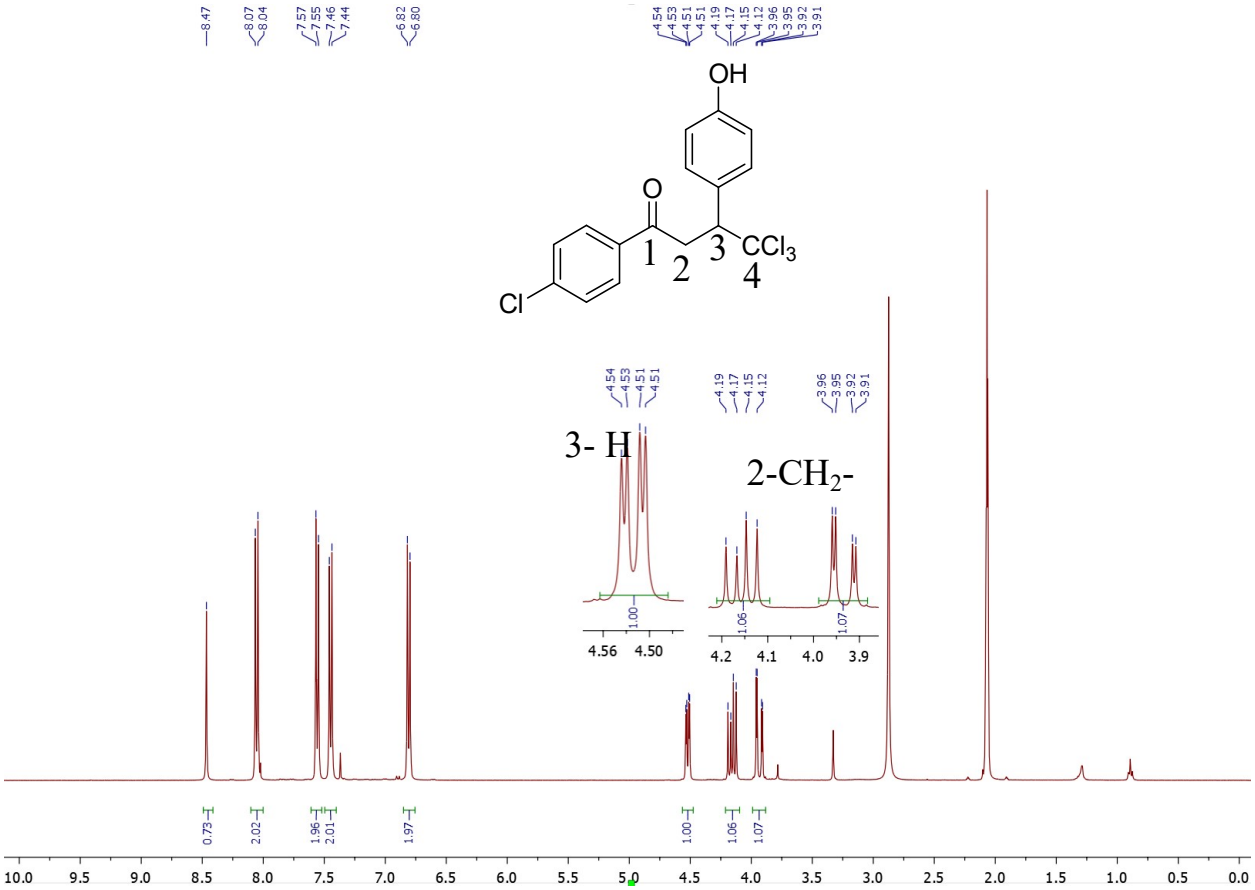


Fig.S63. ^{1}H NMR spectrum of the compound **5eb** ($(CD_3)_2CO$, 400 MHz).

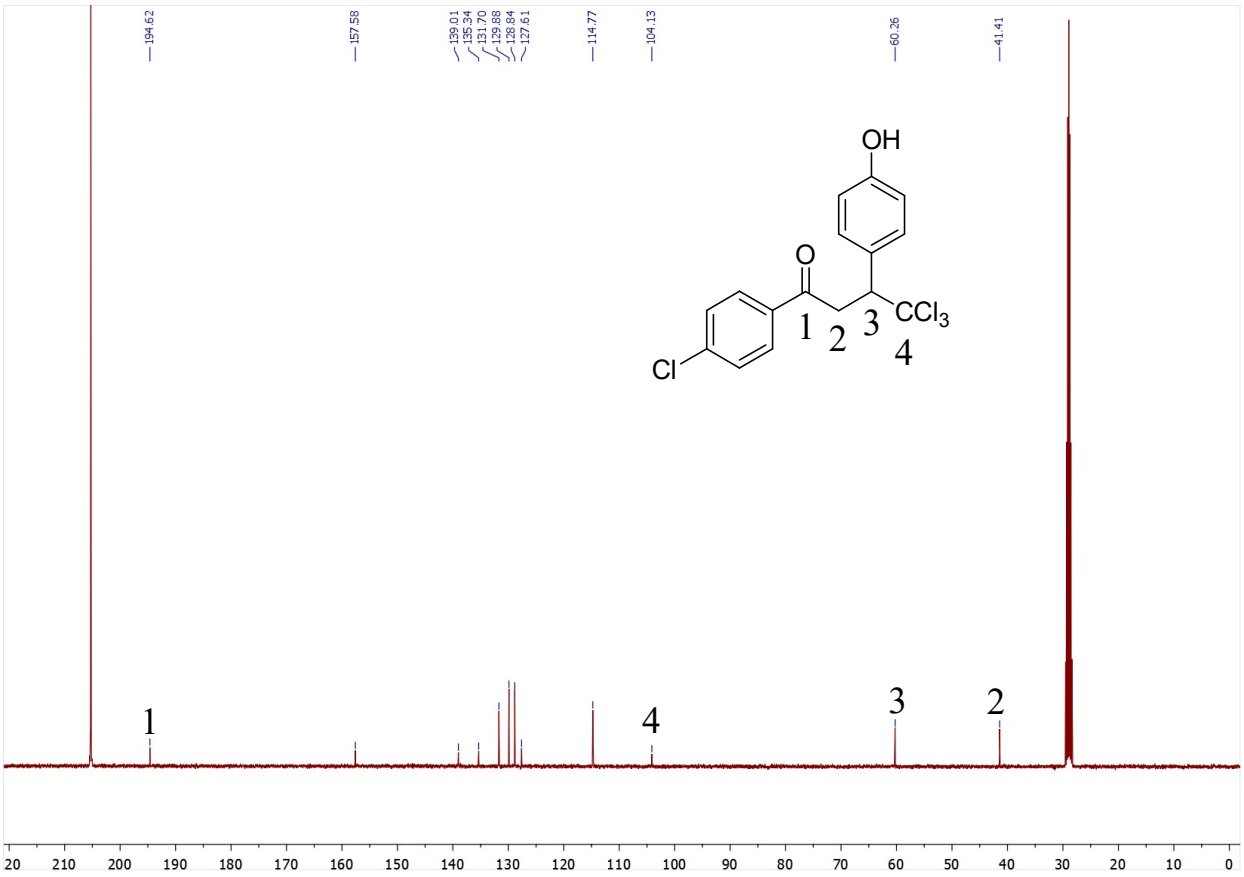


Fig. S64. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5eb** ($(CD_3)_2CO$, 101 MHz).

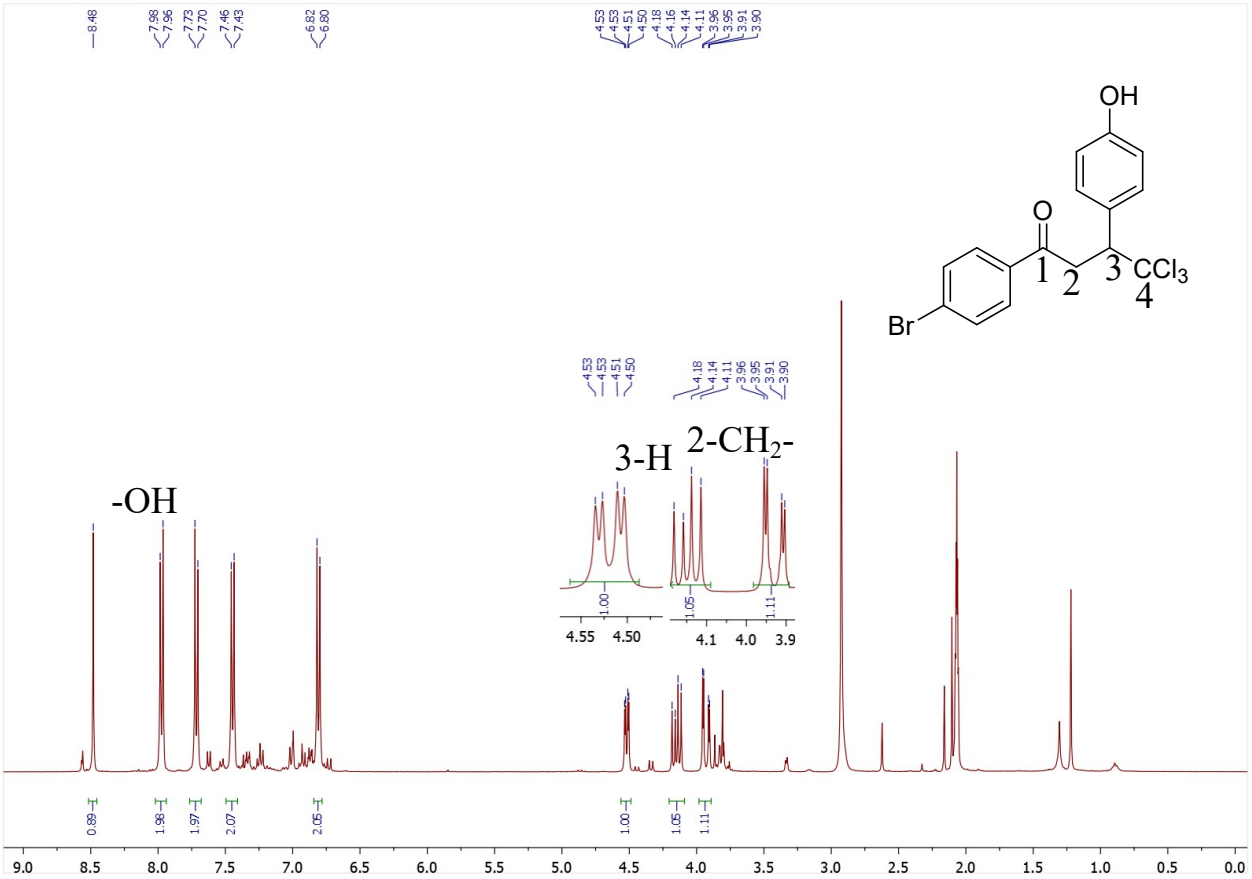


Fig.S65. ^{1}H NMR spectrum of the compound **5fb** ($(CD_3)_2CO$, 400 MHz).

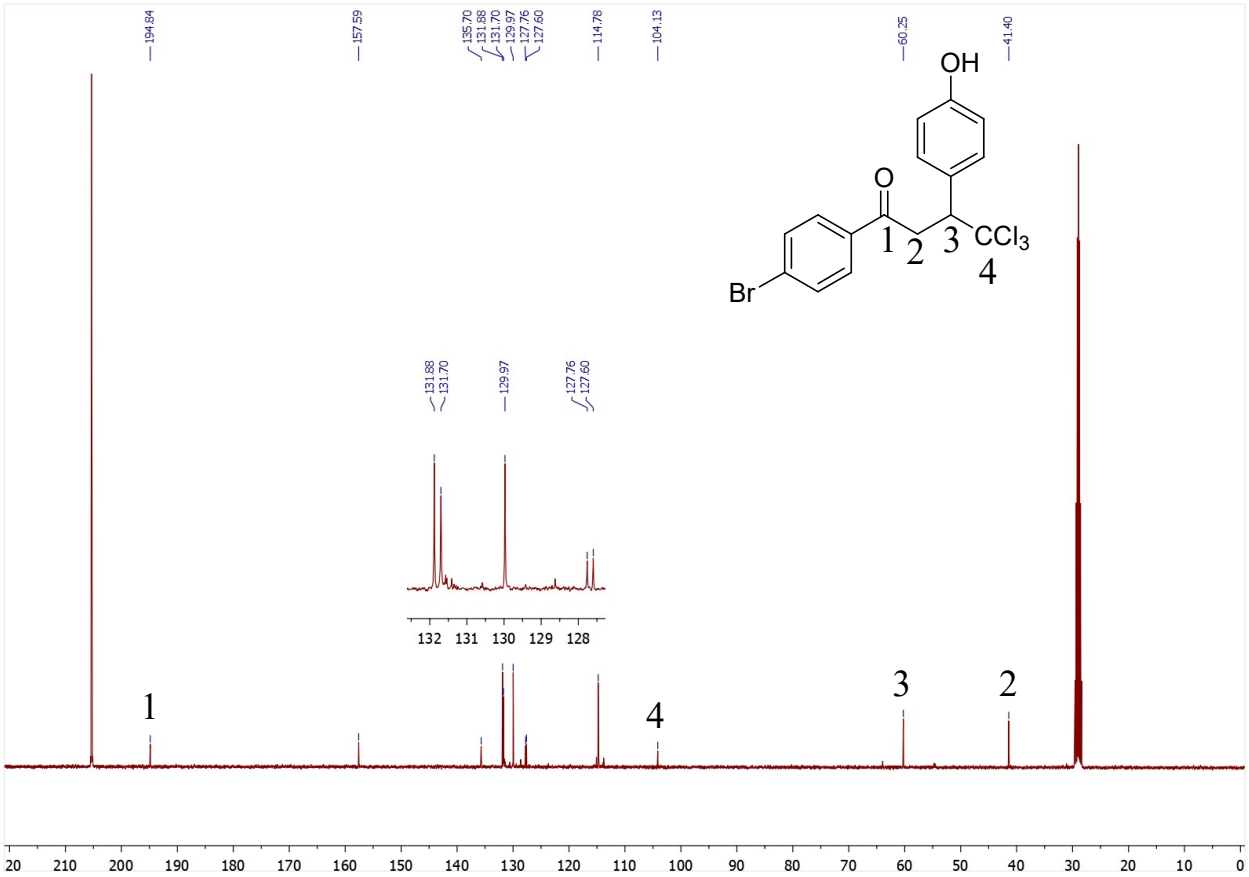


Fig. S66. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5fb** ($(CD_3)_2CO$, 101 MHz).

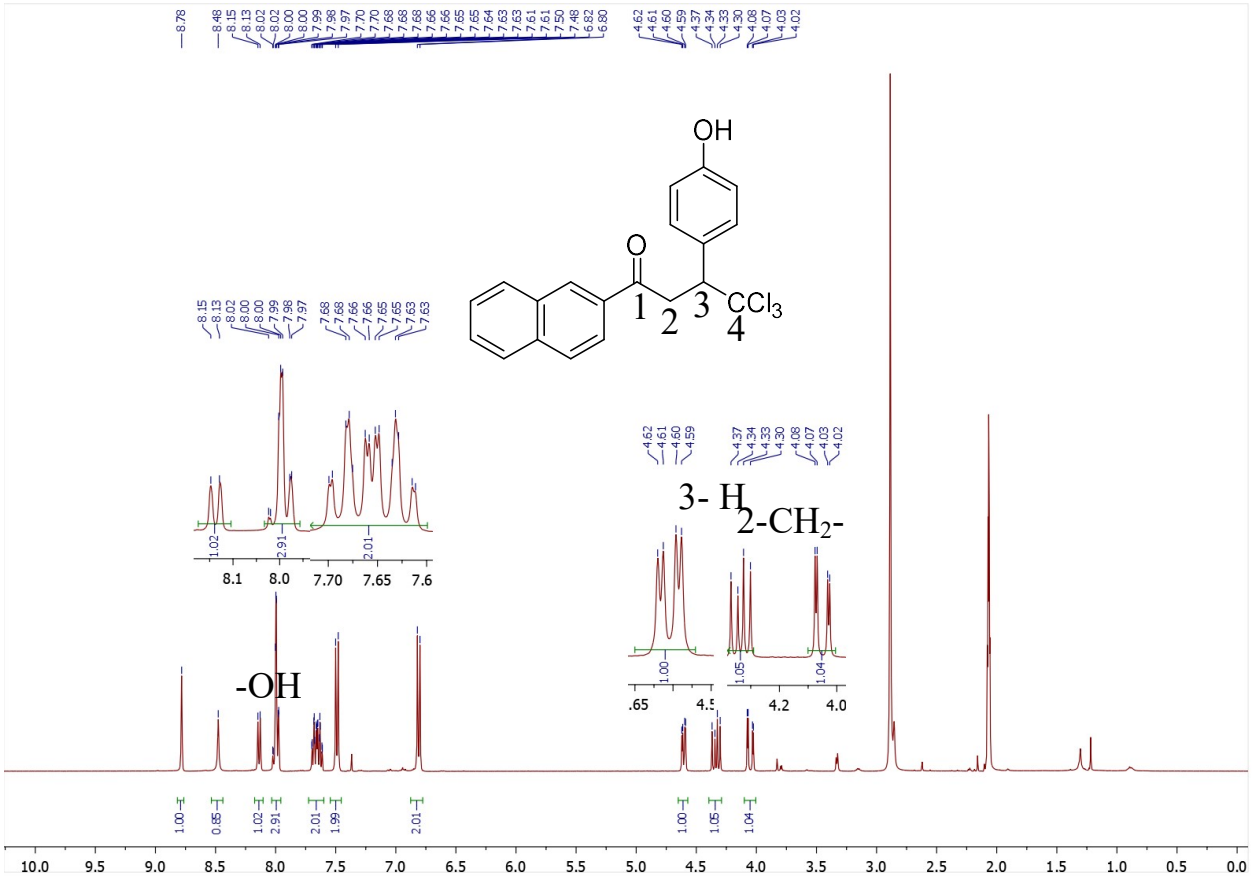


Fig.S67. ^{1}H NMR spectrum of the compound **5l** ($(CD_3)_2CO$, 400 MHz).

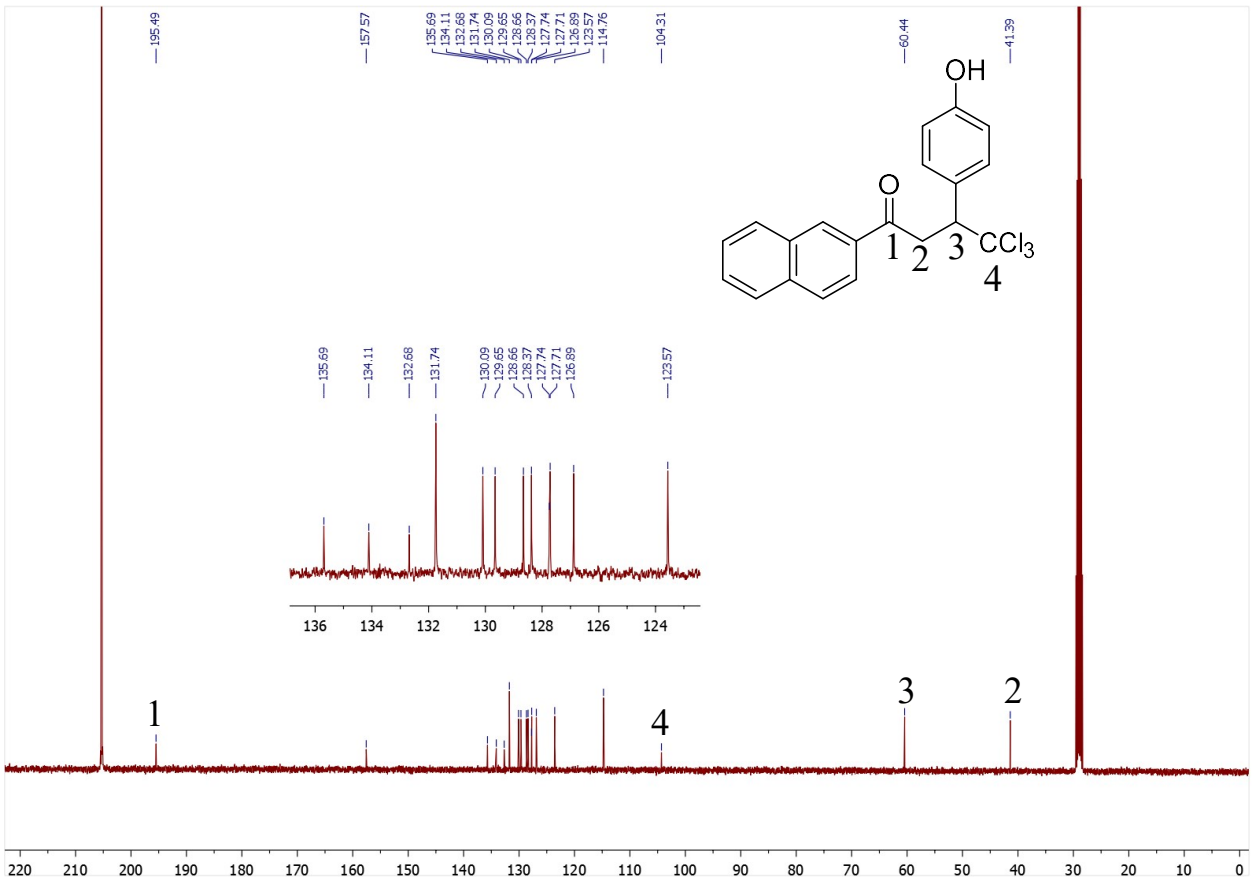


Fig. S68. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5l** ($(CD_3)_2CO$, 101 MHz).

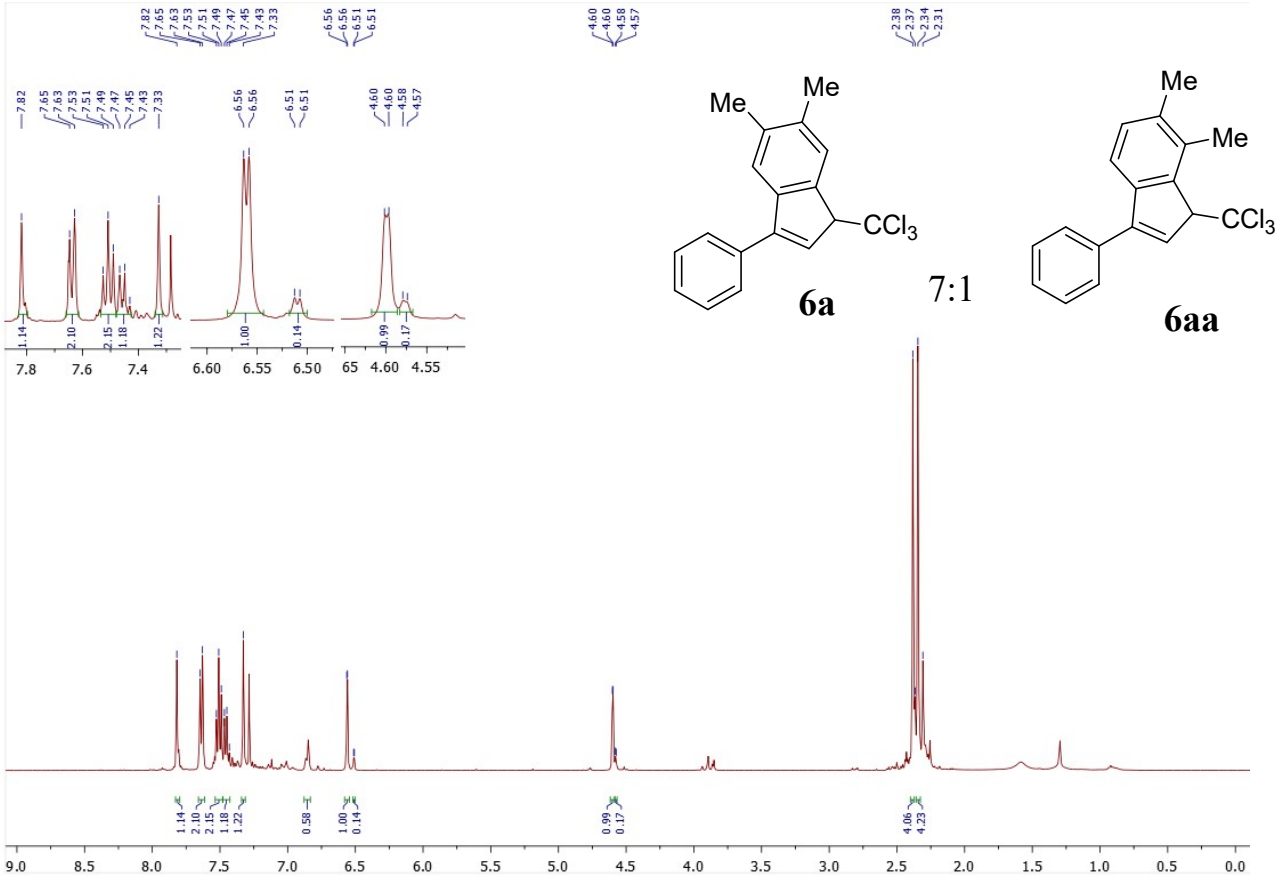


Fig.S69. ^{1}H NMR spectrum of compounds **6a** and **6aa** ($CDCl_3$, 400 MHz).

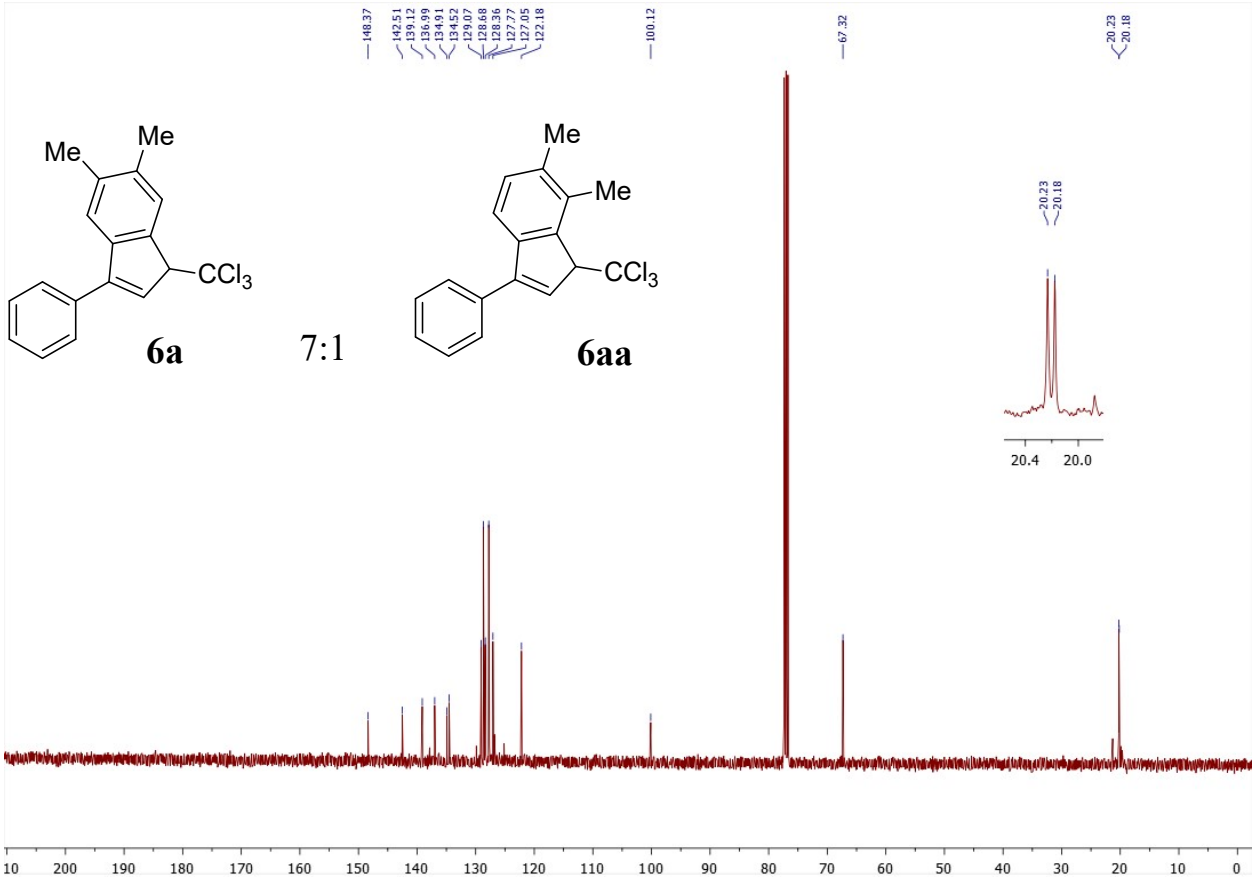


Fig. S70. $^{13}C\{^{1}H\}$ NMR spectrum of compounds **6a** and **6aa** ($CDCl_3$, 101 MHz).

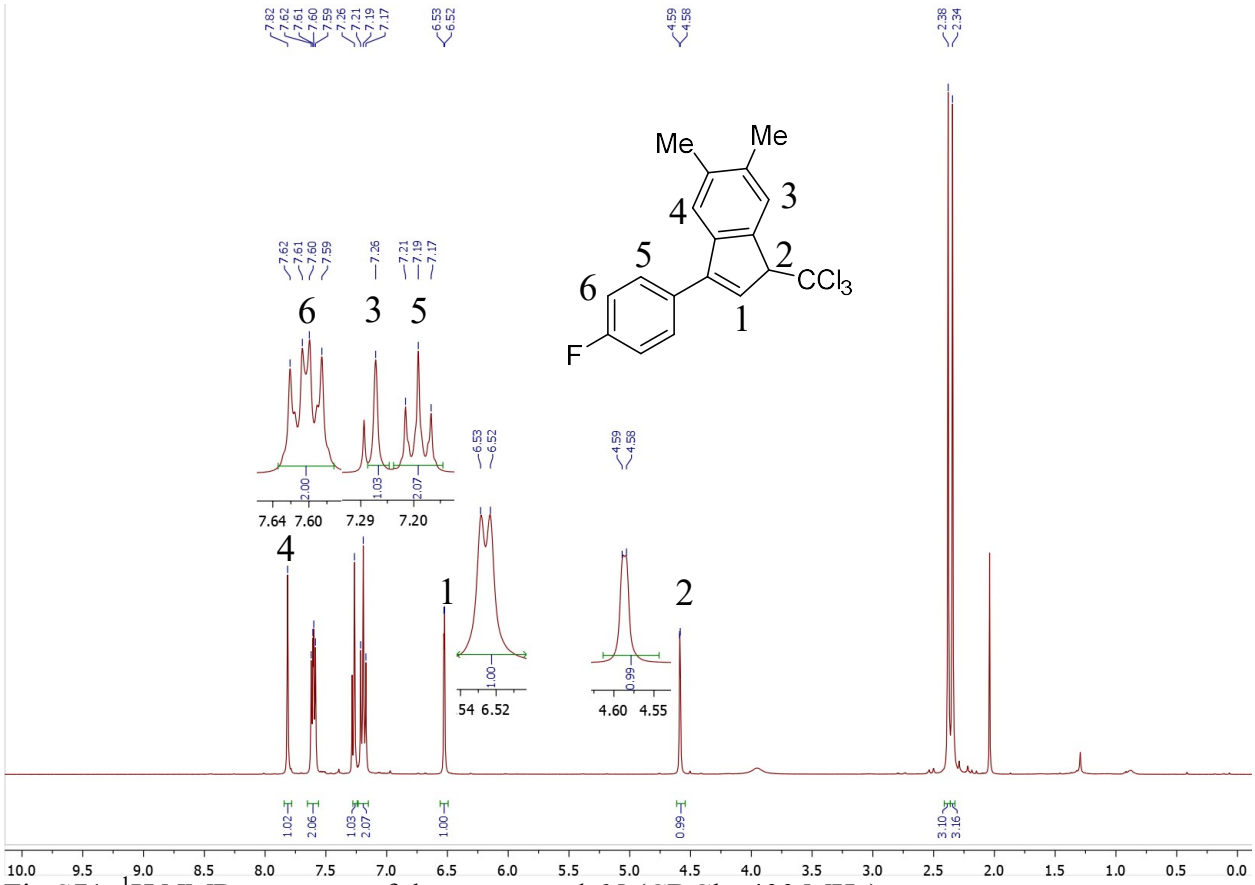


Fig.S71. ^{1}H NMR spectrum of the compound **6d** ($CDCl_3$, 400 MHz).

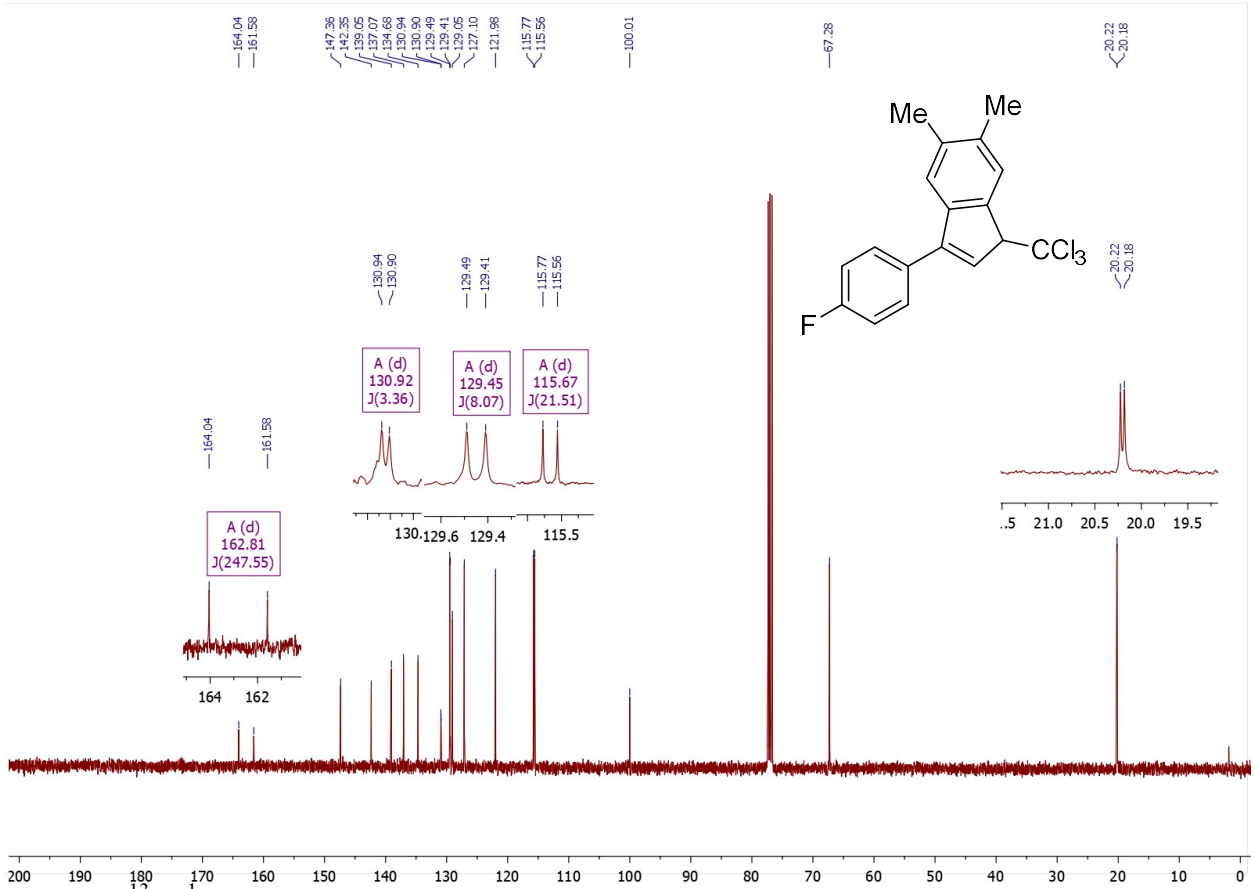


Fig. S72. $^{13}C\{^{1}H\}$ NMR spectrum of the compounds **6d** ($CDCl_3$, 101 MHz).

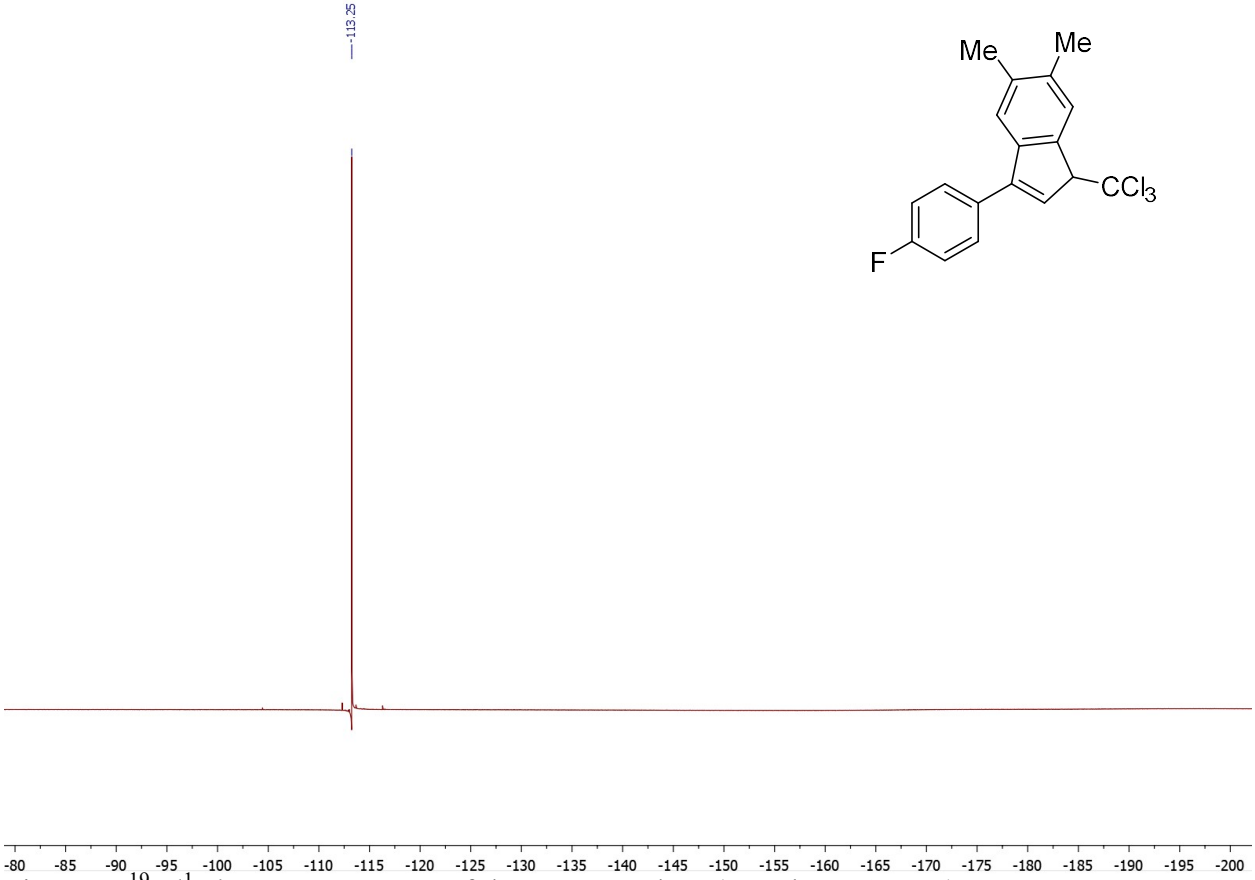


Fig. S73. $^{19}F\{^{1}H\}$ NMR spectrum of the compound **6d** ($CDCl_3$, 376 MHz).

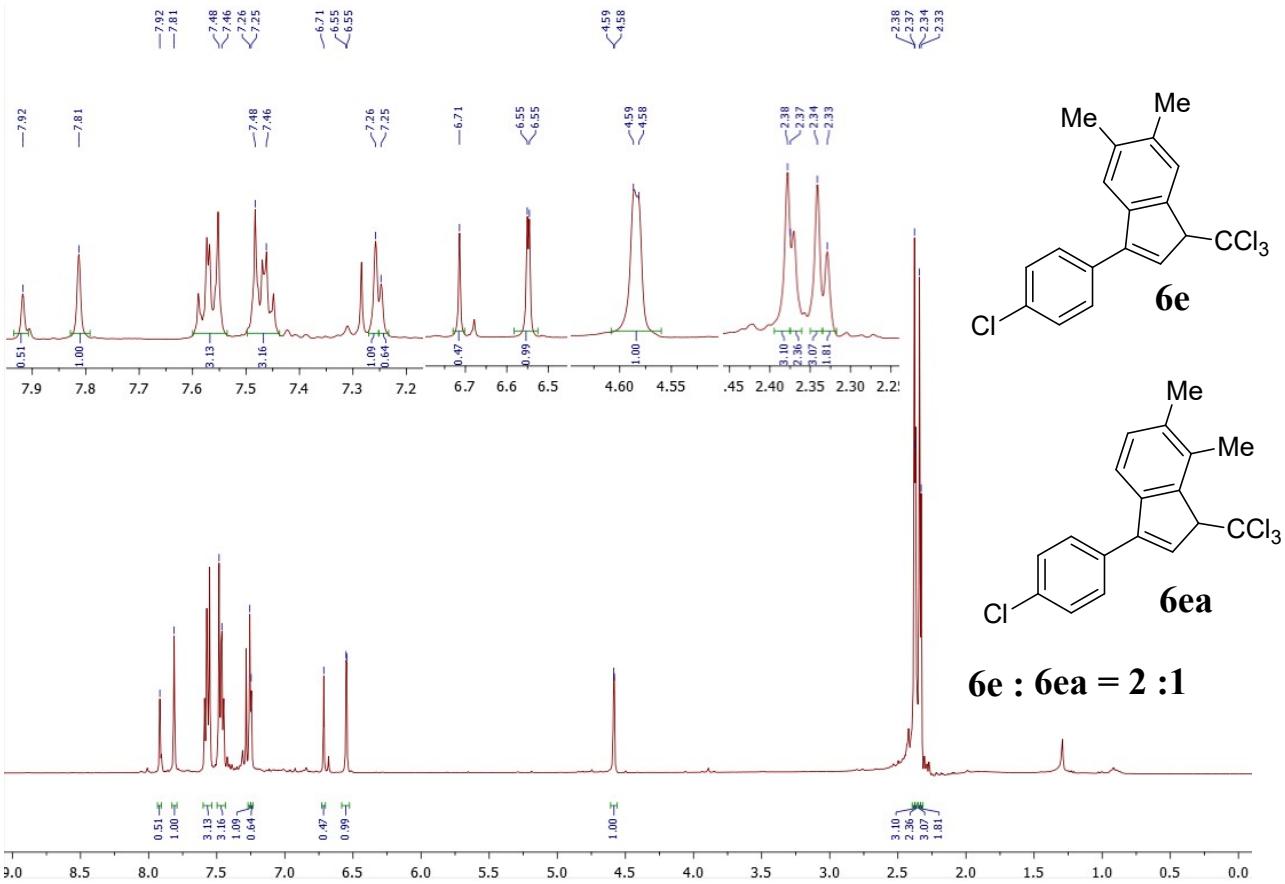


Fig.S74. ^{1}H NMR spectrum of compounds **6e** and **6ea** ($CDCl_3$, 400 MHz).

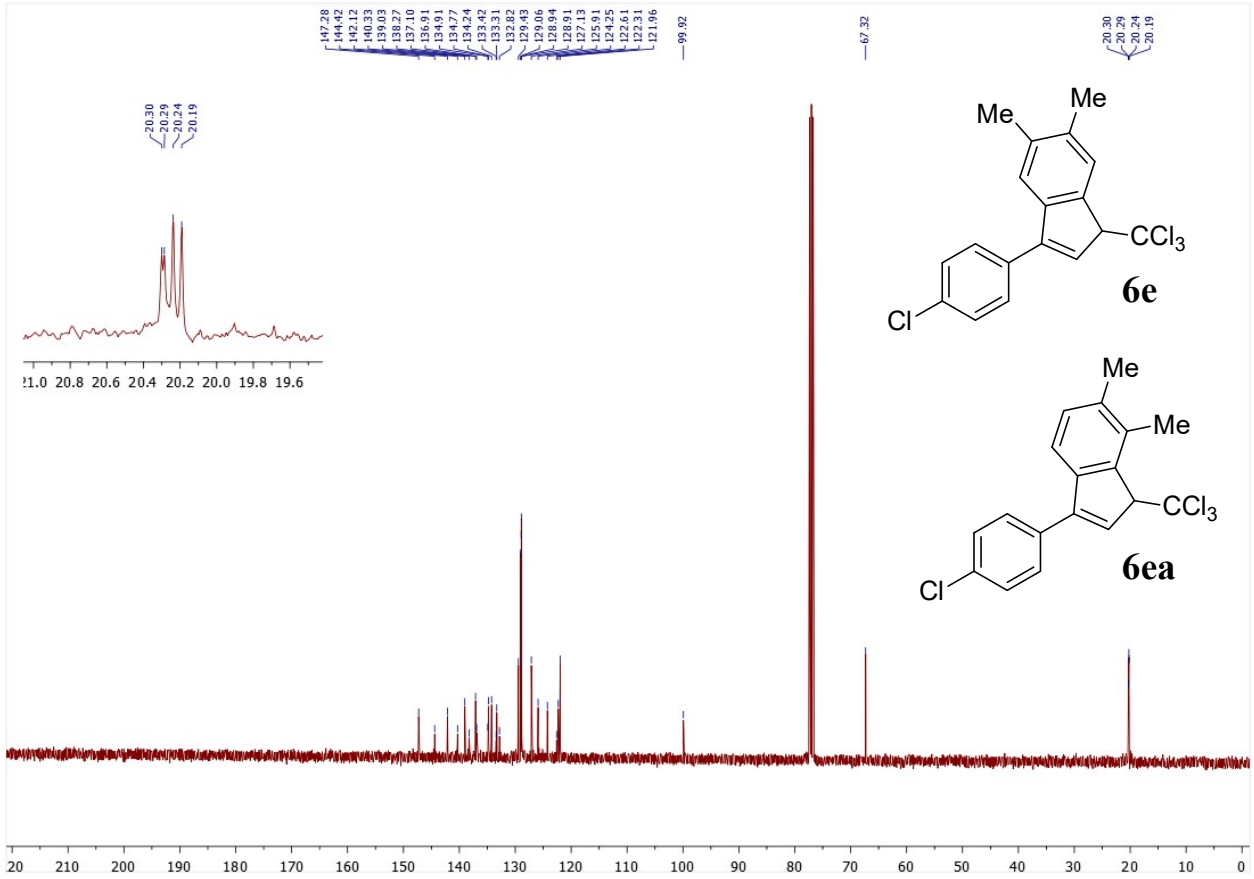


Fig. S75. $^{13}C\{^{1}H\}$ NMR spectrum of compounds **6e** and **6ea** ($CDCl_3$, 101 MHz).

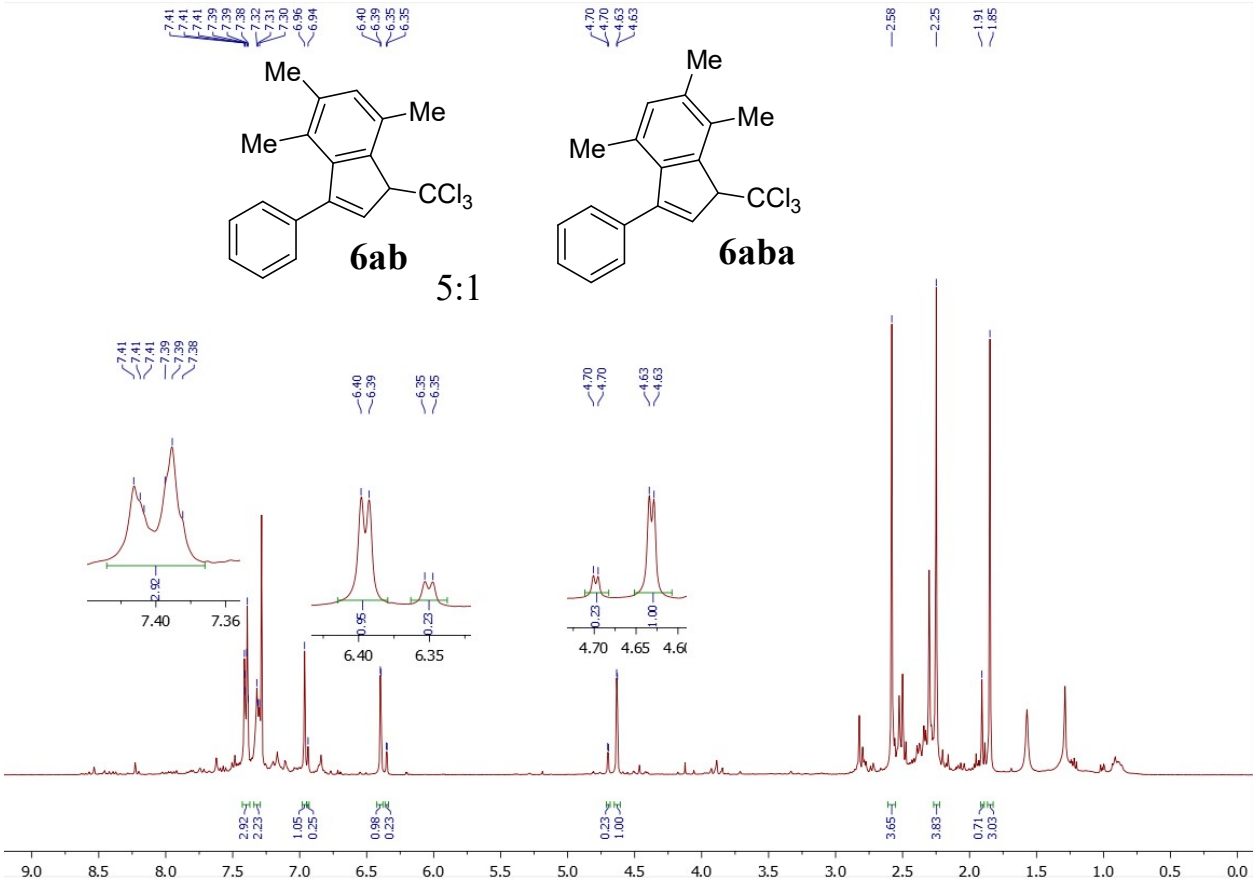


Fig.S76. ^{1}H NMR spectrum of compounds **6ab** and **6aba** ($CDCl_3$, 400 MHz).

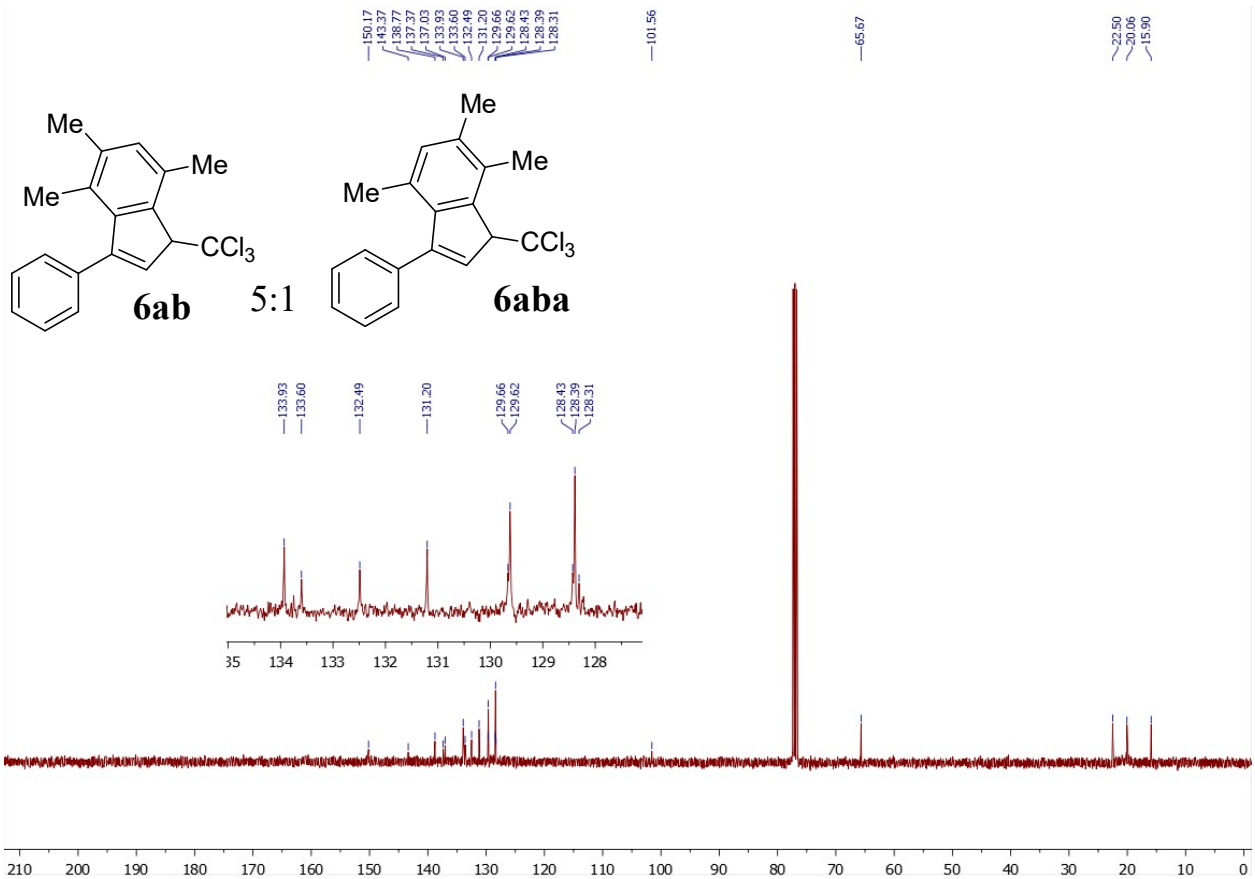


Fig. S77. $^{13}C\{^{1}H\}$ NMR spectrum of compounds **6ab** and **6aba** ($CDCl_3$, 101 MHz).

3. X-ray data of compounds 3a, 3e, 3j, 4e, 4g, 5fb

3a

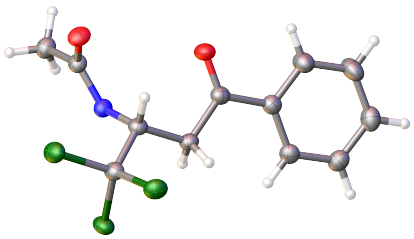


Table S1. Crystal data and structure refinement for 3a.

Empirical formula	$C_{12}H_{11}Cl_3NO_2$
Formula weight	307.57
Temperature /K	99.99(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.7611(4)
b/Å	14.0190(4)
c/Å	9.5719(3)
α/°	90
β/°	109.786(4)
γ/°	90
Volume/Å^3	1358.77(8)
Z	4
ρ_{calc}g/cm^3	1.504
μ/mm^{-1}	6.061
F(000)	628.0
Crystal size/mm^3	? × ? × ?
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.732 to 160.172
Index ranges	$-13 \leq h \leq 13$, $-16 \leq k \leq 17$, $-10 \leq l \leq 12$
Reflections collected	12878
Independent reflections	2855 [R_{int} = 0.0454, R_{sigma} = 0.0356]
Data/restraints/parameters	2855/0/164
Goodness-of-fit on F^2	1.155
Final R indexes [I>=2σ (I)]	R_1 = 0.0430, wR_2 = 0.1183
Final R indexes [all data]	R_1 = 0.0491, wR_2 = 0.1222
Largest diff. peak/hole / e Å^{-3}	0.75/-0.71

3e

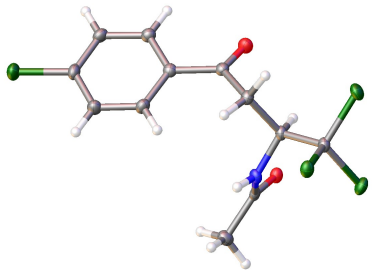


Table S2. Crystal data and structure refinement for 3e.

Empirical formula	$C_{12}H_{11}Cl_4NO_2$
Formula weight	343.02
Temperature/K	100.0(3)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	11.9375(4)
b/Å	13.5556(3)
c/Å	9.6733(3)
α/°	90
β/°	112.902(4)
γ/°	90
Volume/Å^3	1441.94(8)
Z	4
ρ_{calc}g/cm^3	1.580
μ/mm^{-1}	7.442
F(000)	696.0
Crystal size/mm^3	0.1 × 0.08 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.04 to 139.99
Index ranges	$-13 \leq h \leq 14$, $-16 \leq k \leq 16$, $-11 \leq l \leq 11$
Reflections collected	8531
Independent reflections	2661 [R_{int} = 0.0574, R_{sigma} = 0.0388]
Data/restraints/parameters	2661/0/177
Goodness-of-fit on F^2	1.107
Final R indexes [I>=2σ (I)]	R_1 = 0.0411, wR_2 = 0.1199
Final R indexes [all data]	R_1 = 0.0421, wR_2 = 0.1209
Largest diff. peak/hole / e Å^{-3}	0.43/-0.43

3j

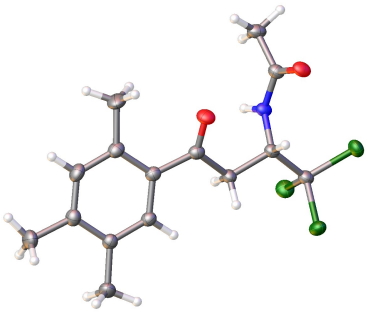


Table S3. Crystal data and structure refinement for 3j.

Empirical formula	$C_{15}H_{18}Cl_3NO_2$
Formula weight	350.65
Temperature/K	100.01(11)
Crystal system	triclinic
Space group	P-1
a/Å	9.2834(2)
b/Å	11.5385(4)
c/Å	16.7356(2)
α/°	76.702(2)
β/°	83.835(2)
γ/°	75.793(2)
Volume/Å^3	1688.77(7)
Z	4
ρ_{calc}g/cm^3	1.379
μ/mm^{-1}	4.941
F(000)	728.0
Crystal size/mm^3	0.28 × 0.09 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.434 to 139.992
Index ranges	-11 ≤ h ≤ 11, -14 ≤ k ≤ 14, -15 ≤ l ≤ 20
Reflections collected	21599
Independent reflections	6387 [R_{int} = 0.0480, R_{sigma} = 0.0441]
Data/restraints/parameters	6387/0/395
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0351, wR_2 = 0.0962
Final R indexes [all data]	R_1 = 0.0386, wR_2 = 0.0988
Largest diff. peak/hole / e Å^{-3}	0.37/-0.33

4e

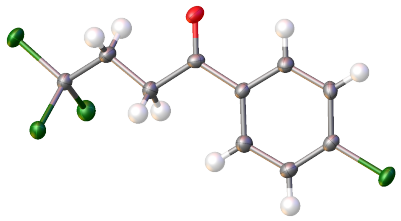


Table S4. Crystal data and structure refinement for 4e.

Empirical formula	$C_{20}H_{16}Cl_8O_2$
Formula weight	571.93
Temperature/K	99.99(11)
Crystal system	monoclinic
Space group	Ia
a/Å	11.2258(2)
b/Å	13.7660(3)
c/Å	15.1288(3)
α/°	90
β/°	93.525(2)
γ/°	90
Volume/Å^3	2333.50(8)
Z	4
ρ_{calc}g/cm^3	1.628
μ/mm^{-1}	8.971
F(000)	1152.0
Crystalsize/mm^3	0.31 × 0.19 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.692 to 138.282
Index ranges	-13 ≤ h ≤ 13, -16 ≤ k ≤ 16, -18 ≤ l ≤ 18
Reflections collected	12181
Independent reflections	3636 [R_{int} = 0.0317, R_{sigma} = 0.0317]
Data/restraints/parameters	3636/2/271
Goodness-of-fit on F^2	0.801
Final R indexes [I>=2σ (I)]	R_1 = 0.0312, wR_2 = 0.0884
Final R indexes [all data]	R_1 = 0.0317, wR_2 = 0.0896
Largest diff. peak/hole / e Å^{-3}	0.44/-0.26

4g

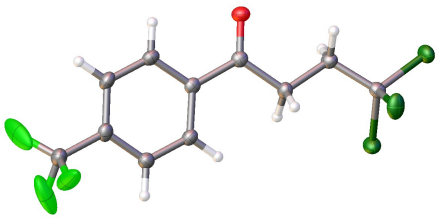


Table S5. Crystal data and structure refinement for 4g.

Empirical formula	$C_{11}H_8Cl_3F_3O$
Formula weight	319.52
Temperature/K	99.98(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	5.76450(10)
b/Å	12.1514(2)
c/Å	18.0507(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1264.39(3)
Z	4
ρ_{calc}g/cm^3	1.679
μ/mm^{-1}	6.806
F(000)	640.0
Crystal size/mm^3	0.16 × 0.14 × 0.07
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.772 to 138.15
Index ranges	$-6 \le h \le 6$, $-14 \le k \le 14$, $-21 \le l \le 21$
Reflections collected	6418
Independent reflections	2348 [R_{int} = 0.0266, R_{sigma} = 0.0281]
Data/restraints/parameters	2348/0/173
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0292, wR_2 = 0.0733
Final R indexes [all data]	R_1 = 0.0296, wR_2 = 0.0737
Largest diff. peak/hole / e Å^{-3}	0.55/-0.33

5fb

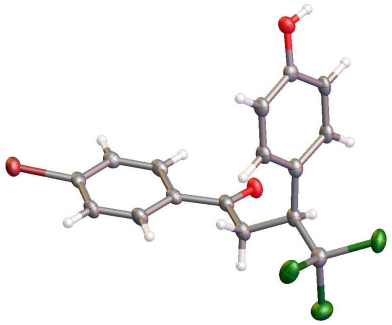


Table S6. Crystal data and structure refinement for 5fb.

Empirical formula	$C_{16}H_{12}BrCl_3O_2$
Formula weight	422.52
Temperature/K	100.01(10)
Crystal system	trigonal
Space group	R-3
a/Å	39.1114(7)
b/Å	39.1114(7)
c/Å	5.87550(10)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	7783.6(3)
Z	18
ρ_{calc}g/cm^3	1.622
μ/mm^{-1}	7.533
F(000)	3780.0
Crystal size/mm^3	0.07 × 0.05 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.044 to 139.986
Index ranges	-47 ≤ h ≤ 35, -47 ≤ k ≤ 46, -7 ≤ l ≤ 7
Reflections collected	8516
Independent reflections	3205 [R_{int} = 0.0253, R_{sigma} = 0.0255]
Data/restraints/parameters	3205/0/200
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0284, wR_2 = 0.0750
Final R indexes [all data]	R_1 = 0.0303, wR_2 = 0.0762
Largest diff. peak/hole / e Å^{-3}	0.65/-0.48

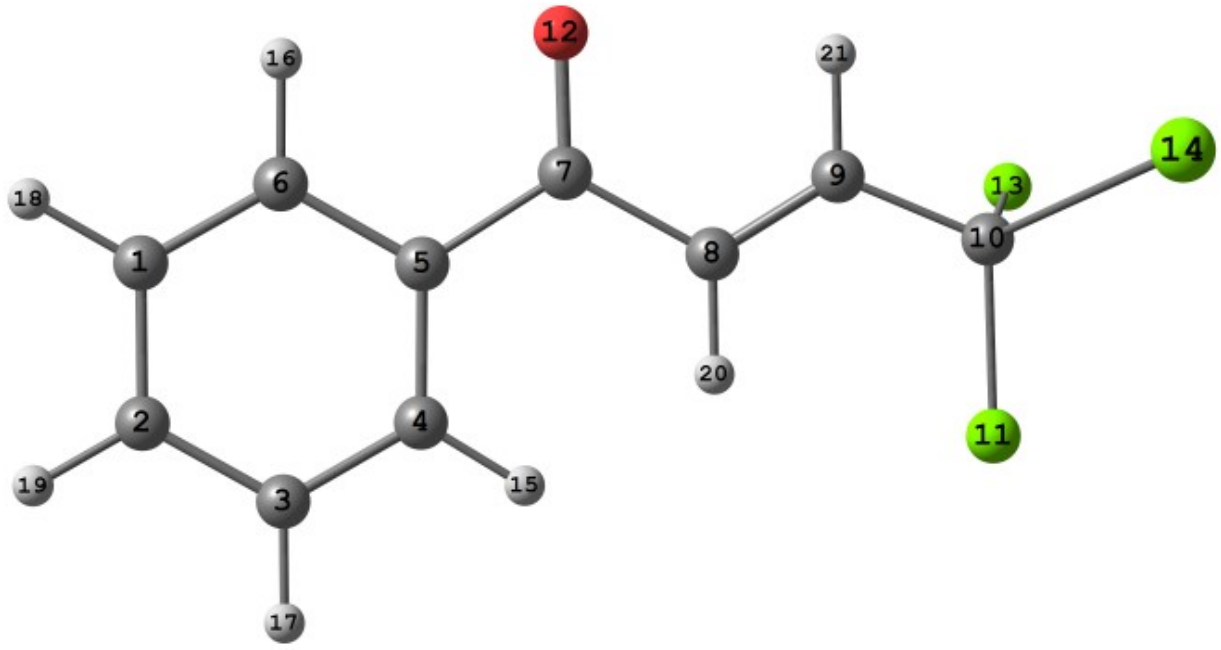
4. Data of DFT calculations of compounds 2 and cations B

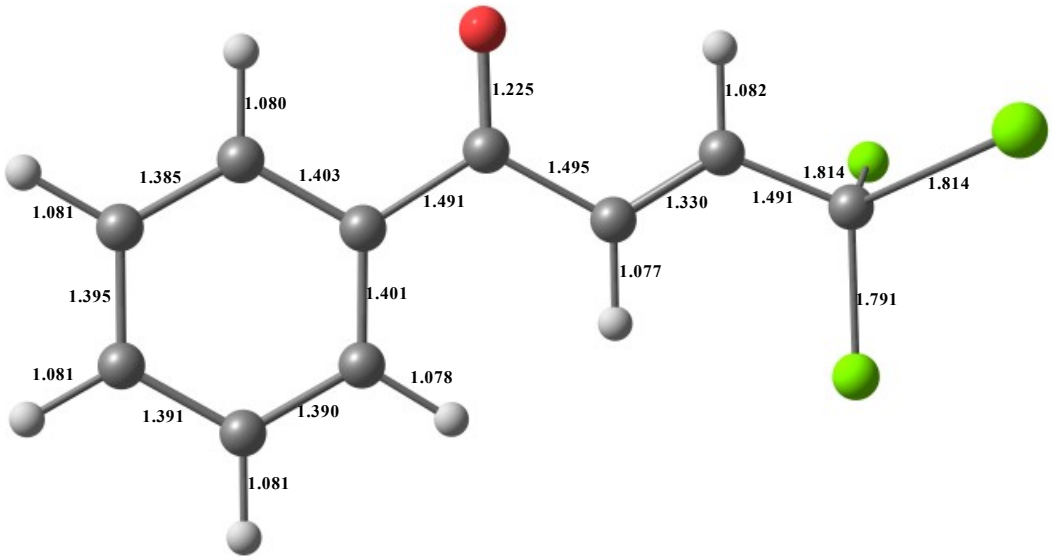
2a

Energy E(B3LYP) = -1841.2941327 h, G^{298} = -1841.195379 h, μ=4.89 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-5.006911	-0.579562	-0.000067
2	C	-5.173853	0.805533	-0.000046
3	C	-4.060459	1.638925	0.000019
4	C	-2.780999	1.094541	0.000059
5	C	-2.600764	-0.294933	0.000034
6	C	-3.732839	-1.123601	-0.000024
7	C	-1.258973	-0.946021	0.000071
8	C	-0.035185	-0.087630	0.000047
9	C	1.169714	-0.649964	0.000081
10	C	2.477986	0.065133	0.000028
11	Cl	2.349476	1.851122	0.000103
12	O	-1.153594	-2.165987	0.000111
13	Cl	3.409722	-0.447671	1.469174
14	Cl	3.409454	-0.447543	-1.469404
15	H	-1.937534	1.766573	0.000111
16	H	-3.592323	-2.194161	-0.000038
17	H	-4.185364	2.712437	0.000038
18	H	-5.871046	-1.229034	-0.000118
19	H	-6.167898	1.230830	-0.000077
20	H	-0.135104	0.984241	0.000007
21	H	1.264637	-1.727942	0.000139





Summary of Natural Population Analysis:

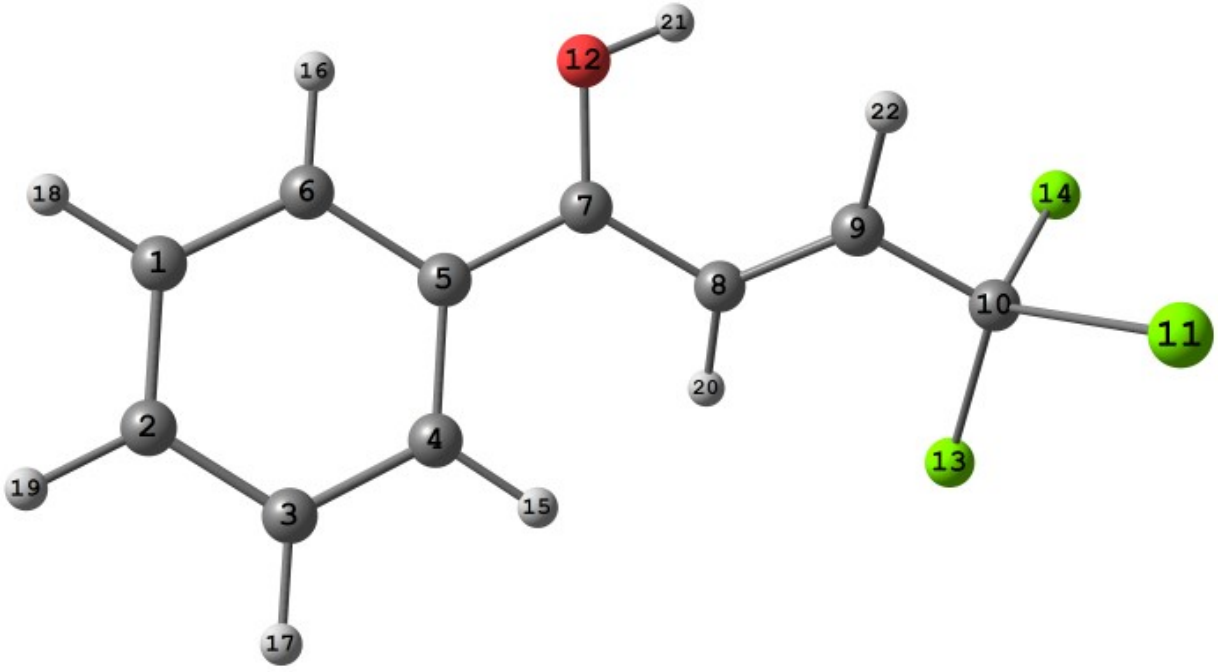
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.20471	1.99915	4.18572	0.01983	6.20471
C	2	-0.16665	1.99915	4.14741	0.02008	6.16665
C	3	-0.20718	1.99916	4.18780	0.02022	6.20718
C	4	-0.16136	1.99908	4.14443	0.01785	6.16136
C	5	-0.15054	1.99893	4.13197	0.01965	6.15054
C	6	-0.15239	1.99907	4.13307	0.02024	6.15239
C	7	0.53790	1.99920	3.42921	0.03369	5.46210
C	8	-0.24562	1.99890	4.22573	0.02099	6.24562
C	9	-0.17688	1.99881	4.15020	0.02787	6.17688
C	10	-0.16140	1.99902	4.09923	0.06314	6.16140
Cl	11	0.04843	9.99948	6.93212	0.01997	16.95157
O	12	-0.60548	1.99977	6.58117	0.02455	8.60548
Cl	13	0.03452	9.99952	6.94717	0.01879	16.96548
Cl	14	0.03448	9.99952	6.94722	0.01879	16.96552
H	15	0.21551	0.00000	0.78266	0.00183	0.78449
H	16	0.22835	0.00000	0.76931	0.00233	0.77165
H	17	0.21988	0.00000	0.77846	0.00166	0.78012
H	18	0.21895	0.00000	0.77937	0.00168	0.78105
H	19	0.21831	0.00000	0.78016	0.00153	0.78169
H	20	0.22689	0.00000	0.77047	0.00264	0.77311
H	21	0.24900	0.00000	0.74771	0.00329	0.75100
* Total *		0.00000	51.98877	73.65060	0.36063	126.00000

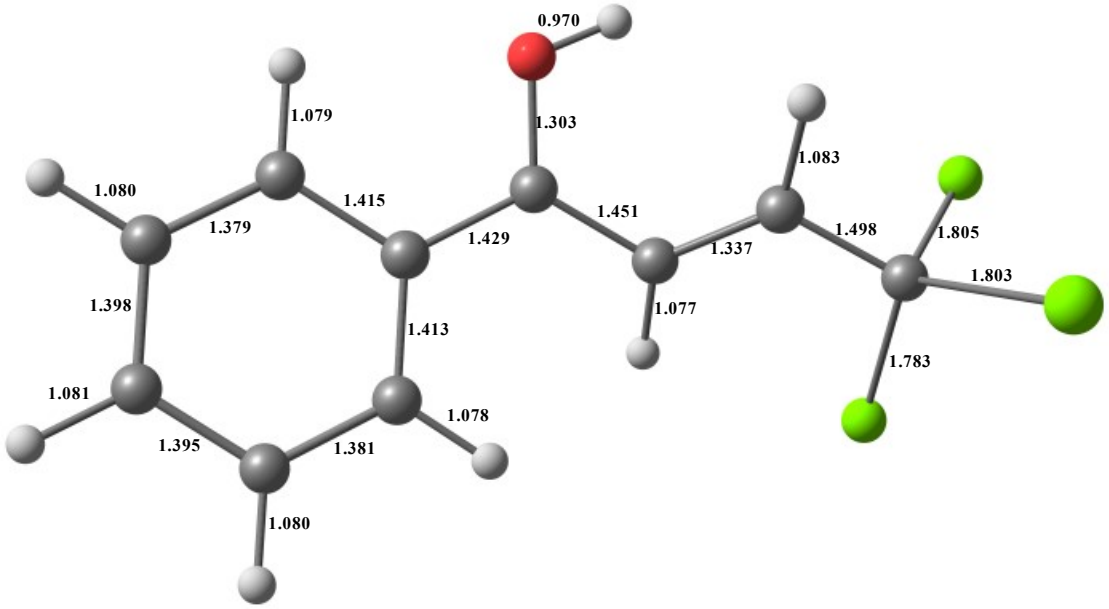
Ba

Energy E(B3LYP) = -1841.70188813 h, G^{298} = -1841. 589006 h, μ=8.85 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.952857	0.493882	0.069798
2	C	-5.054878	-0.900001	0.078096
3	C	-3.913098	-1.700029	0.028877
4	C	-2.664283	-1.114150	-0.033156
5	C	-2.545182	0.294018	-0.041278
6	C	-3.712281	1.092368	0.012806
7	C	-1.260901	0.918889	-0.081025
8	C	-0.026522	0.181925	-0.279065
9	C	1.149901	0.615107	0.185107
10	C	2.459853	-0.094551	0.028412
11	Cl	3.082132	-0.459189	1.681122
12	O	-1.244661	2.212485	0.070320
13	Cl	2.368547	-1.605135	-0.915252
14	Cl	3.584626	1.053349	-0.792765
15	H	-1.789112	-1.743590	-0.058206
16	H	-3.626779	2.167430	-0.001258
17	H	-4.003036	-2.775775	0.039549
18	H	-5.844458	1.101888	0.104402
19	H	-6.030376	-1.363520	0.120950
20	H	-0.095561	-0.763796	-0.790406
21	H	-0.377086	2.613000	-0.093803
22	H	1.244988	1.526301	0.761995





Summary of Natural Population Analysis:

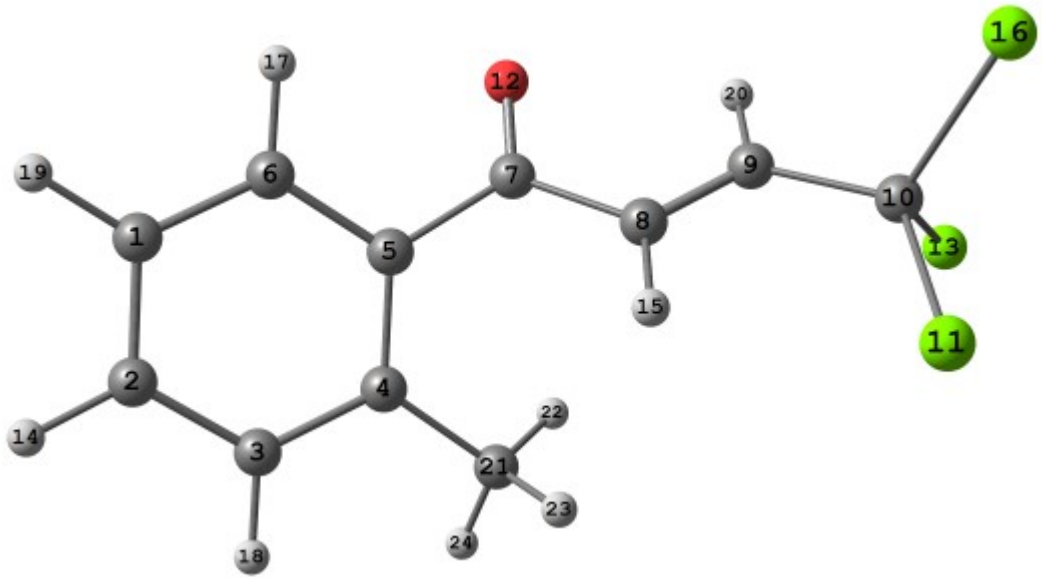
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.19978	1.99915	4.18096	0.01966	6.19978
C	2	-0.08891	1.99917	4.07053	0.01921	6.08891
C	3	-0.20409	1.99915	4.18496	0.01997	6.20409
C	4	-0.09761	1.99909	4.08173	0.01679	6.09761
C	5	-0.16484	1.99893	4.14666	0.01924	6.16484
C	6	-0.09815	1.99908	4.08004	0.01902	6.09815
C	7	0.58844	1.99897	3.38703	0.02556	5.41156
C	8	-0.27137	1.99891	4.25149	0.02097	6.27137
C	9	-0.11103	1.99883	4.08554	0.02666	6.11103
C	10	-0.18471	1.99906	4.12021	0.06545	6.18471
Cl	11	0.06553	9.99951	6.91590	0.01906	16.93447
O	12	-0.57642	1.99969	6.55285	0.02387	8.57642
Cl	13	0.07116	9.99948	6.90933	0.02002	16.92884
Cl	14	0.06682	9.99951	6.91471	0.01896	16.93318
H	15	0.23038	0.00000	0.76779	0.00182	0.76962
H	16	0.23868	0.00000	0.75931	0.00201	0.76132
H	17	0.23382	0.00000	0.76459	0.00159	0.76618
H	18	0.23305	0.00000	0.76534	0.00161	0.76695
H	19	0.22884	0.00000	0.76977	0.00139	0.77116
H	20	0.26395	0.00000	0.73357	0.00248	0.73605
H	21	0.52857	0.00000	0.46860	0.00282	0.47143
H	22	0.24766	0.00000	0.74944	0.00290	0.75234
* Total *		1.00000	51.98854	73.66036	0.35110	126.00000

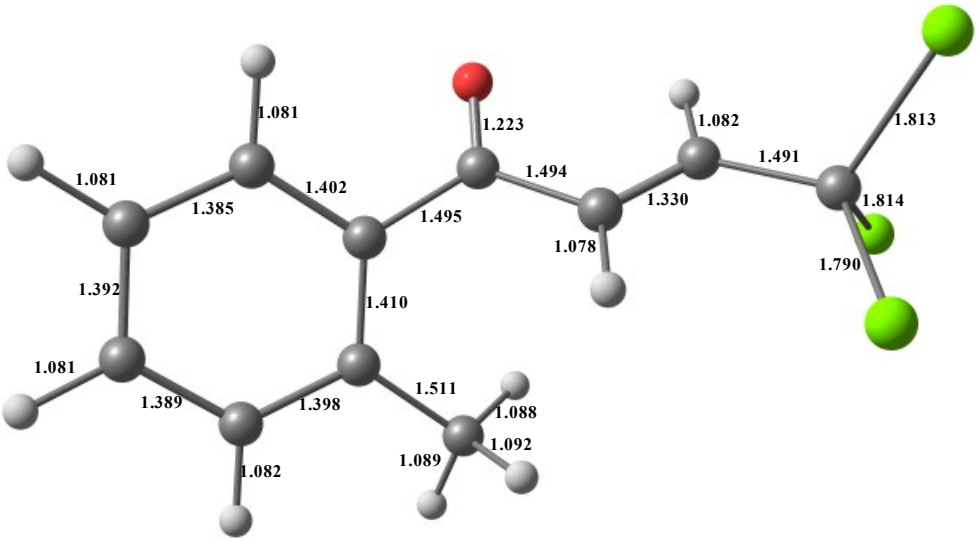
2b

Energy E(B3LYP) =-1880.61759134 h, G^{298} = -1880.492944 h, μ=4.48 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.726640	-0.992939	-0.562340
2	C	-5.072411	0.354161	-0.503483
3	C	-4.132671	1.295286	-0.101429
4	C	-2.822060	0.937078	0.226861
5	C	-2.478152	-0.428186	0.157897
6	C	-3.440854	-1.376252	-0.217028
7	C	-1.123006	-0.969225	0.484587
8	C	0.079857	-0.243160	-0.023532
9	C	1.298734	-0.605094	0.365249
10	C	2.585632	0.000493	-0.082291
11	Cl	2.407393	1.322439	-1.276449
12	O	-1.003447	-2.023605	1.093086
13	Cl	3.450266	0.648094	1.374376
14	H	-6.074133	0.671172	-0.759443
15	H	-0.066733	0.560328	-0.727108
16	Cl	3.607415	-1.306852	-0.813750
17	H	-3.156281	-2.418143	-0.248293
18	H	-4.421223	2.335597	-0.028705
19	H	-5.451460	-1.733882	-0.868754
20	H	1.423410	-1.411859	1.075729
21	C	-1.873723	2.020854	0.685062
22	H	-1.187250	1.678094	1.456525
23	H	-1.276119	2.407218	-0.142857
24	H	-2.437134	2.859651	1.089891





Summary of Natural Population Analysis:

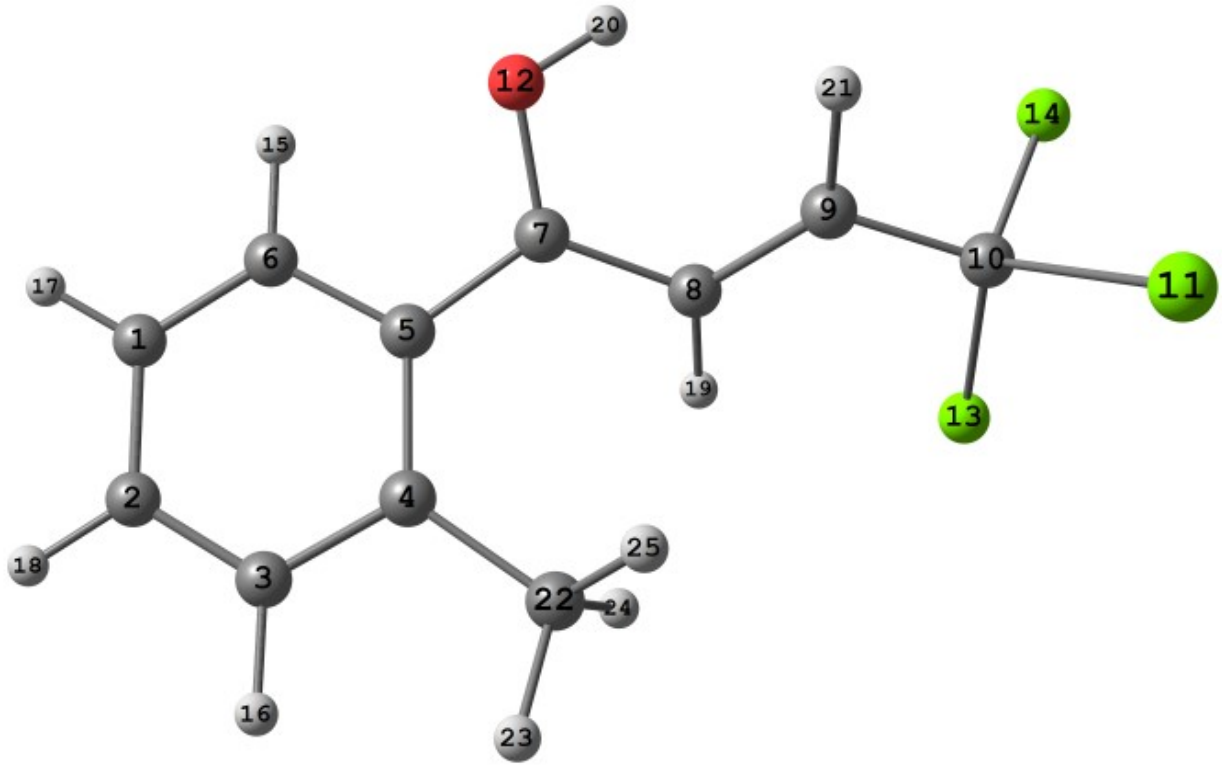
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.21529	1.99914	4.19618	0.01997	6.21529
C	2	-0.17355	1.99915	4.15428	0.02012	6.17355
C	3	-0.20694	1.99905	4.18800	0.01989	6.20694
C	4	0.00534	1.99898	3.97914	0.01655	5.99466
C	5	-0.15017	1.99884	4.12826	0.02307	6.15017
C	6	-0.15588	1.99907	4.13764	0.01917	6.15588
C	7	0.54788	1.99919	3.41751	0.03541	5.45212
C	8	-0.24923	1.99891	4.22890	0.02142	6.24923
C	9	-0.17735	1.99880	4.15099	0.02755	6.17735
C	10	-0.16178	1.99902	4.09981	0.06294	6.16178
Cl	11	0.04925	9.99948	6.93130	0.01996	16.95075
O	12	-0.59430	1.99976	6.56968	0.02486	8.59430
Cl	13	0.03508	9.99952	6.94666	0.01874	16.96492
H	14	0.21638	0.00000	0.78194	0.00168	0.78362
H	15	0.23315	0.00000	0.76440	0.00245	0.76685
Cl	16	0.03550	9.99952	6.94624	0.01875	16.96450
H	17	0.22228	0.00000	0.77560	0.00211	0.77772
H	18	0.21465	0.00000	0.78345	0.00189	0.78535
H	19	0.21784	0.00000	0.78049	0.00167	0.78216
H	20	0.24866	0.00000	0.74819	0.00316	0.75134
C	21	-0.60094	1.99928	4.58948	0.01218	6.60094
H	22	0.21748	0.00000	0.78103	0.00150	0.78252
H	23	0.22128	0.00000	0.77695	0.00177	0.77872
H	24	0.22067	0.00000	0.77779	0.00154	0.77933
* Total *		0.00000	53.98771	79.63392	0.37837	134.00000

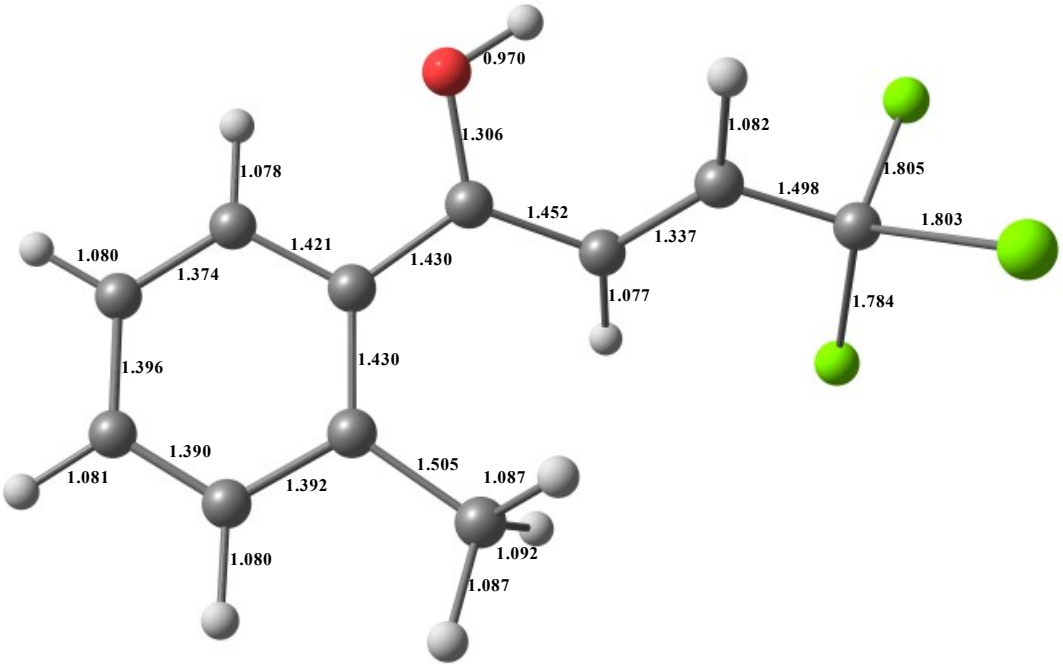
Bb

Energy E(B3LYP) =-1881.026114 h, G^{298} = -1880. 887232 h, μ=7.94 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.827661	0.882078	-0.174781
2	C	-5.076359	-0.491200	-0.135140
3	C	-4.031890	-1.396932	0.005080
4	C	-2.703743	-0.989687	0.090143
5	C	-2.448256	0.415960	0.034590
6	C	-3.531681	1.328303	-0.078235
7	C	-1.139001	0.987950	0.092399
8	C	0.090321	0.293267	-0.245760
9	C	1.265345	0.618138	0.302689
10	C	2.581093	-0.023903	-0.012591
11	Cl	3.215262	-0.746931	1.512892
12	O	-1.084835	2.247259	0.434932
13	Cl	2.498904	-1.282950	-1.273448
14	Cl	3.690826	1.291866	-0.555586
15	H	-3.321567	2.384666	-0.125843
16	H	-4.254414	-2.452628	0.062973
17	H	-5.639505	1.584989	-0.285924
18	H	-6.090713	-0.857983	-0.207148
19	H	0.019041	-0.509504	-0.959877
20	H	-0.209997	2.643366	0.300889
21	H	1.348579	1.370496	1.076533
22	C	-1.657238	-2.051946	0.291613
23	H	-2.129880	-2.964184	0.647363
24	H	-1.156889	-2.298835	-0.647015
25	H	-0.896419	-1.764364	1.012950





Summary of Natural Population Analysis:

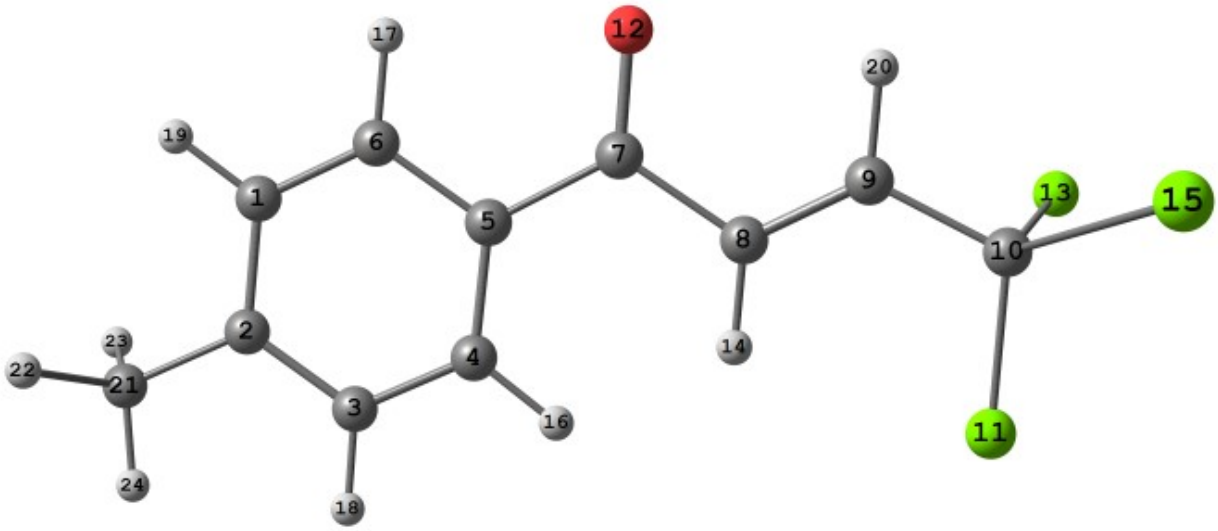
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.21028	1.99914	4.19150	0.01964	6.21028
C	2	-0.08700	1.99916	4.06867	0.01917	6.08700
C	3	-0.21013	1.99904	4.19141	0.01968	6.21013
C	4	0.08566	1.99901	3.89942	0.01591	5.91434
C	5	-0.16994	1.99885	4.14946	0.02163	6.16994
C	6	-0.09501	1.99909	4.07751	0.01841	6.09501
C	7	0.58773	1.99897	3.38793	0.02537	5.41227
C	8	-0.27364	1.99890	4.25312	0.02161	6.27364
C	9	-0.11844	1.99882	4.09285	0.02677	6.11844
C	10	-0.18400	1.99905	4.11975	0.06520	6.18400
Cl	11	0.06468	9.99951	6.91673	0.01908	16.93532
O	12	-0.57925	1.99970	6.55587	0.02369	8.57925
Cl	13	0.07076	9.99948	6.90975	0.02001	16.92924
Cl	14	0.06635	9.99951	6.91520	0.01893	16.93365
H	15	0.23649	0.00000	0.76151	0.00200	0.76351
H	16	0.22828	0.00000	0.76991	0.00182	0.77172
H	17	0.23196	0.00000	0.76644	0.00160	0.76804
H	18	0.22774	0.00000	0.77078	0.00148	0.77226
H	19	0.26741	0.00000	0.73004	0.00255	0.73259
H	20	0.52698	0.00000	0.47013	0.00289	0.47302
H	21	0.24956	0.00000	0.74759	0.00285	0.75044
C	22	-0.61057	1.99926	4.59736	0.01394	6.61057
H	23	0.23114	0.00000	0.76730	0.00156	0.76886
H	24	0.23471	0.00000	0.76372	0.00157	0.76529
H	25	0.22880	0.00000	0.76950	0.00169	0.77120
* Total *		1.00000	53.98749	79.64345	0.36906	134.00000

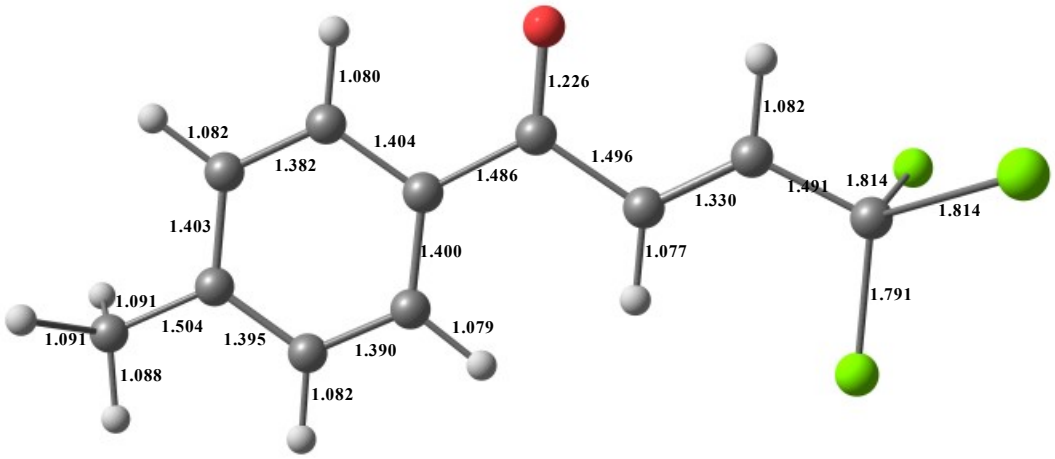
2c

Energy E(B3LYP) =-1880.62520485 h, G^{298} = -1880.501976 h, μ=5.87 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.557409	-0.907032	0.000146
2	C	-4.823232	0.470509	0.000023
3	C	-3.738491	1.347978	-0.000119
4	C	-2.430908	0.876760	-0.000138
5	C	-2.168628	-0.498581	-0.000032
6	C	-3.260190	-1.382318	0.000107
7	C	-0.798843	-1.075494	-0.000075
8	C	0.377581	-0.152058	-0.000018
9	C	1.610375	-0.650280	0.000043
10	C	2.880389	0.129972	0.000061
11	Cl	2.661552	1.907091	0.000258
12	O	-0.624616	-2.289098	-0.000148
13	Cl	3.838426	-0.334433	1.469061
14	H	0.219459	0.912862	-0.000005
15	Cl	3.838157	-0.334105	-1.469286
16	H	-1.629251	1.598732	-0.000268
17	H	-3.067783	-2.444898	0.000191
18	H	-3.915737	2.414992	-0.000210
19	H	-5.382320	-1.607583	0.000266
20	H	1.759010	-1.722166	0.000056
21	C	-6.240188	0.975724	0.000066
22	H	-6.780577	0.615625	-0.877009
23	H	-6.780528	0.615636	0.877173
24	H	-6.276367	2.063117	0.000054





Summary of Natural Population Analysis:

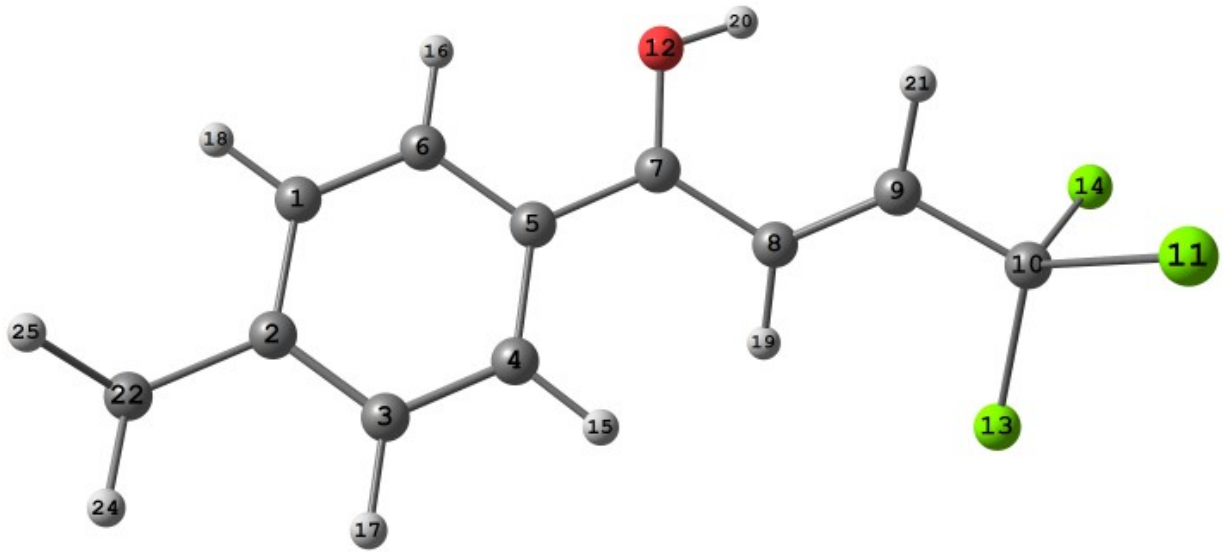
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.20569	1.99904	4.18748	0.01917	6.20569
C	2	0.01535	1.99905	3.96790	0.01771	5.98465
C	3	-0.21352	1.99904	4.19499	0.01949	6.21352
C	4	-0.15081	1.99908	4.13422	0.01750	6.15081
C	5	-0.16874	1.99894	4.14881	0.02100	6.16874
C	6	-0.14469	1.99908	4.12580	0.01981	6.14469
C	7	0.54543	1.99900	3.42053	0.03504	5.45457
C	8	-0.23715	1.99881	4.21715	0.02119	6.23715
C	9	-0.18816	1.99882	4.16014	0.02920	6.18816
C	10	-0.16040	1.99902	4.09825	0.06313	6.16040
Cl	11	0.04777	9.99948	6.93271	0.02003	16.95223
O	12	-0.61343	1.99977	6.58906	0.02460	8.61343
Cl	13	0.03318	9.99952	6.94846	0.01885	16.96682
H	14	0.22498	0.00000	0.77249	0.00253	0.77502
Cl	15	0.03314	9.99952	6.94850	0.01884	16.96686
H	16	0.21462	0.00000	0.78352	0.00186	0.78538
H	17	0.22714	0.00000	0.77049	0.00237	0.77286
H	18	0.21691	0.00000	0.78111	0.00198	0.78309
H	19	0.21608	0.00000	0.78203	0.00188	0.78392
H	20	0.24890	0.00000	0.74779	0.00330	0.75110
C	21	-0.59768	1.99928	4.58630	0.01209	6.59768
H	22	0.22196	0.00000	0.77648	0.00156	0.77804
H	23	0.22196	0.00000	0.77648	0.00156	0.77804
H	24	0.21288	0.00000	0.78561	0.00152	0.78712
* Total *		0.00005	53.98743	79.63630	0.37622	133.99995

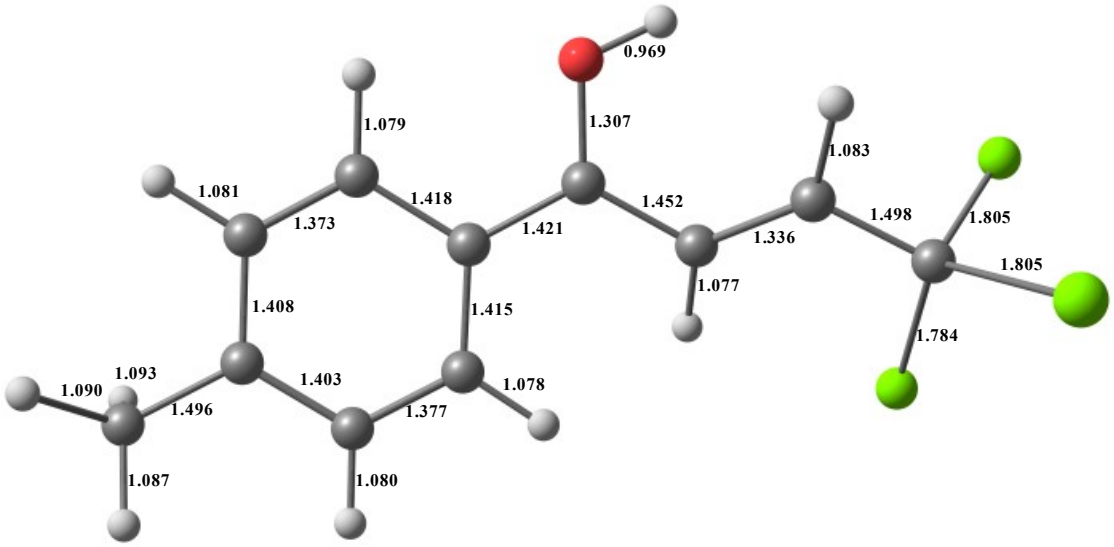
Bc

Energy E(B3LYP) =-1881.0359443 h, G^{298} = -1880. 899239 h, μ=8.68 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.513318	0.864890	0.065810
2	C	-4.731892	-0.525894	0.049269
3	C	-3.622537	-1.382099	-0.016061
4	C	-2.341254	-0.880336	-0.071846
5	C	-2.122094	0.517033	-0.057837
6	C	-3.242538	1.382615	0.014493
7	C	-0.807539	1.056823	-0.089893
8	C	0.380747	0.241636	-0.269223
9	C	1.584456	0.621736	0.169058
10	C	2.849978	-0.166966	0.031023
11	Cl	3.466532	-0.503879	1.693318
12	O	-0.706742	2.351565	0.055844
13	Cl	2.664015	-1.706294	-0.851100
14	Cl	4.035908	0.878322	-0.840742
15	H	-1.512774	-1.569549	-0.109013
16	H	-3.092408	2.450747	0.022227
17	H	-3.775216	-2.451617	-0.020595
18	H	-5.360964	1.533456	0.117916
19	H	0.254666	-0.715018	-0.747425
20	H	0.188274	2.688760	-0.098676
21	H	1.737630	1.547486	0.708872
22	C	-6.124753	-1.071206	0.080575
23	H	-6.590975	-0.948235	-0.900669
24	H	-6.137822	-2.129661	0.328282
25	H	-6.741745	-0.526807	0.795019





Summary of Natural Population Analysis:

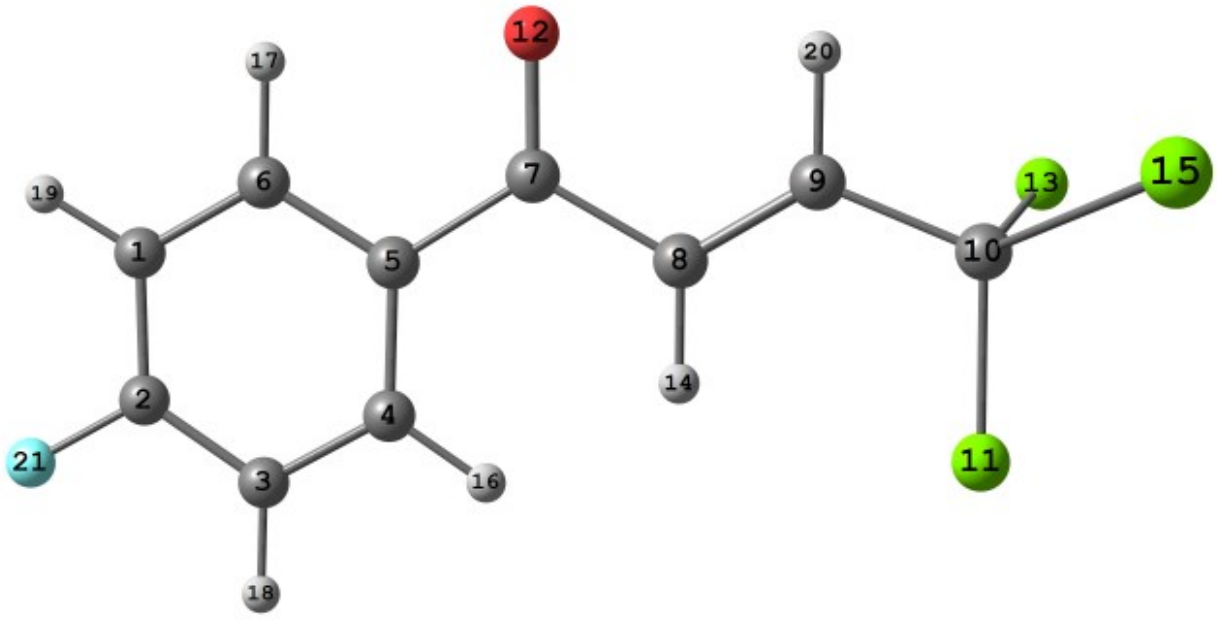
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.20170	1.99903	4.18334	0.01932	6.20170
C	2	0.09860	1.99907	3.88499	0.01734	5.90140
C	3	-0.21047	1.99904	4.19186	0.01957	6.21047
C	4	-0.08760	1.99909	4.07187	0.01664	6.08760
C	5	-0.16799	1.99893	4.15016	0.01890	6.16799
C	6	-0.09318	1.99908	4.07526	0.01883	6.09318
C	7	0.57194	1.99895	3.40377	0.02534	5.42806
C	8	-0.26502	1.99891	4.24530	0.02082	6.26502
C	9	-0.12063	1.99882	4.09518	0.02663	6.12063
C	10	-0.18245	1.99906	4.11807	0.06532	6.18245
Cl	11	0.06232	9.99951	6.91915	0.01901	16.93768
O	12	-0.58511	1.99970	6.56165	0.02376	8.58511
Cl	13	0.06959	9.99948	6.91092	0.02001	16.93041
Cl	14	0.06391	9.99951	6.91761	0.01896	16.93609
H	15	0.22942	0.00000	0.76873	0.00185	0.77058
H	16	0.23819	0.00000	0.75975	0.00206	0.76181
H	17	0.23134	0.00000	0.76676	0.00190	0.76866
H	18	0.23057	0.00000	0.76759	0.00184	0.76943
H	19	0.26103	0.00000	0.73647	0.00250	0.73897
H	20	0.52561	0.00000	0.47154	0.00284	0.47439
H	21	0.24513	0.00000	0.75194	0.00293	0.75487
C	22	-0.60944	1.99926	4.59757	0.01261	6.60944
H	23	0.24160	0.00000	0.75687	0.00153	0.75840
H	24	0.22294	0.00000	0.77555	0.00150	0.77706
H	25	0.23138	0.00000	0.76710	0.00152	0.76862
* Total *		1.00000	53.98745	79.64902	0.36353	134.00000

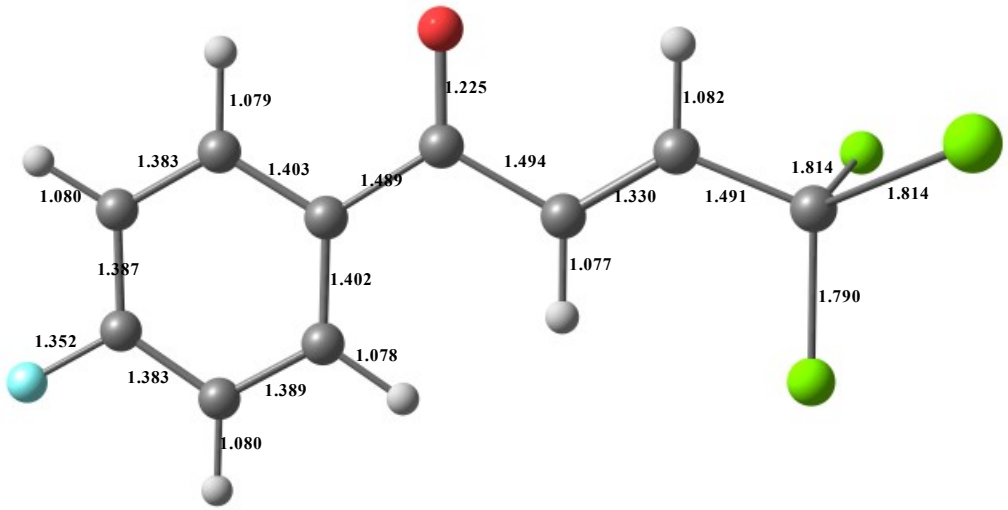
2d

Energy E(B3LYP) = -1940.56558947 h, G^{298} = -1940.476241 h, μ=3.12 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.589664	-0.885391	-0.000270
2	C	-4.790300	0.487048	-0.000053
3	C	-3.747711	1.395620	0.000220
4	C	-2.447720	0.907574	0.000265
5	C	-2.198022	-0.471514	0.000047
6	C	-3.288373	-1.355144	-0.000217
7	C	-0.828878	-1.058017	0.000091
8	C	0.353187	-0.143788	-0.000043
9	C	1.581882	-0.652186	-0.000171
10	C	2.858137	0.118611	-0.000078
11	Cl	2.652450	1.897023	-0.000901
12	O	-0.668130	-2.272116	0.000236
13	Cl	3.810131	-0.353144	1.469737
14	H	0.204596	0.922485	-0.000087
15	Cl	3.811199	-0.354346	-1.468796
16	H	-1.640891	1.622729	0.000515
17	H	-3.097013	-2.417351	-0.000370
18	H	-3.952188	2.455695	0.000396
19	H	-5.435989	-1.556130	-0.000478
20	H	1.722387	-1.725145	-0.000222
21	F	-6.058372	0.955080	-0.000119





Summary of Natural Population Analysis:

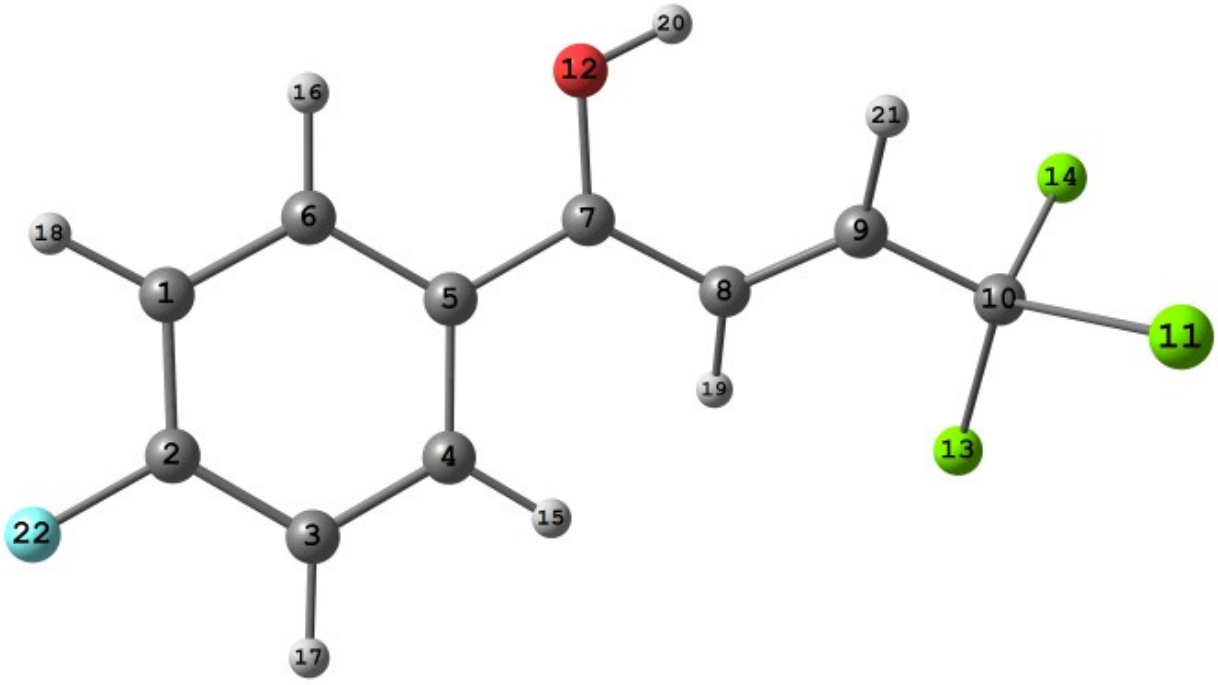
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.26337	1.99902	4.24432	0.02003	6.26337
C	2	0.44333	1.99848	3.53297	0.02522	5.55667
C	3	-0.26739	1.99902	4.24789	0.02048	6.26739
C	4	-0.13982	1.99910	4.12371	0.01701	6.13982
C	5	-0.16056	1.99893	4.14249	0.01915	6.16056
C	6	-0.12996	1.99909	4.11142	0.01946	6.12996
C	7	0.53718	1.99920	3.42995	0.03366	5.46282
C	8	-0.24613	1.99890	4.22631	0.02092	6.24613
C	9	-0.17567	1.99881	4.14895	0.02790	6.17567
C	10	-0.16171	1.99902	4.09953	0.06316	6.16171
Cl	11	0.04880	9.99948	6.93173	0.01998	16.95120
O	12	-0.60642	1.99977	6.58213	0.02452	8.60642
Cl	13	0.03495	9.99952	6.94674	0.01879	16.96505
H	14	0.22676	0.00000	0.77059	0.00265	0.77324
Cl	15	0.03495	9.99952	6.94675	0.01879	16.96505
H	16	0.22134	0.00000	0.77682	0.00184	0.77866
H	17	0.23419	0.00000	0.76344	0.00237	0.76581
H	18	0.23810	0.00000	0.75980	0.00210	0.76190
H	19	0.23717	0.00000	0.76070	0.00213	0.76283
H	20	0.24943	0.00000	0.74730	0.00327	0.75057
F	21	-0.35515	1.99992	7.34555	0.00968	9.35515
* Total *		0.00000	53.98779	79.63910	0.37312	134.00000

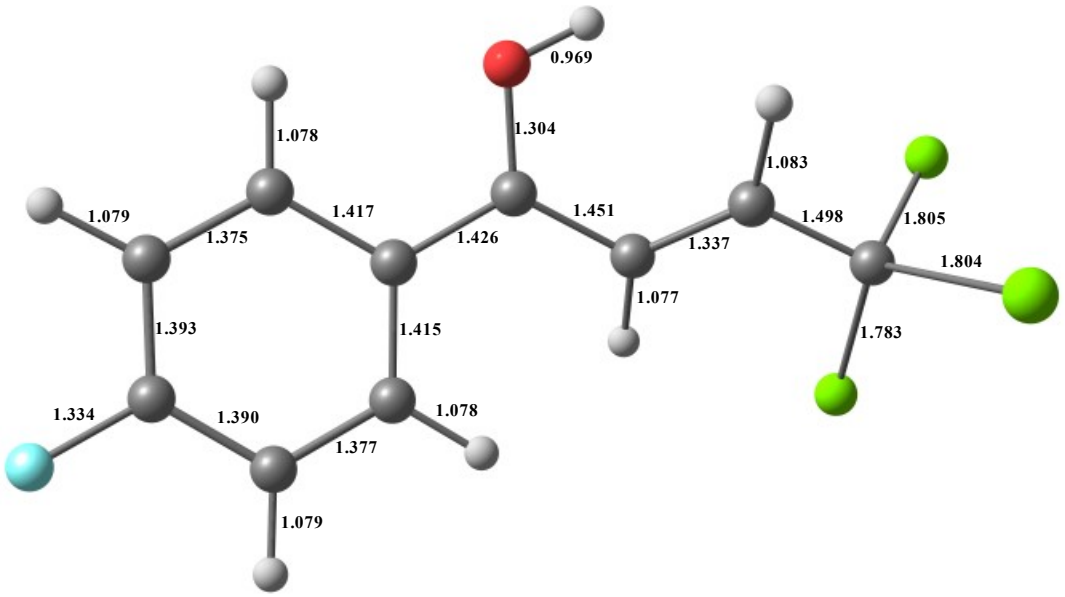
Bd

Energy E(B3LYP) = - 1940.97318867 h, G^{298} = -1940.869737 h, μ=6.45 D

Cartesian coordinates, Å

1	C	-4.547291	0.835662	0.049068
2	C	-4.696965	-0.548840	0.042834
3	C	-3.625162	-1.432640	-0.008096
4	C	-2.352147	-0.910461	-0.059221
5	C	-2.151301	0.489888	-0.054459
6	C	-3.273937	1.352206	0.002797
7	C	-0.837426	1.042110	-0.083409
8	C	0.355707	0.239588	-0.276122
9	C	1.554103	0.620147	0.177565
10	C	2.827065	-0.155260	0.029834
11	Cl	3.430394	-0.529083	1.687822
12	O	-0.751862	2.333440	0.075891
13	Cl	2.660146	-1.671921	-0.893485
14	Cl	4.008346	0.923871	-0.804920
15	H	-1.516092	-1.590255	-0.085835
16	H	-3.129718	2.420784	-0.000105
17	H	-3.802261	-2.496863	-0.006034
18	H	-5.418375	1.471507	0.085282
19	H	0.238983	-0.707580	-0.775513
20	H	0.137615	2.686005	-0.079484
21	H	1.695019	1.534867	0.739154
22	F	-5.931913	-1.052126	0.085617





Summary of Natural Population Analysis:

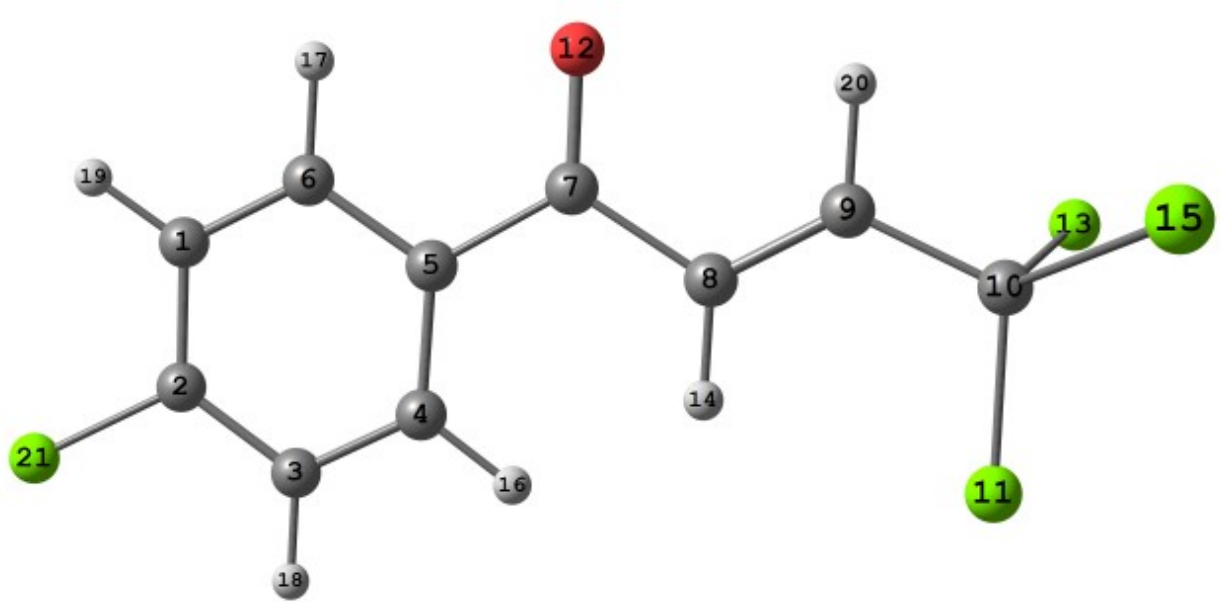
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.25403	1.99902	4.23489	0.02012	6.25403
C	2	0.50857	1.99856	3.46726	0.02561	5.49143
C	3	-0.25915	1.99902	4.23963	0.02050	6.25915
C	4	-0.08053	1.99911	4.06524	0.01618	6.08053
C	5	-0.17044	1.99893	4.15284	0.01867	6.17044
C	6	-0.08036	1.99910	4.06283	0.01843	6.08036
C	7	0.58125	1.99896	3.39430	0.02549	5.41875
C	8	-0.27000	1.99891	4.25023	0.02086	6.27000
C	9	-0.11124	1.99883	4.08574	0.02667	6.11124
C	10	-0.18460	1.99906	4.12008	0.06546	6.18460
Cl	11	0.06544	9.99951	6.91600	0.01905	16.93456
O	12	-0.57959	1.99970	6.55614	0.02376	8.57959
Cl	13	0.07120	9.99948	6.90930	0.02002	16.92880
Cl	14	0.06676	9.99951	6.91476	0.01897	16.93324
H	15	0.23625	0.00000	0.76190	0.00185	0.76375
H	16	0.24485	0.00000	0.75311	0.00204	0.75515
H	17	0.25196	0.00000	0.74598	0.00206	0.74804
H	18	0.25122	0.00000	0.74668	0.00210	0.74878
H	19	0.26286	0.00000	0.73465	0.00249	0.73714
H	20	0.52822	0.00000	0.46896	0.00282	0.47178
H	21	0.24662	0.00000	0.75048	0.00291	0.75338
F	22	-0.32526	1.99992	7.31509	0.01026	9.32526
* Total *		1.00000	53.98762	79.64608	0.36630	134.00000

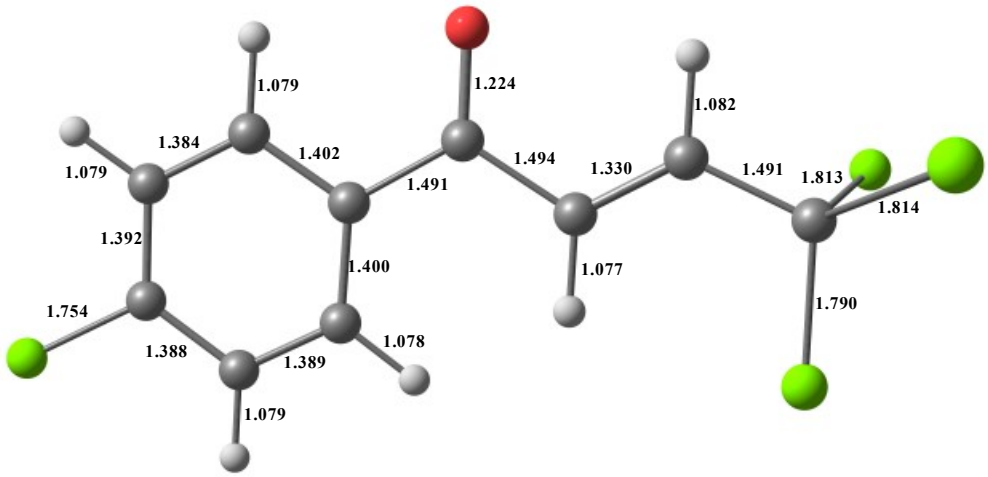
2e

Energy E(B3LYP) = -2300.91852572 h, G^{298} = -2300.831657 h, μ=2.94 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	4.161373	1.111071	-0.017285
2	C	4.431503	-0.254246	-0.001019
3	C	3.410772	-1.194009	0.019166
4	C	2.092061	-0.758284	0.021611
5	C	1.787975	0.608461	0.005617
6	C	2.843281	1.531442	-0.012897
7	C	0.395735	1.142749	0.011274
8	C	-0.750163	0.184691	-0.007994
9	C	-1.996962	0.646620	0.014466
10	C	-3.244542	-0.169680	-0.001573
11	Cl	-2.974838	-1.938461	-0.054032
12	O	0.191541	2.349630	0.029729
13	Cl	-4.203937	0.226068	1.485516
14	H	-0.560472	-0.874538	-0.042295
15	Cl	-4.221844	0.310902	-1.451660
16	H	1.315485	-1.506292	0.039127
17	H	2.613781	2.586152	-0.024409
18	H	3.638632	-2.248770	0.032721
19	H	4.969099	1.826908	-0.032927
20	H	-2.176356	1.713193	0.047775
21	Cl	6.099521	-0.797720	-0.006060





Summary of Natural Population Analysis:

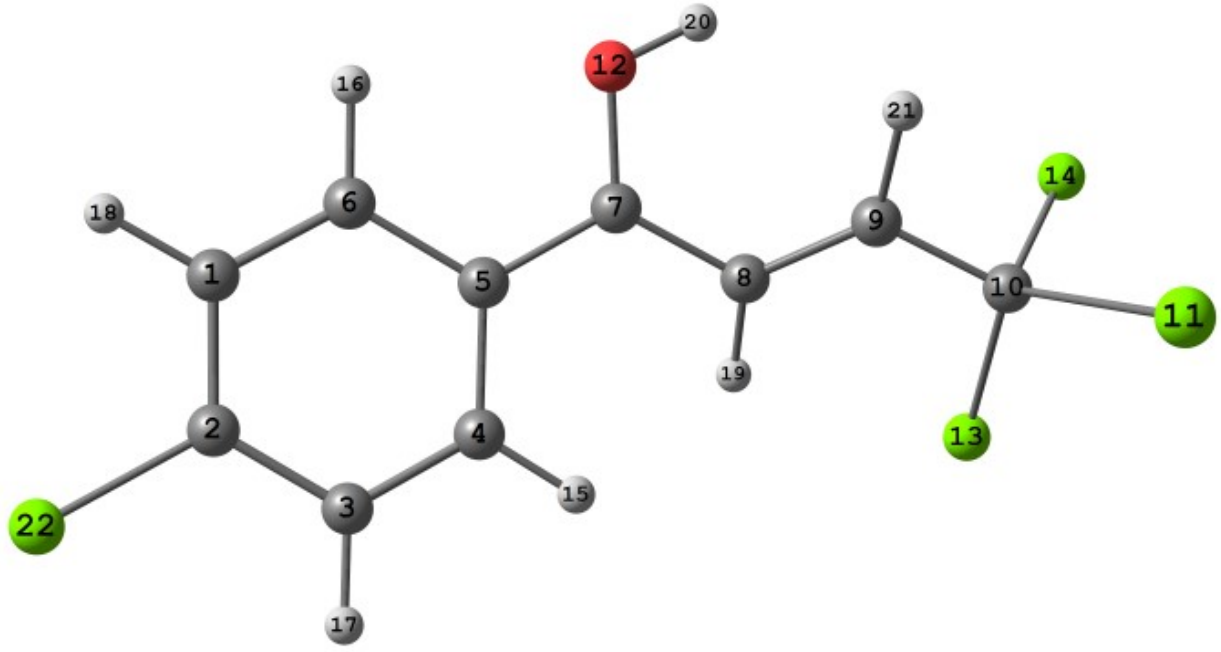
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.22593	1.99895	4.20494	0.02203	6.22593
C	2	-0.01364	1.99855	3.98738	0.02771	6.01364
C	3	-0.22877	1.99896	4.20749	0.02232	6.22877
C	4	-0.14242	1.99908	4.12601	0.01733	6.14242
C	5	-0.14867	1.99893	4.13041	0.01934	6.14867
C	6	-0.13251	1.99907	4.11371	0.01974	6.13251
C	7	0.53734	1.99920	3.42984	0.03361	5.46266
C	8	-0.24728	1.99890	4.22752	0.02085	6.24728
C	9	-0.17358	1.99881	4.14692	0.02785	6.17358
C	10	-0.16216	1.99902	4.09996	0.06317	6.16216
Cl	11	0.04929	9.99948	6.93124	0.01999	16.95071
O	12	-0.60228	1.99977	6.57799	0.02453	8.60228
Cl	13	0.03549	9.99952	6.94620	0.01879	16.96451
H	14	0.22729	0.00000	0.77006	0.00265	0.77271
Cl	15	0.03549	9.99952	6.94621	0.01879	16.96451
H	16	0.22246	0.00000	0.77571	0.00184	0.77754
H	17	0.23520	0.00000	0.76245	0.00235	0.76480
H	18	0.23574	0.00000	0.76216	0.00210	0.76426
H	19	0.23481	0.00000	0.76306	0.00213	0.76519
H	20	0.24946	0.00000	0.74728	0.00326	0.75054
Cl	21	0.01468	9.99959	6.96767	0.01807	16.98532
* Total *		0.00000	61.98735	79.62422	0.38843	142.00000

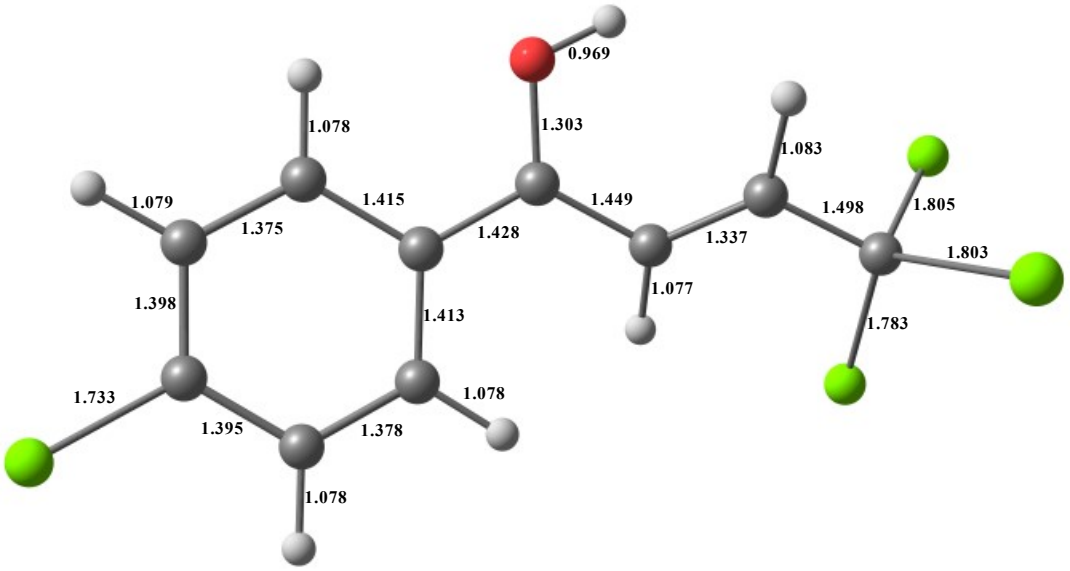
Be

Energy E(B3LYP) = -2301.32523173 h, G^{298} = -2301.223987 h, μ=5.48 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.126464	1.086360	0.035177
2	C	-4.357455	-0.292067	0.019189
3	C	-3.309888	-1.211965	-0.031814
4	C	-2.012957	-0.749029	-0.071734
5	C	-1.747443	0.638922	-0.057093
6	C	-2.831038	1.547086	-0.000686
7	C	-0.408772	1.134424	-0.075948
8	C	0.747161	0.278820	-0.255398
9	C	1.966010	0.618879	0.176344
10	C	3.203184	-0.212871	0.031005
11	Cl	3.820276	-0.561692	1.689344
12	O	-0.271123	2.421248	0.079508
13	Cl	2.957676	-1.747760	-0.842914
14	Cl	4.411062	0.791913	-0.856629
15	H	-1.211019	-1.469116	-0.098247
16	H	-2.642423	2.608823	0.005289
17	H	-3.515341	-2.270676	-0.038891
18	H	-4.955938	1.774926	0.071717
19	H	0.586682	-0.674225	-0.730230
20	H	0.635493	2.735683	-0.057560
21	H	2.153951	1.539685	0.713566
22	Cl	-5.989981	-0.873429	0.062201





Summary of Natural Population Analysis:

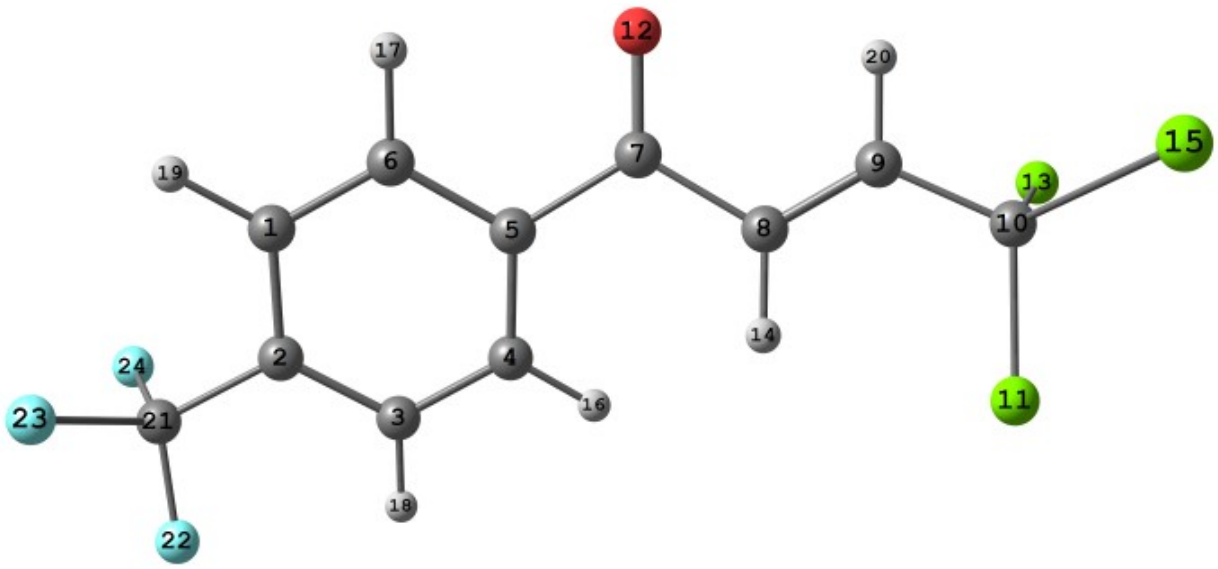
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.21842	1.99896	4.19720	0.02227	6.21842
C	2	0.03398	1.99862	3.93865	0.02875	5.96602
C	3	-0.22343	1.99896	4.20195	0.02251	6.22343
C	4	-0.08348	1.99909	4.06795	0.01644	6.08348
C	5	-0.16225	1.99893	4.14447	0.01884	6.16225
C	6	-0.08378	1.99908	4.06598	0.01872	6.08378
C	7	0.58108	1.99897	3.39460	0.02536	5.41892
C	8	-0.27031	1.99891	4.25062	0.02079	6.27031
C	9	-0.10784	1.99883	4.08243	0.02658	6.10784
C	10	-0.18513	1.99906	4.12055	0.06553	6.18513
Cl	11	0.06590	9.99951	6.91555	0.01905	16.93410
O	12	-0.57821	1.99970	6.55473	0.02378	8.57821
Cl	13	0.07169	9.99948	6.90880	0.02003	16.92831
Cl	14	0.06754	9.99951	6.91398	0.01897	16.93246
H	15	0.23624	0.00000	0.76193	0.00183	0.76376
H	16	0.24513	0.00000	0.75285	0.00203	0.75487
H	17	0.24820	0.00000	0.74975	0.00205	0.75180
H	18	0.24742	0.00000	0.75049	0.00209	0.75258
H	19	0.26241	0.00000	0.73509	0.00250	0.73759
H	20	0.52817	0.00000	0.46902	0.00281	0.47183
H	21	0.24590	0.00000	0.75118	0.00292	0.75410
Cl	22	0.07919	9.99955	6.90298	0.01828	16.92081
* Total *		1.00000	61.98714	79.63073	0.38213	142.00000

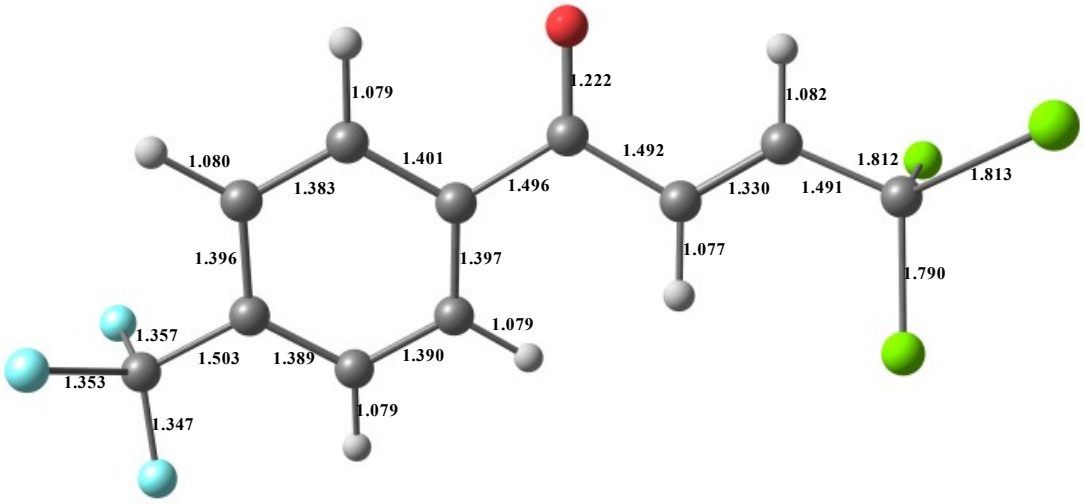
2g

Energy E(B3LYP) = -2178.45007197 h, G^{298} = -2178.353476 h, μ=1.95 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	3.454828	1.293624	-0.159525
2	C	3.777568	-0.056812	-0.010298
3	C	2.778540	-1.003324	0.178682
4	C	1.447621	-0.602756	0.207034
5	C	1.109942	0.745136	0.062765
6	C	2.130416	1.688436	-0.116168
7	C	-0.301663	1.238560	0.114963
8	C	-1.411494	0.251507	-0.029097
9	C	-2.673465	0.644832	0.116106
10	C	-3.886542	-0.212517	-0.017500
11	Cl	-3.545266	-1.926009	-0.407072
12	O	-0.536116	2.429196	0.259149
13	Cl	-4.807632	-0.144583	1.541953
14	H	-1.179453	-0.772968	-0.268228
15	Cl	-4.930045	0.483528	-1.326221
16	H	0.689380	-1.354166	0.361495
17	H	1.868057	2.729540	-0.226733
18	H	3.028775	-2.045777	0.300085
19	H	4.233012	2.027487	-0.311280
20	H	-2.895959	1.677282	0.351972
21	C	5.225415	-0.461507	-0.030985
22	F	5.394516	-1.796433	-0.093115
23	F	5.884382	0.069852	-1.086841
24	F	5.882008	-0.036301	1.077336





Summary of Natural Population Analysis:

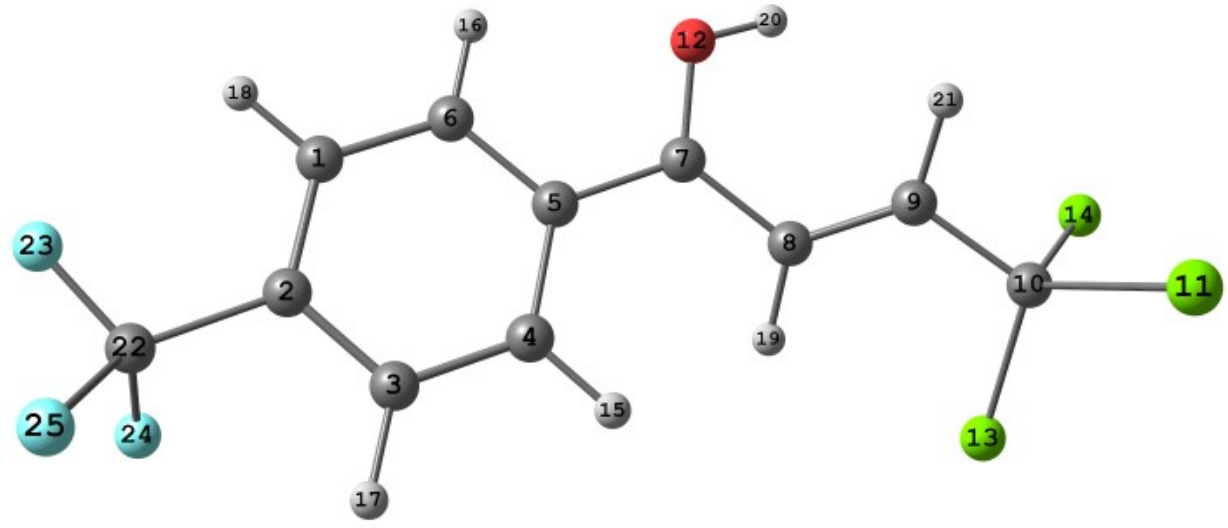
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.17470	1.99906	4.15583	0.01981	6.17470
C	2	-0.12395	1.99886	4.10323	0.02186	6.12395
C	3	-0.17535	1.99906	4.15652	0.01976	6.17535
C	4	-0.15529	1.99908	4.13881	0.01739	6.15529
C	5	-0.12437	1.99893	4.10534	0.02009	6.12437
C	6	-0.14467	1.99908	4.12589	0.01971	6.14467
C	7	0.53969	1.99920	3.42661	0.03450	5.46031
C	8	-0.25196	1.99891	4.23190	0.02115	6.25196
C	9	-0.16769	1.99881	4.14130	0.02758	6.16769
C	10	-0.16362	1.99903	4.10138	0.06322	6.16362
Cl	11	0.05020	9.99948	6.93038	0.01993	16.94980
O	12	-0.58962	1.99977	6.56516	0.02469	8.58962
Cl	13	0.03751	9.99951	6.94417	0.01880	16.96249
H	14	0.23056	0.00000	0.76684	0.00261	0.76944
Cl	15	0.03748	9.99952	6.94423	0.01878	16.96252
H	16	0.22488	0.00000	0.77331	0.00181	0.77512
H	17	0.23503	0.00000	0.76273	0.00224	0.76497
H	18	0.23645	0.00000	0.76157	0.00197	0.76355
H	19	0.23264	0.00000	0.76525	0.00211	0.76736
H	20	0.24965	0.00000	0.74720	0.00315	0.75035
C	21	1.08343	1.99910	2.86496	0.05251	4.91657
F	22	-0.35926	1.99991	7.34996	0.00938	9.35926
F	23	-0.36279	1.99992	7.35348	0.00939	9.36279
F	24	-0.36423	1.99992	7.35498	0.00933	9.36423
* Total *		0.00000	59.98716	97.57106	0.44178	158.00000

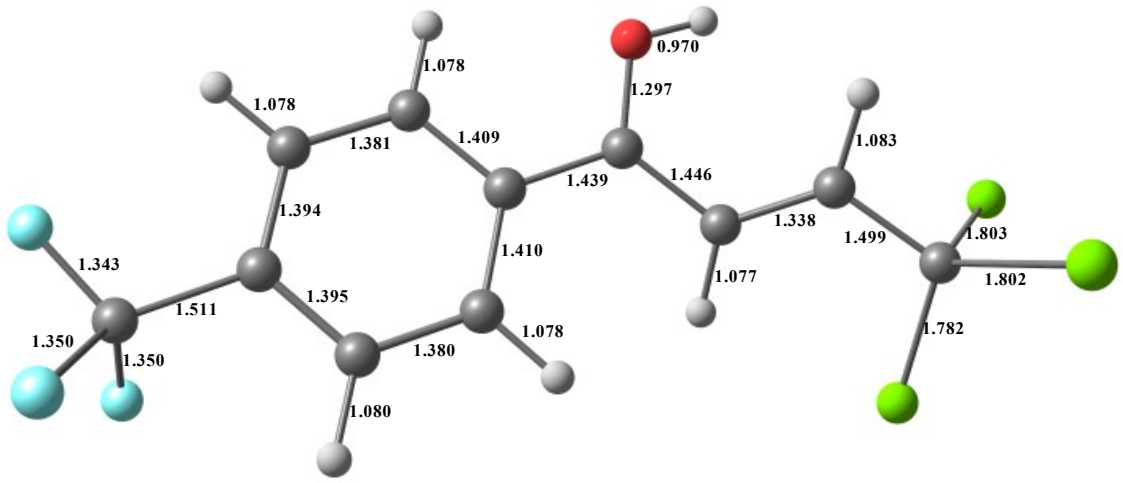
Bg

Energy E(B3LYP) = -2178.85233737 h, G^{298} = -2178.740529 h, μ=6.61 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-3.437537	1.338712	0.000123
2	C	-3.730077	-0.023823	0.009180
3	C	-2.714371	-0.980361	0.000494
4	C	-1.395271	-0.575427	-0.025306
5	C	-1.081097	0.798935	-0.037225
6	C	-2.119746	1.751088	-0.020071
7	C	0.287638	1.242930	-0.049904
8	C	1.401865	0.342091	-0.245822
9	C	2.636843	0.620268	0.188231
10	C	3.833012	-0.267608	0.025241
11	Cl	4.432085	-0.671578	1.675945
12	O	0.468898	2.516334	0.120099
13	Cl	3.512275	-1.772208	-0.874813
14	Cl	5.079568	0.699336	-0.848574
15	H	-0.620771	-1.325243	-0.017035
16	H	-1.887586	2.803854	-0.034748
17	H	-2.952310	-2.033254	0.014827
18	H	-4.231731	2.068007	0.005667
19	H	1.196256	-0.595530	-0.734191
20	H	1.385983	2.805180	-0.009056
21	H	2.868986	1.521772	0.740885
22	C	-5.162889	-0.503000	0.022221
23	F	-6.045499	0.507803	0.073359
24	F	-5.444339	-1.226970	-1.082501
25	F	-5.402050	-1.301124	1.084299





Summary of Natural Population Analysis:

Natural Population

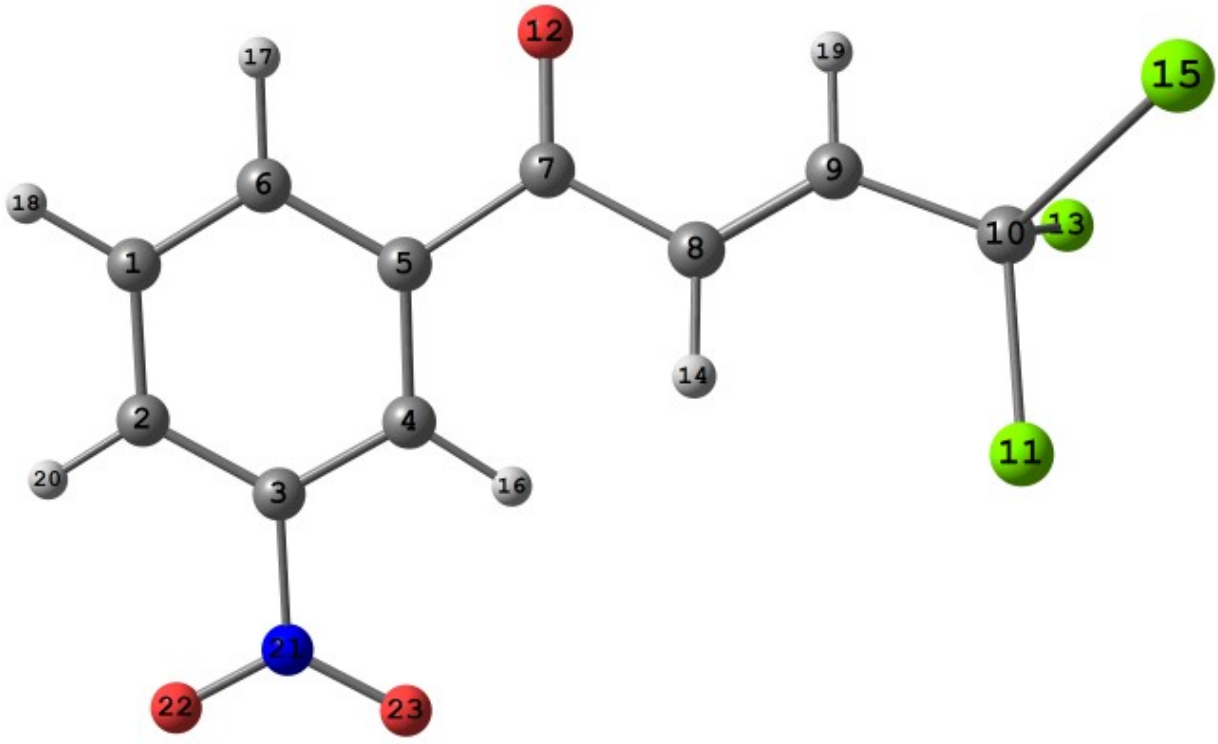
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.17552	1.99905	4.15684	0.01962	6.17552
C	2	-0.05595	1.99888	4.03486	0.02221	6.05595
C	3	-0.17546	1.99906	4.15610	0.02031	6.17546
C	4	-0.09488	1.99909	4.07903	0.01676	6.09488
C	5	-0.14963	1.99893	4.13133	0.01937	6.14963
C	6	-0.08836	1.99908	4.07053	0.01875	6.08836
C	7	0.60028	1.99898	3.37476	0.02598	5.39972
C	8	-0.26802	1.99879	4.24899	0.02024	6.26802
C	9	-0.09666	1.99884	4.06994	0.02788	6.09666
C	10	-0.18899	1.99906	4.12415	0.06578	6.18899
Cl	11	0.07100	9.99951	6.91037	0.01912	16.92900
O	12	-0.56574	1.99969	6.54213	0.02392	8.56574
Cl	13	0.07474	9.99948	6.90582	0.01996	16.92526
Cl	14	0.07278	9.99951	6.90870	0.01902	16.92722
H	15	0.23717	0.00000	0.76105	0.00178	0.76283
H	16	0.24538	0.00000	0.75262	0.00200	0.75462
H	17	0.24583	0.00000	0.75208	0.00209	0.75417
H	18	0.24850	0.00000	0.74953	0.00197	0.75150
H	19	0.26438	0.00000	0.73325	0.00237	0.73562
H	20	0.53152	0.00000	0.46566	0.00281	0.46848
H	21	0.24827	0.00000	0.74905	0.00268	0.75173
C	22	1.07964	1.99914	2.86869	0.05253	4.92036
F	23	-0.35179	1.99991	7.34248	0.00940	9.35179
F	24	-0.35432	1.99992	7.34497	0.00944	9.35432
F	25	-0.35413	1.99992	7.34477	0.00944	9.35413
* Total *		1.00004	59.98685	97.57769	0.43543	157.99996

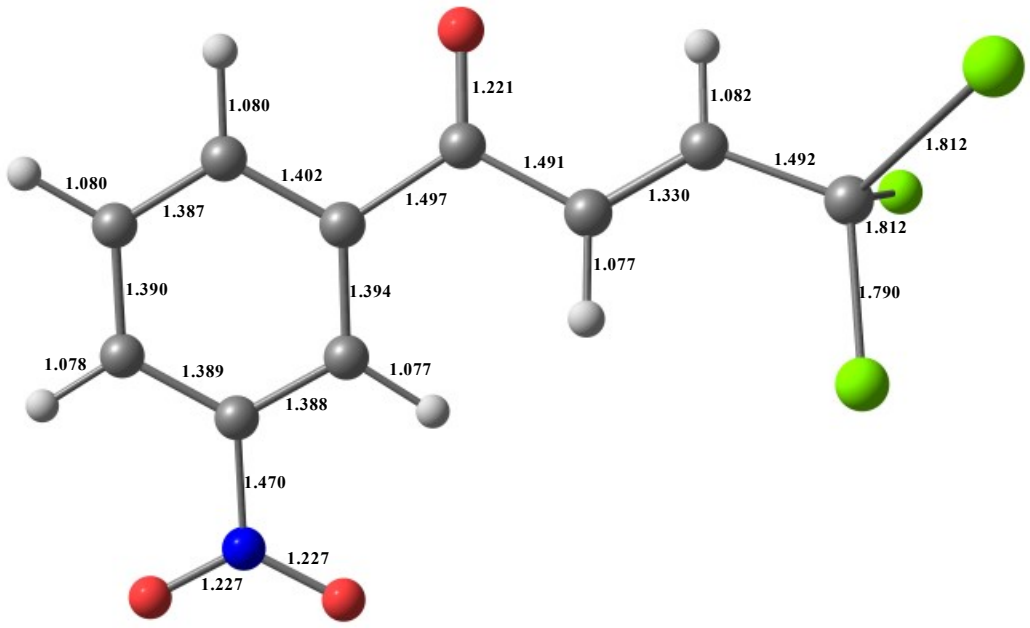
2h

Energy E(B3LYP) = -2045.8648157 h, G^{298} = -2045.768094 h, μ=3.64 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	4.029808	2.005839	-0.152652
2	C	4.495173	0.696860	-0.114493
3	C	3.568774	-0.331427	-0.003370
4	C	2.202417	-0.097219	0.060990
5	C	1.741553	1.217936	0.024976
6	C	2.668972	2.264112	-0.077452
7	C	0.288355	1.566071	0.119834
8	C	-0.722066	0.486002	-0.071031
9	C	-2.009515	0.736044	0.148883
10	C	-3.136539	-0.227845	-0.012506
11	Cl	-2.644399	-1.861207	-0.553303
12	O	-0.054145	2.717566	0.339263
13	Cl	-3.989835	-0.375483	1.579360
14	H	-0.400894	-0.487996	-0.401067
15	Cl	-4.298230	0.459321	-1.222065
16	H	1.538466	-0.939451	0.154987
17	H	2.302915	3.279506	-0.100972
18	H	4.732730	2.820860	-0.240099
19	H	-2.322800	1.718648	0.476831
20	H	5.548187	0.472820	-0.168497
21	N	4.048165	-1.720099	0.045761
22	O	5.257255	-1.915377	-0.027650
23	O	3.216207	-2.615523	0.157331





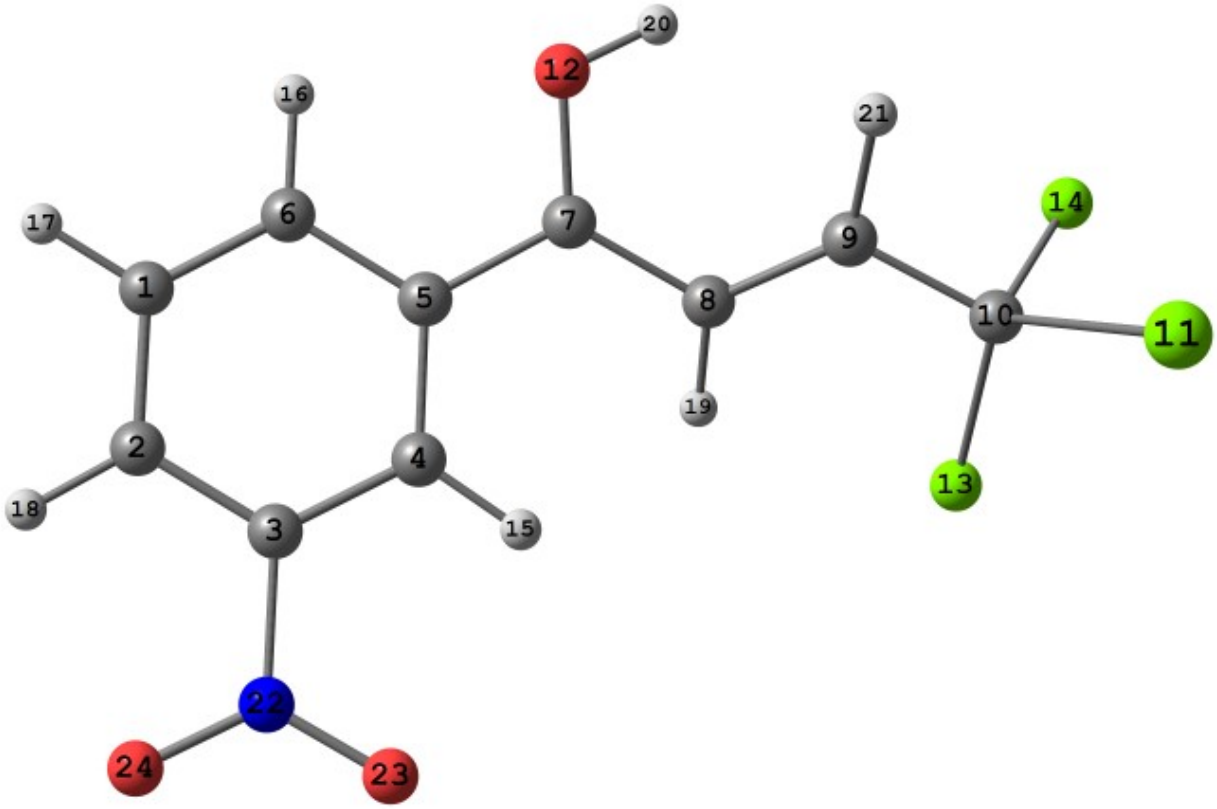
Summary of Natural Population Analysis:

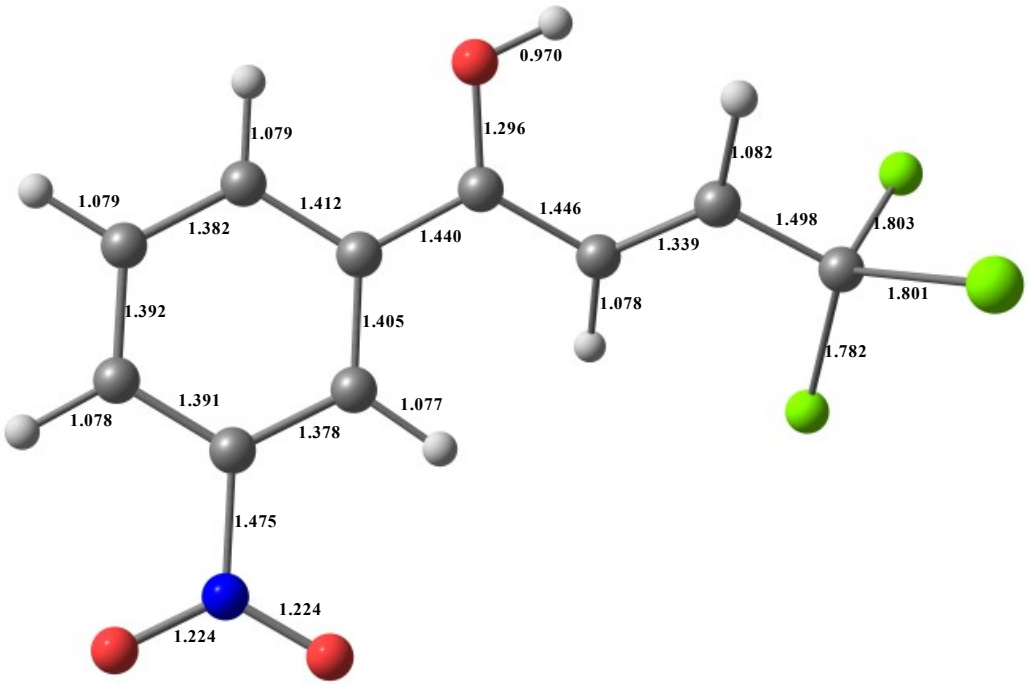
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.18940	1.99916	4.17105	0.01919	6.18940
C	2	-0.14305	1.99904	4.12332	0.02069	6.14305
C	3	0.06914	1.99876	3.91047	0.02163	5.93086
C	4	-0.14264	1.99896	4.12439	0.01929	6.14264
C	5	-0.13258	1.99894	4.11388	0.01977	6.13258
C	6	-0.10887	1.99908	4.09026	0.01953	6.10887
C	7	0.54140	1.99921	3.42492	0.03448	5.45860
C	8	-0.25407	1.99891	4.23417	0.02099	6.25407
C	9	-0.16409	1.99882	4.13772	0.02756	6.16409
C	10	-0.16451	1.99903	4.10221	0.06327	6.16451
Cl	11	0.05125	9.99948	6.92932	0.01995	16.94875
O	12	-0.58622	1.99976	6.56179	0.02466	8.58622
Cl	13	0.03850	9.99951	6.94318	0.01881	16.96150
H	14	0.23089	0.00000	0.76653	0.00258	0.76911
Cl	15	0.03866	9.99952	6.94303	0.01879	16.96134
H	16	0.24866	0.00000	0.74876	0.00258	0.75134
H	17	0.23681	0.00000	0.76102	0.00217	0.76319
H	18	0.23126	0.00000	0.76714	0.00161	0.76874
H	19	0.25000	0.00000	0.74685	0.00314	0.75000
H	20	0.24921	0.00000	0.74874	0.00205	0.75079
N	21	0.50629	1.99944	4.44286	0.05141	6.49371
O	22	-0.40238	1.99979	6.38080	0.02178	8.40238
O	23	-0.40425	1.99979	6.38251	0.02195	8.40425
* Total *		0.00000	57.98720	89.55494	0.45786	148.00000

Bh

Energy E(B3LYP) = -2046.26523658 h, G^{298} = --2046.155533 h, μ=11.8 D

1	C	-4.021672	1.966713	0.000619
2	C	-4.441133	0.639714	0.011054
3	C	-3.486264	-0.371730	0.006305
4	C	-2.133493	-0.107869	-0.015434
5	C	-1.712608	1.232601	-0.027223
6	C	-2.673019	2.267625	-0.014725
7	C	-0.309218	1.555806	-0.031961
8	C	0.721869	0.566570	-0.253803
9	C	1.972137	0.717027	0.199854
10	C	3.085549	-0.269037	0.018153
11	Cl	3.632435	-0.766459	1.660974
12	O	-0.024202	2.803891	0.170776
13	Cl	2.640714	-1.714219	-0.924102
14	Cl	4.417863	0.609135	-0.821621
15	H	-1.441074	-0.932483	-0.002196
16	H	-2.349548	3.296382	-0.030634
17	H	-4.753693	2.759393	0.000805
18	H	-5.489370	0.386508	0.021607
19	H	0.438386	-0.331000	-0.778348
20	H	0.912681	3.023739	0.046274
21	H	2.277939	1.573090	0.787094
22	N	-3.930911	-1.778466	0.024535
23	O	-3.069815	-2.648688	0.031850
24	O	-5.135861	-1.992037	0.030793





Summary of Natural Population Analysis:

Natural Population

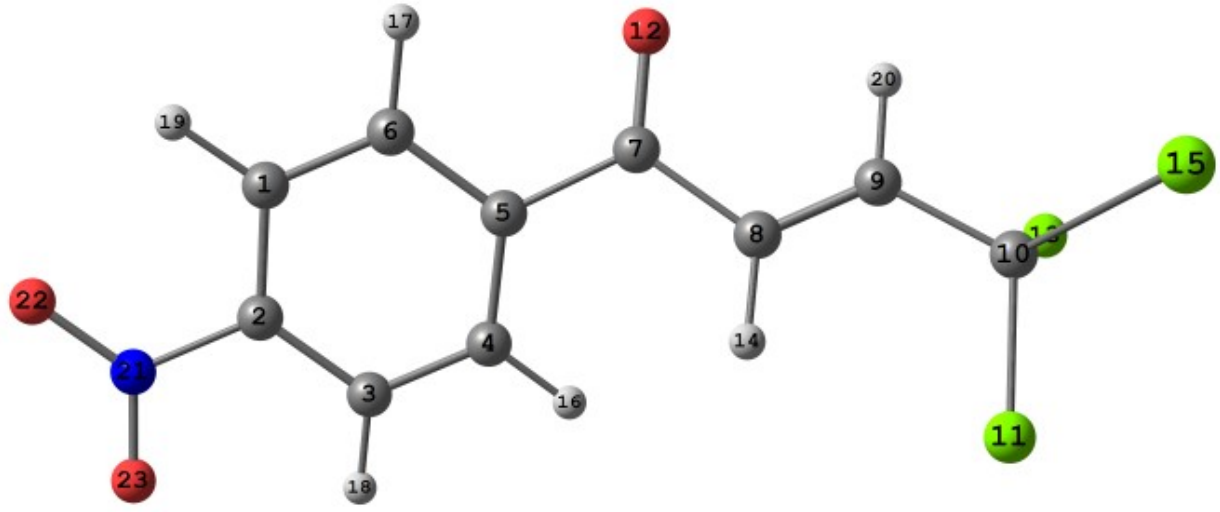
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.18316	1.99916	4.16479	0.01920	6.18316
C	2	-0.08426	1.99905	4.06490	0.02031	6.08426
C	3	0.06898	1.99875	3.91040	0.02187	5.93102
C	4	-0.08600	1.99896	4.06821	0.01883	6.08600
C	5	-0.15315	1.99894	4.13521	0.01901	6.15315
C	6	-0.06640	1.99909	4.04857	0.01875	6.06640
C	7	0.60547	1.99899	3.36998	0.02555	5.39453
C	8	-0.28199	1.99891	4.26216	0.02092	6.28199
C	9	-0.08532	1.99883	4.05993	0.02656	6.08532
C	10	-0.18995	1.99906	4.12504	0.06584	6.18995
Cl	11	0.07224	9.99950	6.90915	0.01910	16.92776
O	12	-0.56278	1.99969	6.53929	0.02380	8.56278
Cl	13	0.07599	9.99948	6.90446	0.02007	16.92401
Cl	14	0.07411	9.99951	6.90740	0.01898	16.92589
H	15	0.26127	0.00000	0.73611	0.00262	0.73873
H	16	0.24686	0.00000	0.75121	0.00194	0.75314
H	17	0.24377	0.00000	0.75469	0.00155	0.75623
H	18	0.25855	0.00000	0.73949	0.00195	0.74145
H	19	0.26686	0.00000	0.73067	0.00247	0.73314
H	20	0.53338	0.00000	0.46386	0.00276	0.46662
H	21	0.24892	0.00000	0.74817	0.00290	0.75108
N	22	0.50862	1.99945	4.44024	0.05169	6.49138
O	23	-0.38784	1.99979	6.36621	0.02185	8.38784
O	24	-0.38415	1.99979	6.36266	0.02170	8.38415
* Total *		1.00000	57.98695	89.56282	0.45023	148.00000

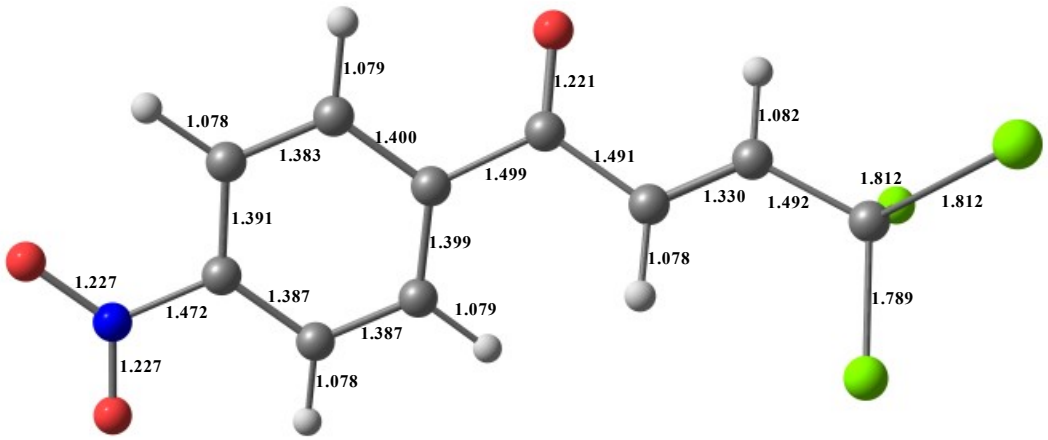
2i

Energy E(B3LYP) = -2045.86407 h, G^{298} = -2045.767482 h, μ=2.99 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-3.865086	-1.202184	-0.162380
2	C	-4.146610	0.150869	-0.006512
3	C	-3.151813	1.095999	0.198729
4	C	-1.831119	0.672558	0.238165
5	C	-1.516231	-0.682061	0.088907
6	C	-2.545075	-1.611712	-0.105771
7	C	-0.109693	-1.196890	0.159986
8	C	1.013003	-0.235774	-0.035303
9	C	2.267747	-0.636964	0.147700
10	C	3.495915	0.191276	-0.027652
11	Cl	3.185888	1.881047	-0.527713
12	O	0.099520	-2.382837	0.360385
13	Cl	4.399916	0.205404	1.542803
14	H	0.794673	0.773940	-0.342101
15	Cl	4.538197	-0.603728	-1.278997
16	H	-1.060523	1.407994	0.407978
17	H	-2.295832	-2.655759	-0.216868
18	H	-3.406990	2.135454	0.323639
19	H	-4.664065	-1.907633	-0.321917
20	H	2.471727	-1.655469	0.451211
21	N	-5.548709	0.595814	-0.058721
22	O	-6.416102	-0.253017	-0.238225
23	O	-5.779953	1.792576	0.080379





Summary of Natural Population Analysis:

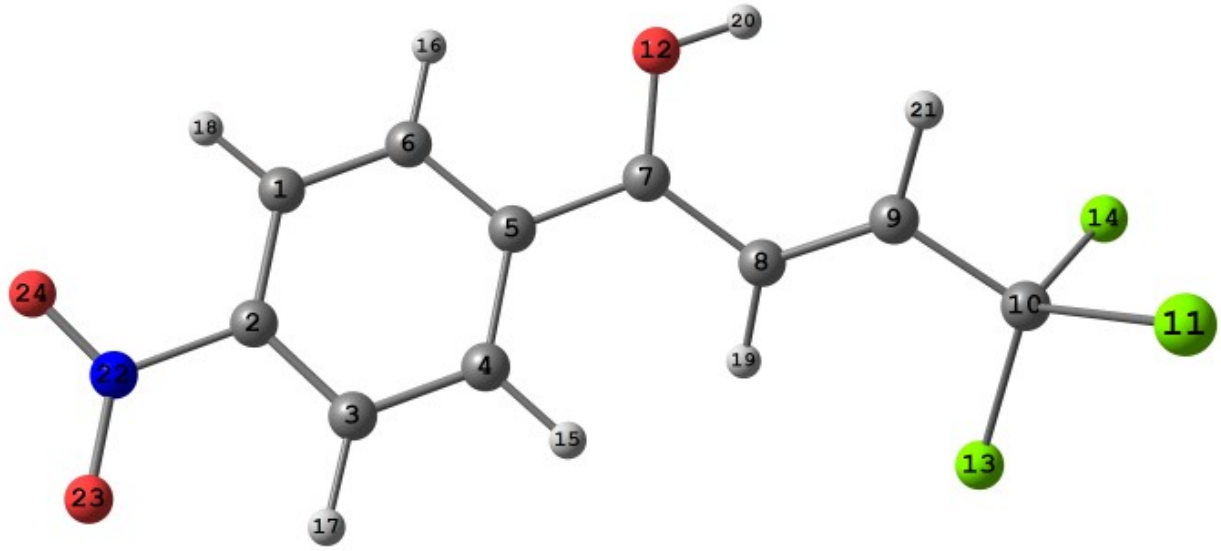
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.17572	1.99903	4.15590	0.02079	6.17572
C	2	0.09290	1.99876	3.88677	0.02158	5.90710
C	3	-0.17364	1.99904	4.15352	0.02109	6.17364
C	4	-0.15756	1.99908	4.14128	0.01720	6.15756
C	5	-0.10233	1.99893	4.08325	0.02015	6.10233
C	6	-0.14434	1.99907	4.12592	0.01934	6.14434
C	7	0.53949	1.99921	3.42676	0.03454	5.46051
C	8	-0.25544	1.99891	4.23551	0.02102	6.25544
C	9	-0.16236	1.99882	4.13603	0.02751	6.16236
C	10	-0.16497	1.99903	4.10265	0.06329	6.16497
Cl	11	0.05158	9.99948	6.92899	0.01994	16.94842
O	12	-0.58047	1.99976	6.55599	0.02471	8.58047
Cl	13	0.03893	9.99951	6.94275	0.01880	16.96107
H	14	0.23249	0.00000	0.76492	0.00258	0.76751
Cl	15	0.03916	9.99952	6.94254	0.01878	16.96084
H	16	0.22984	0.00000	0.76839	0.00177	0.77016
H	17	0.23873	0.00000	0.75911	0.00216	0.76127
H	18	0.25045	0.00000	0.74741	0.00214	0.74955
H	19	0.24957	0.00000	0.74826	0.00217	0.75043
H	20	0.25003	0.00000	0.74688	0.00310	0.74997
N	21	0.50382	1.99944	4.44520	0.05154	6.49618
O	22	-0.39992	1.99979	6.37847	0.02166	8.39992
O	23	-0.40025	1.99979	6.37883	0.02163	8.40025
* Total *		0.00000	57.98719	89.55532	0.45749	148.00000

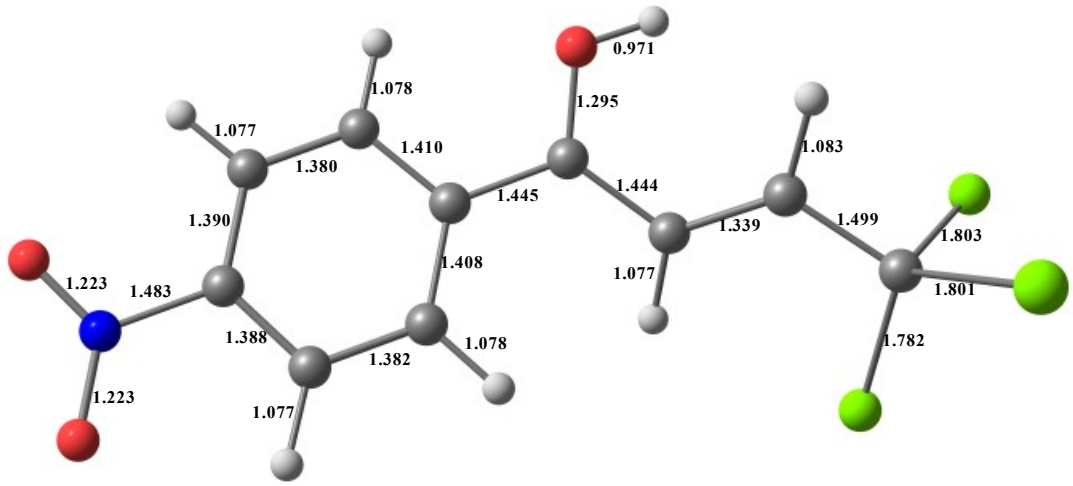
Bi

Energy E(B3LYP) = -2046.26340239 h, G^{298} = -2046.154357 h, μ=7.29 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C6	0	-3.849092	1.195758	-0.016961
2	C	-4.085029	-0.173760	0.009355
3	C	-3.066831	-1.116318	0.020643
4	C	-1.757812	-0.672490	-0.002539
5	C	-1.481648	0.707544	-0.031929
6	C	-2.541428	1.636861	-0.035198
7	C	-0.118718	1.186005	-0.041651
8	C	1.014028	0.313087	-0.242920
9	C	2.242990	0.619880	0.191507
10	C	3.461315	-0.236303	0.023188
11	Cl	4.071698	-0.629320	1.671638
12	O	0.025979	2.460821	0.135245
13	Cl	3.178869	-1.744546	-0.882357
14	Cl	4.677427	0.769059	-0.848952
15	H	-0.964306	-1.401474	0.022956
16	H	-2.334335	2.694354	-0.064374
17	H	-3.297579	-2.168181	0.047648
18	H	-4.673005	1.889883	-0.026585
19	H	0.830049	-0.628061	-0.733416
20	H	0.934600	2.779312	0.011663
21	H	2.452236	1.525109	0.747206
22	N	-5.489145	-0.649900	0.025512
23	O	-5.678250	-1.858388	0.017655
24	O	-6.373505	0.194878	0.045819





Summary of Natural Population Analysis:

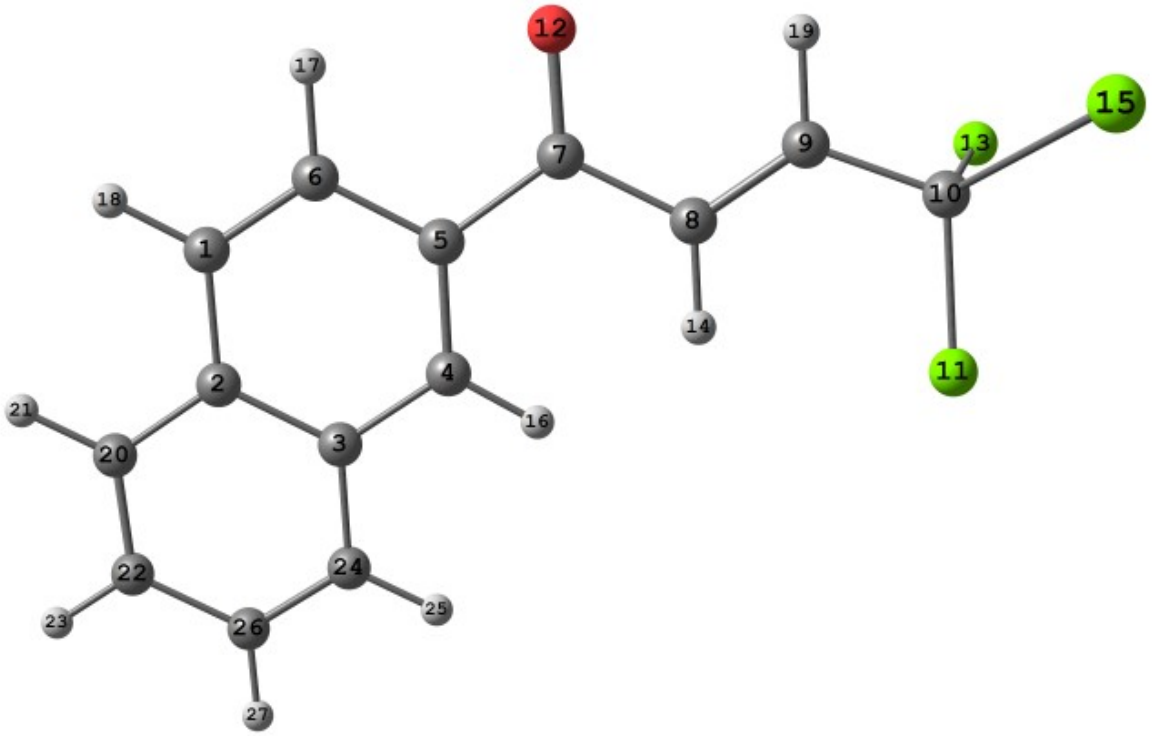
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.17701	1.99903	4.15703	0.02095	6.17701
C	2	0.14845	1.99876	3.83095	0.02184	5.85155
C	3	-0.17872	1.99903	4.15847	0.02123	6.17872
C	4	-0.09361	1.99910	4.07805	0.01647	6.09361
C	5	-0.13616	1.99893	4.11803	0.01920	6.13616
C	6	-0.09215	1.99909	4.07444	0.01863	6.09215
C	7	0.60789	1.99900	3.36755	0.02556	5.39211
C	8	-0.28277	1.99891	4.26293	0.02093	6.28277
C	9	-0.08009	1.99884	4.05471	0.02654	6.08009
C	10	-0.19104	1.99906	4.12606	0.06592	6.19104
Cl	11	0.07370	9.99950	6.90769	0.01910	16.92630
O	12	-0.55980	1.99969	6.53620	0.02391	8.55980
Cl	13	0.07645	9.99948	6.90400	0.02006	16.92355
Cl	14	0.07574	9.99951	6.90576	0.01899	16.92426
H	15	0.24071	0.00000	0.75752	0.00176	0.75929
H	16	0.24874	0.00000	0.74931	0.00195	0.75126
H	17	0.26242	0.00000	0.73548	0.00210	0.73758
H	18	0.26164	0.00000	0.73622	0.00213	0.73836
H	19	0.26737	0.00000	0.73014	0.00249	0.73263
H	20	0.53351	0.00000	0.46375	0.00275	0.46649
H	21	0.24860	0.00000	0.74850	0.00290	0.75140
N	22	0.50169	1.99945	4.44715	0.05171	6.49831
O	23	-0.37799	1.99979	6.35677	0.02142	8.37799
O	24	-0.37758	1.99979	6.35635	0.02144	8.37758
* Total *		1.00000	57.98695	89.56307	0.44998	148.00000

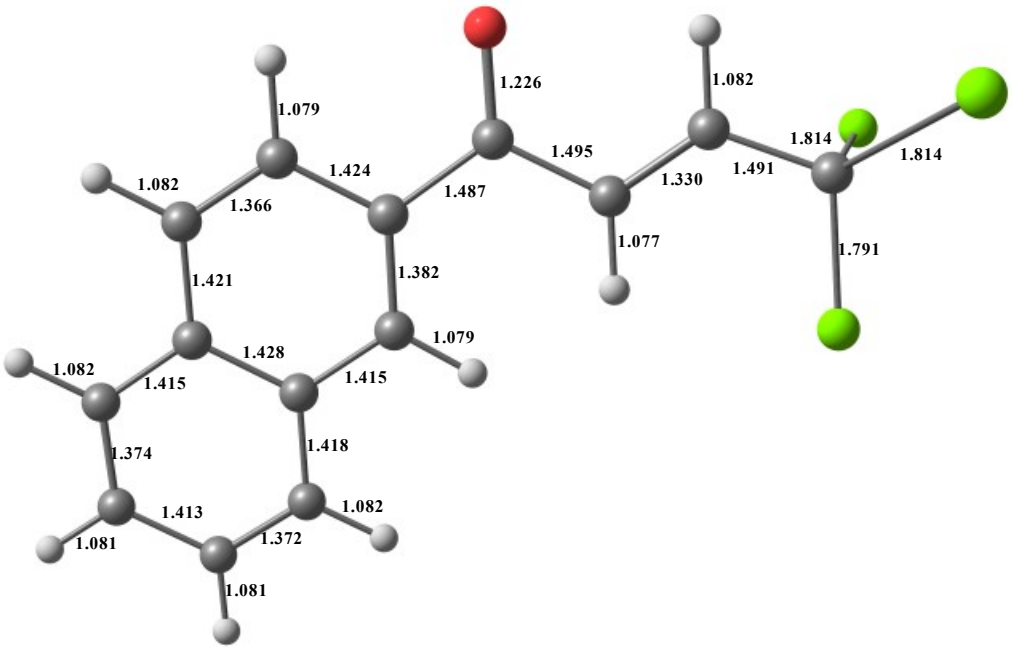
2l

Energy E(B3LYP) = -1994.97958331 h, G^{298} = -1994.837725 h, μ=5.83 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	3.723413	1.840002	-0.038402
2	C	4.194534	0.499269	-0.019525
3	C	3.238845	-0.560685	0.015652
4	C	1.860225	-0.244104	0.027418
5	C	1.423591	1.066936	0.009998
6	C	2.385996	2.115958	-0.022016
7	C	-0.015263	1.443172	0.034913
8	C	-1.051550	0.367249	-0.016611
9	C	-2.341327	0.685233	0.042242
10	C	-3.488576	-0.265366	-0.004216
11	Cl	-3.022662	-1.987333	-0.160726
12	O	-0.353192	2.619902	0.092375
13	Cl	-4.460133	-0.065960	1.514725
14	H	-0.749734	-0.662034	-0.108458
15	Cl	-4.542836	0.178740	-1.412084
16	H	1.164260	-1.068344	0.057710
17	H	2.032990	3.135901	-0.034775
18	H	4.445203	2.645471	-0.066024
19	H	-2.639931	1.721523	0.131870
20	C	5.572125	0.177621	-0.033812
21	H	6.297893	0.979484	-0.060916
22	C	5.983968	-1.133292	-0.013301
23	H	7.039499	-1.367604	-0.024255
24	C	3.695588	-1.903062	0.036838
25	H	2.967849	-2.703136	0.064046
26	C	5.038956	-2.183005	0.022582
27	H	5.380083	-3.208645	0.038692





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.17348	1.99907	4.15514	0.01927	6.17348
C	2	-0.04380	1.99898	4.02682	0.01801	6.04380
C	3	-0.07511	1.99898	4.05759	0.01854	6.07511
C	4	-0.10802	1.99889	4.09142	0.01770	6.10802
C	5	-0.15654	1.99896	4.13636	0.02123	6.15654

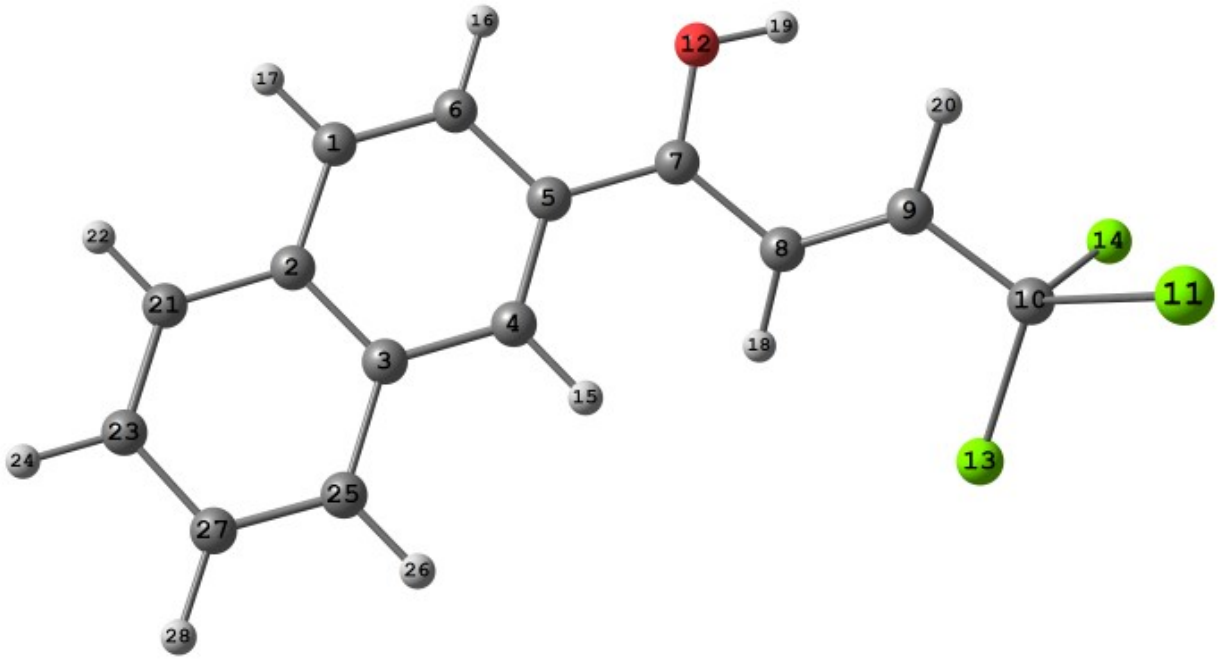
C	6	-0.17148	1.99908	4.15266	0.01973	6.17148
C	7	0.54594	1.99901	3.42115	0.03390	5.45406
C	8	-0.24995	1.99893	4.22878	0.02225	6.24995
C	9	-0.18004	1.99881	4.15358	0.02764	6.18004
C	10	-0.16059	1.99902	4.09848	0.06308	6.16059
Cl	11	0.04798	9.99948	6.93258	0.01996	16.95202
O	12	-0.60817	1.99977	6.58355	0.02485	8.60817
Cl	13	0.03361	9.99952	6.94811	0.01877	16.96639
H	14	0.22641	0.00000	0.77121	0.00238	0.77359
Cl	15	0.03366	9.99952	6.94806	0.01877	16.96634
H	16	0.21474	0.00000	0.78323	0.00203	0.78526
H	17	0.22912	0.00000	0.76860	0.00229	0.77088
H	18	0.21837	0.00000	0.77962	0.00201	0.78163
H	19	0.24886	0.00000	0.74792	0.00322	0.75114
C	20	-0.18602	1.99907	4.16742	0.01952	6.18602
H	21	0.21786	0.00000	0.78021	0.00194	0.78214
C	22	-0.18414	1.99916	4.16509	0.01989	6.18414
H	23	0.21735	0.00000	0.78103	0.00162	0.78265
C	24	-0.16725	1.99908	4.14906	0.01911	6.16725
H	25	0.21753	0.00000	0.78066	0.00181	0.78247
C	26	-0.20472	1.99915	4.18547	0.02009	6.20472
H	27	0.21790	0.00000	0.78041	0.00169	0.78210
* Total *		0.00003	59.98446	91.57420	0.44131	151.99997

Bl

Energy E(B3LYP) = -1995.38975127 h, G^{298} = -1995.233958 h, μ=6.29 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-3.700223	1.826878	0.045215
2	C	-4.143657	0.472434	0.032198
3	C	-3.169261	-0.576505	-0.025129
4	C	-1.810974	-0.242919	-0.070774
5	C	-1.394494	1.094216	-0.055380
6	C	-2.377060	2.136393	0.006207
7	C	-0.009643	1.421618	-0.073068
8	C	1.046920	0.438611	-0.224254
9	C	2.307673	0.662330	0.160000
10	C	3.439635	-0.309163	0.029974
11	Cl	4.066849	-0.643032	1.689039
12	O	0.274829	2.691179	0.056795
13	Cl	2.999305	-1.850223	-0.753848
14	Cl	4.730201	0.501871	-0.938827
15	H	-1.094610	-1.048953	-0.104288
16	H	-2.056610	3.165624	0.013596
17	H	-4.439703	2.614296	0.084528
18	H	0.777122	-0.513659	-0.647654
19	H	1.213397	2.892049	-0.069106
20	H	2.616787	1.580837	0.642214
21	C	-5.507234	0.127659	0.072653
22	H	-6.249904	0.912113	0.114032
23	C	-5.891119	-1.195846	0.059715
24	H	-6.941886	-1.447759	0.091960
25	C	-3.597738	-1.931773	-0.035949
26	H	-2.854269	-2.715465	-0.077589
27	C	-4.933749	-2.232754	0.005675
28	H	-5.261435	-3.262058	-0.002738



Summary of Natural Population Analysis:

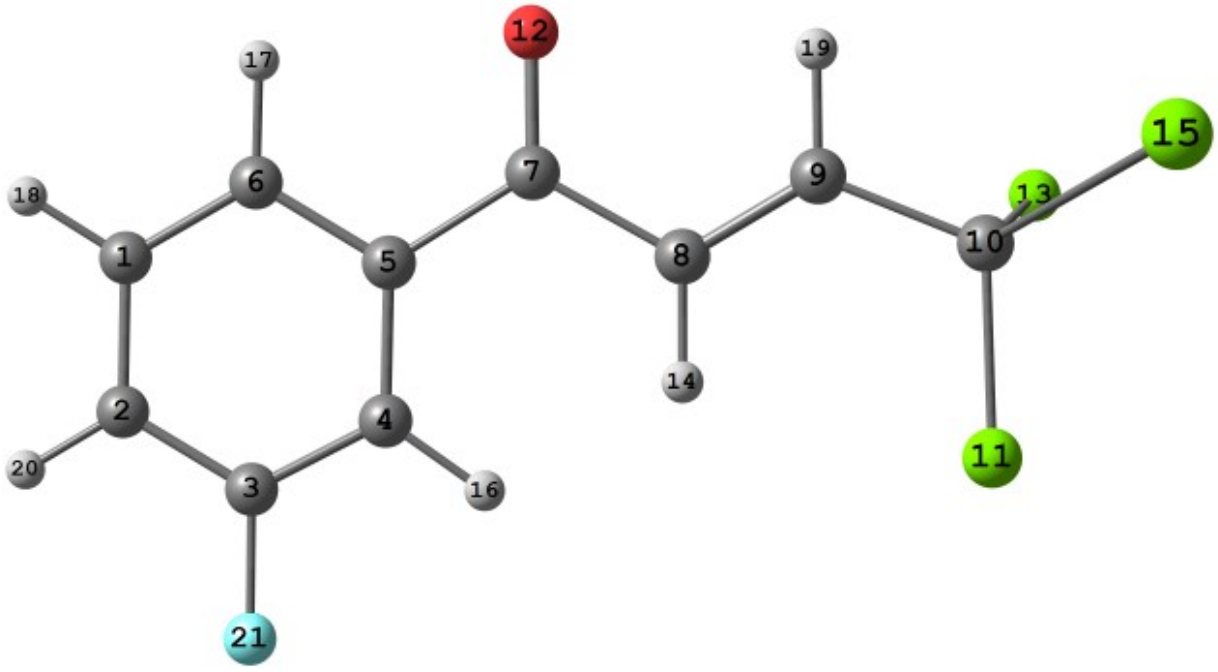
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.15747	1.99907	4.13927	0.01912	6.15747
C	2	-0.00582	1.99898	3.98907	0.01778	6.00582
C	3	-0.08607	1.99897	4.06864	0.01846	6.08607
C	4	-0.02101	1.99892	4.00504	0.01705	6.02101
C	5	-0.16490	1.99897	4.14598	0.01995	6.16490
C	6	-0.15344	1.99908	4.13561	0.01875	6.15344
C	7	0.57607	1.99879	3.39878	0.02636	5.42393
C	8	-0.26851	1.99893	4.24843	0.02115	6.26851
C	9	-0.12205	1.99882	4.09683	0.02640	6.12205
C	10	-0.18174	1.99906	4.11741	0.06527	6.18174
Cl	11	0.06184	9.99951	6.91963	0.01902	16.93816
O	12	-0.58533	1.99969	6.56208	0.02356	8.58533
Cl	13	0.06919	9.99948	6.91135	0.01998	16.93081
Cl	14	0.06261	9.99951	6.91894	0.01894	16.93739
H	15	0.22800	0.00000	0.77005	0.00196	0.77200
H	16	0.23794	0.00000	0.76000	0.00205	0.76206
H	17	0.22970	0.00000	0.76836	0.00194	0.77030
H	18	0.25838	0.00000	0.73933	0.00229	0.74162
H	19	0.52453	0.00000	0.47270	0.00277	0.47547
H	20	0.24308	0.00000	0.75401	0.00291	0.75692
C	21	-0.18555	1.99907	4.16710	0.01938	6.18555
H	22	0.22706	0.00000	0.77107	0.00188	0.77294
C	23	-0.13234	1.99917	4.11397	0.01920	6.13234
H	24	0.22452	0.00000	0.77397	0.00150	0.77548
C	25	-0.13205	1.99908	4.11426	0.01872	6.13205
H	26	0.22608	0.00000	0.77221	0.00171	0.77392
C	27	-0.19914	1.99915	4.18022	0.01976	6.19914
H	28	0.22643	0.00000	0.77194	0.00164	0.77357
* Total *		1.00002	59.98424	91.58624	0.42949	151.99998

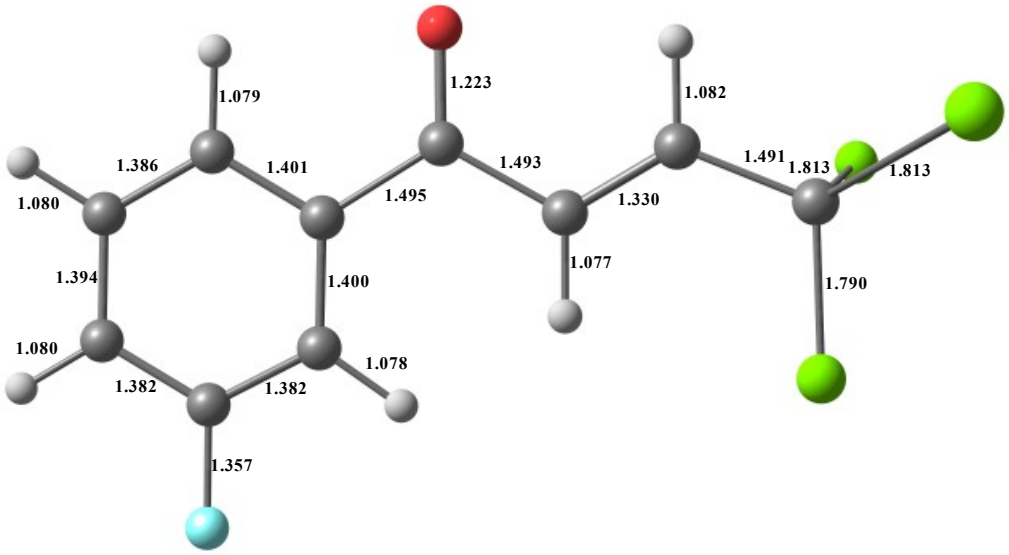
2m

Energy E(B3LYP) = -1940.56380258 h, G^{298} = -1940.47527 h, μ=3.21 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.677159	-1.144147	-0.026096
2	C	-4.969168	0.218581	-0.015245
3	C	-3.913595	1.110863	0.005470
4	C	-2.591377	0.710381	0.014255
5	C	-2.304345	-0.660309	0.003779
6	C	-3.361311	-1.580080	-0.015703
7	C	-0.908761	-1.196320	0.016653
8	C	0.237694	-0.239758	-0.008955
9	C	1.483964	-0.702778	0.019386
10	C	2.732315	0.112613	-0.001689
11	Cl	2.463820	1.880936	-0.067660
12	O	-0.708062	-2.402305	0.046010
13	Cl	3.689001	-0.273156	1.489405
14	H	0.049689	0.819376	-0.052946
15	Cl	3.709786	-0.380155	-1.447164
16	H	-1.826721	1.469927	0.032464
17	H	-3.132346	-2.634445	-0.023037
18	H	-5.485199	-1.861130	-0.042552
19	H	1.662605	-1.769147	0.061999
20	H	-5.986046	0.582622	-0.022541
21	F	-4.183480	2.440815	0.017725





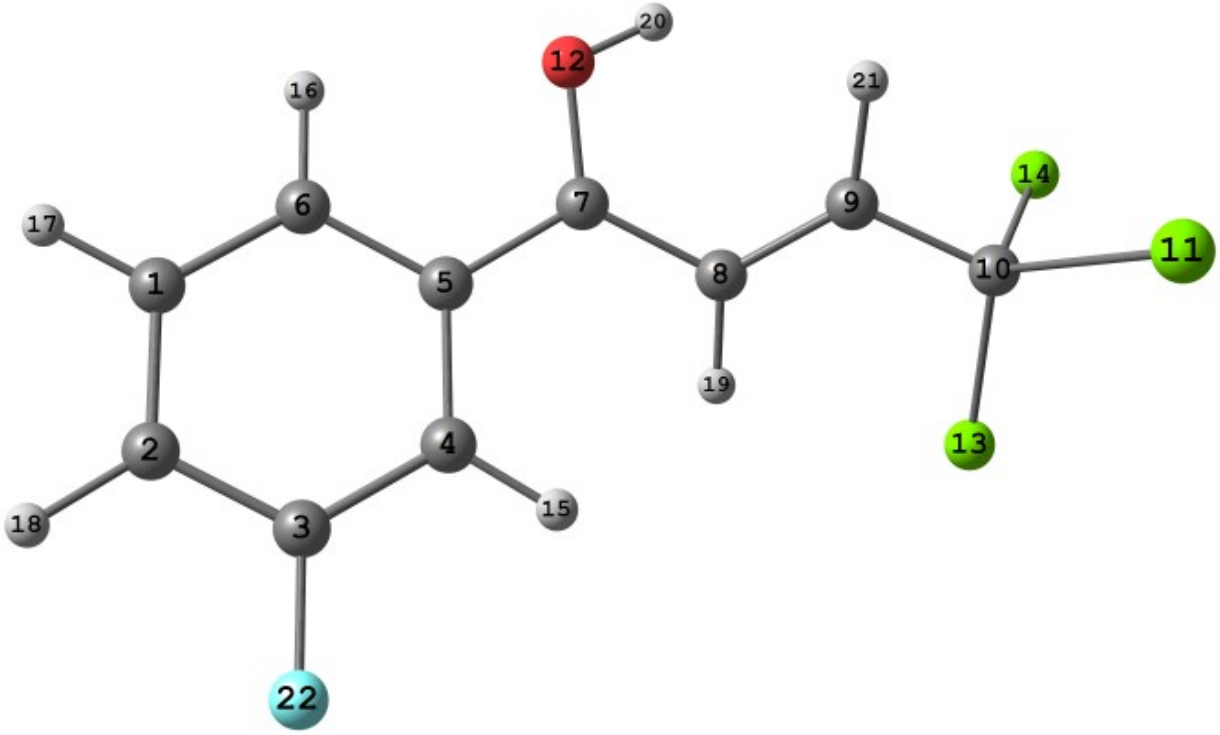
Summary of Natural Population Analysis:

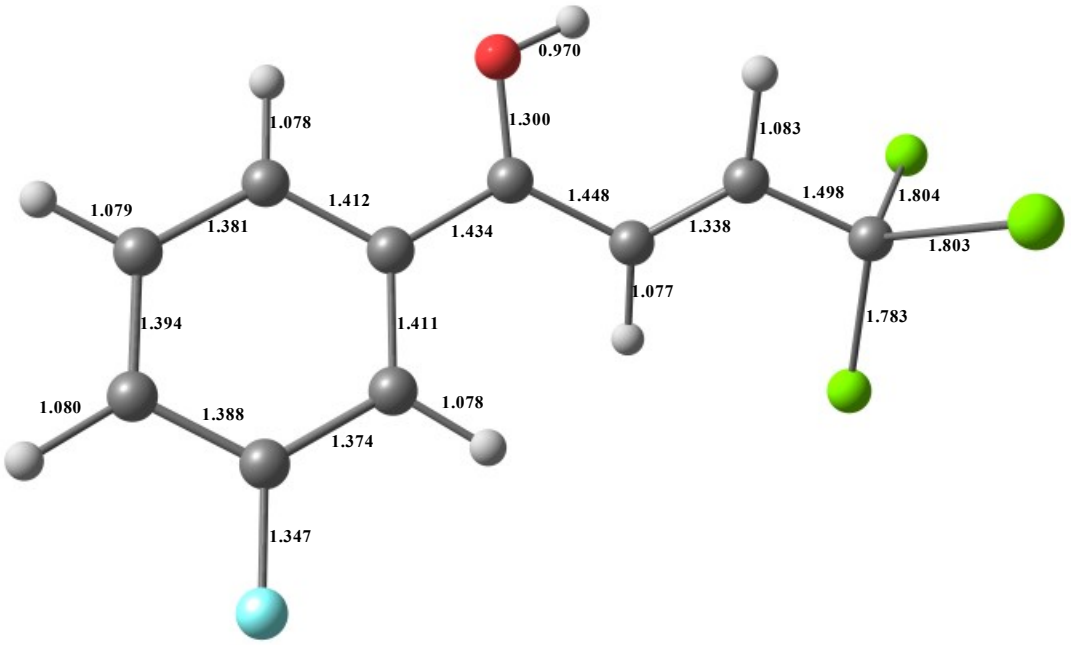
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.18249	1.99917	4.16408	0.01924	6.18249
C	2	-0.23028	1.99902	4.21121	0.02005	6.23028
C	3	0.40729	1.99847	3.56930	0.02495	5.59271
C	4	-0.22766	1.99895	4.21039	0.01832	6.22766
C	5	-0.12713	1.99895	4.10917	0.01901	6.12713
C	6	-0.16486	1.99907	4.14599	0.01979	6.16486
C	7	0.53933	1.99920	3.42793	0.03353	5.46067
C	8	-0.24891	1.99890	4.22913	0.02088	6.24891
C	9	-0.17081	1.99881	4.14416	0.02784	6.17081
C	10	-0.16283	1.99902	4.10060	0.06321	6.16283
Cl	11	0.04987	9.99948	6.93067	0.01998	16.95013
O	12	-0.59637	1.99977	6.57203	0.02458	8.59637
Cl	13	0.03628	9.99952	6.94541	0.01880	16.96372
H	14	0.22745	0.00000	0.76996	0.00259	0.77255
Cl	15	0.03632	9.99952	6.94537	0.01879	16.96368
H	16	0.23337	0.00000	0.76432	0.00231	0.76663
H	17	0.23273	0.00000	0.76505	0.00223	0.76727
H	18	0.22448	0.00000	0.77379	0.00173	0.77552
H	19	0.24961	0.00000	0.74711	0.00327	0.75039
H	20	0.23622	0.00000	0.76178	0.00200	0.76378
F	21	-0.36161	1.99992	7.35275	0.00893	9.36161
* Total *		0.00000	53.98778	79.64020	0.37202	134.00000

Bm

Energy E(B3LYP) = -1940,96824727 h, G^{298} = -1940.864957 h, μ=8.67 D

1	C	-4.642298	1.070816	0.038566
2	C	-4.874649	-0.303734	0.049593
3	C	-3.791188	-1.171411	0.018949
4	C	-2.491179	-0.728372	-0.025959
5	C	-2.259454	0.663514	-0.035154
6	C	-3.350581	1.558962	-0.000739
7	C	-0.920107	1.176413	-0.060589
8	C	0.241031	0.334560	-0.259982
9	C	1.456950	0.676202	0.180269
10	C	2.700750	-0.143992	0.022917
11	Cl	3.309482	-0.522783	1.676816
12	O	-0.798875	2.459729	0.104901
13	Cl	2.469861	-1.660828	-0.884801
14	Cl	3.902330	0.890550	-0.836808
15	H	-1.692164	-1.451671	-0.031853
16	H	-3.172210	2.621920	-0.016558
17	H	-5.478626	1.752754	0.058090
18	H	-5.877405	-0.704376	0.079755
19	H	0.086723	-0.610807	-0.752507
20	H	0.101865	2.790347	-0.037459
21	H	1.635415	1.588190	0.735571
22	F	-4.024078	-2.497768	0.035557





Summary of Natural Population Analysis:

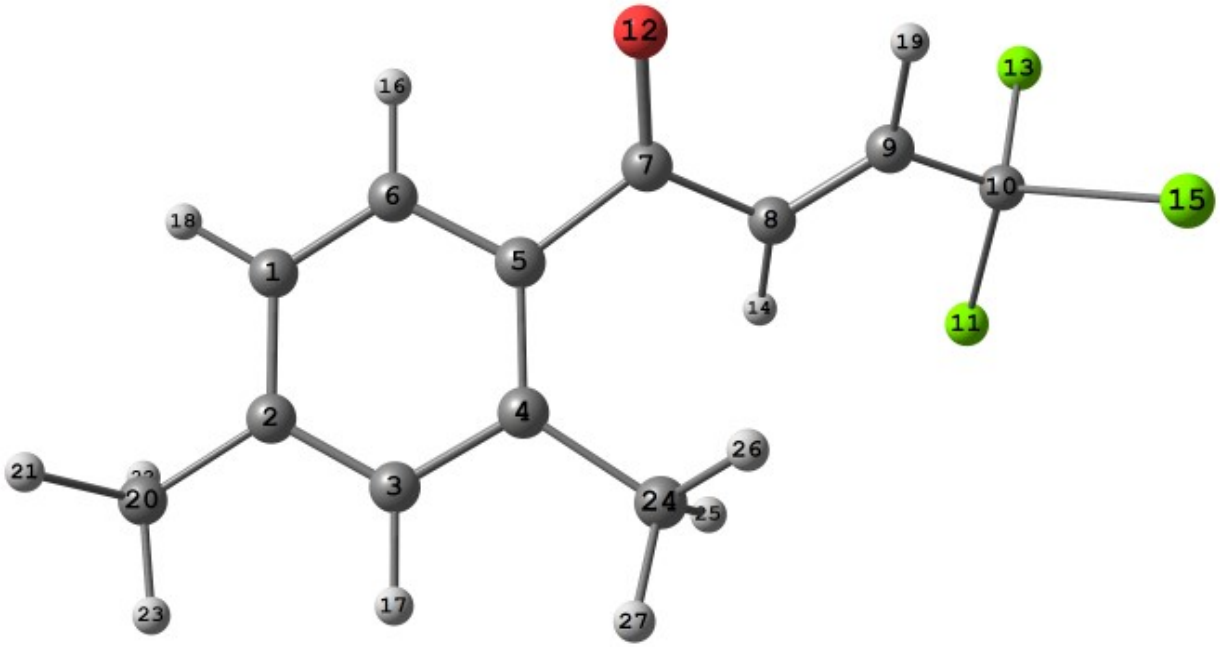
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.18018	1.99917	4.16178	0.01923	6.18018
C	2	-0.15440	1.99904	4.13604	0.01932	6.15440
C	3	0.40743	1.99848	3.56887	0.02522	5.59257
C	4	-0.17089	1.99896	4.15447	0.01746	6.17089
C	5	-0.14601	1.99895	4.12842	0.01865	6.14601
C	6	-0.10631	1.99908	4.08859	0.01864	6.10631
C	7	0.59469	1.99898	3.38082	0.02551	5.40531
C	8	-0.27579	1.99891	4.25591	0.02098	6.27579
C	9	-0.09760	1.99883	4.07215	0.02661	6.09760
C	10	-0.18739	1.99906	4.12267	0.06565	6.18739
Cl	11	0.06889	9.99951	6.91254	0.01906	16.93111
O	12	-0.56978	1.99969	6.54628	0.02381	8.56978
Cl	13	0.07351	9.99948	6.90699	0.02002	16.92649
Cl	14	0.07072	9.99951	6.91079	0.01899	16.92928
H	15	0.24770	0.00000	0.75002	0.00228	0.75230
H	16	0.24268	0.00000	0.75539	0.00194	0.75732
H	17	0.23825	0.00000	0.76009	0.00166	0.76175
H	18	0.24642	0.00000	0.75167	0.00191	0.75358
H	19	0.26463	0.00000	0.73291	0.00246	0.73537
H	20	0.53017	0.00000	0.46703	0.00280	0.46983
H	21	0.24721	0.00000	0.74987	0.00293	0.75279
F	22	-0.34393	1.99992	7.33495	0.00906	9.34393
* Total *		1.00000	53.98757	79.64823	0.36420	134.00000

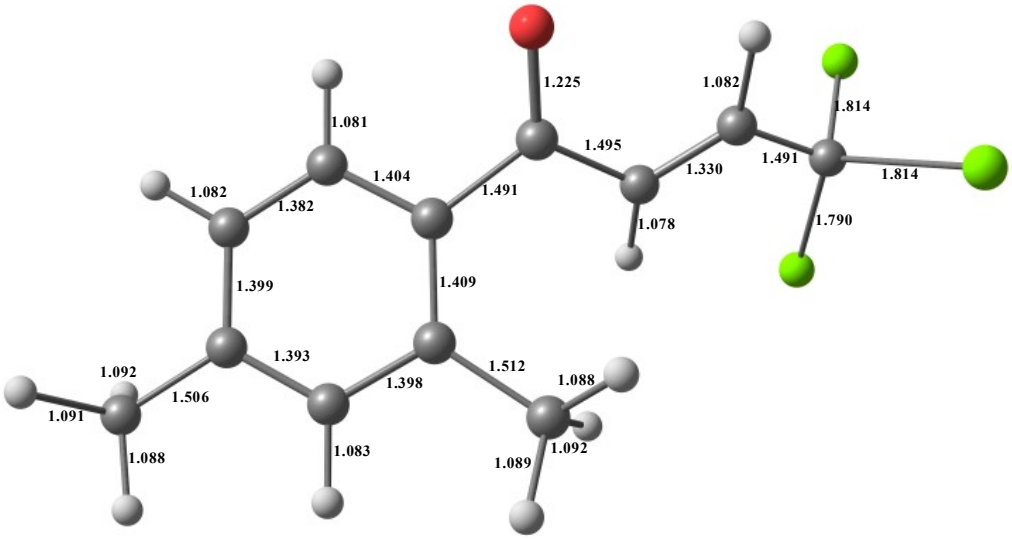
2n

Energy E(B3LYP) = -1919.9481281 h, G^{298} = -1919.799233 h, μ=5.33 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.353098	-1.145518	0.385093
2	C	-4.747097	0.192245	0.270126
3	C	-3.788131	1.127434	-0.113549
4	C	-2.452869	0.793466	-0.357648
5	C	-2.076484	-0.557667	-0.226523
6	C	-3.046086	-1.510342	0.124901
7	C	-0.699967	-1.081840	-0.458760
8	C	0.468372	-0.283109	0.022767
9	C	1.705653	-0.624788	-0.323691
10	C	2.963228	0.050062	0.106947
11	Cl	2.721411	1.436076	1.213903
12	O	-0.527197	-2.181528	-0.969595
13	Cl	4.013089	-1.175447	0.935855
14	H	0.282522	0.556089	0.673142
15	Cl	3.836197	0.635098	-1.371621
16	H	-2.746086	-2.545217	0.206539
17	H	-4.089753	2.159671	-0.240361
18	H	-5.074461	-1.898464	0.674420
19	H	1.870562	-1.467726	-0.982100
20	C	-6.169010	0.602465	0.547521
21	H	-6.869036	0.017699	-0.050918
22	H	-6.424221	0.431826	1.595164
23	H	-6.329615	1.656327	0.329061
24	C	-1.515617	1.893804	-0.800260
25	H	-0.977129	2.325813	0.045590
26	H	-0.777454	1.551281	-1.522236
27	H	-2.082966	2.700276	-1.261414





Summary of Natural Population Analysis:

Natural Population

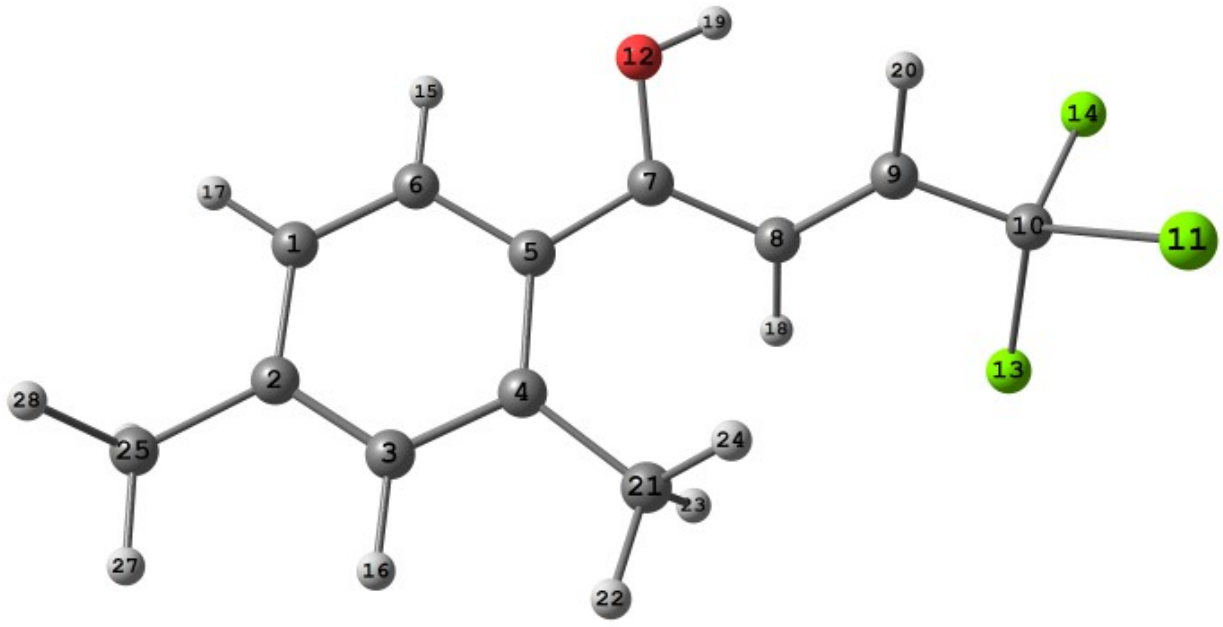
Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.21706	1.99903	4.19896	0.01907	6.21706
C	2	0.00887	1.99904	3.97476	0.01733	5.99113
C	3	-0.21348	1.99895	4.19537	0.01917	6.21348
C	4	0.01661	1.99898	3.96819	0.01622	5.98339
C	5	-0.16292	1.99884	4.14131	0.02277	6.16292
C	6	-0.14554	1.99908	4.12754	0.01893	6.14554
C	7	0.54441	1.99919	3.42115	0.03525	5.45559
C	8	-0.24622	1.99891	4.22583	0.02148	6.24622
C	9	-0.18174	1.99880	4.15537	0.02757	6.18174
C	10	-0.16068	1.99902	4.09879	0.06287	6.16068
Cl	11	0.04888	9.99948	6.93167	0.01997	16.95112
O	12	-0.60155	1.99976	6.57710	0.02468	8.60155
Cl	13	0.03396	9.99952	6.94780	0.01872	16.96604
H	14	0.23251	0.00000	0.76503	0.00246	0.76749
Cl	15	0.03375	9.99952	6.94800	0.01873	16.96625
H	16	0.22178	0.00000	0.77603	0.00220	0.77822
H	17	0.21131	0.00000	0.78655	0.00214	0.78869
H	18	0.21501	0.00000	0.78315	0.00184	0.78499
H	19	0.24826	0.00000	0.74857	0.00316	0.75174
C	20	-0.59458	1.99928	4.58342	0.01187	6.59458
H	21	0.21865	0.00000	0.77981	0.00155	0.78135
H	22	0.22027	0.00000	0.77819	0.00154	0.77973
H	23	0.21141	0.00000	0.78708	0.00151	0.78859
C	24	-0.60019	1.99927	4.58870	0.01222	6.60019
H	25	0.22075	0.00000	0.77751	0.00175	0.77925
H	26	0.21750	0.00000	0.78101	0.00150	0.78250
H	27	0.22005	0.00000	0.77842	0.00154	0.77995
* Total *		0.00000	55.98667	85.62530	0.38803	142.00000

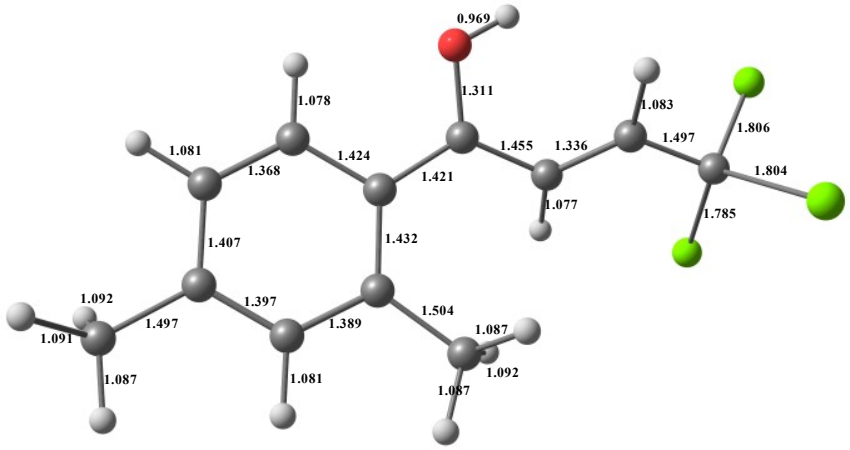
Bn

Energy E(B3LYP) = -1929,36007971 h, G^{298} = -1920.197239 h, μ=1.95 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.419513	1.107308	-0.050647
2	C	-4.741730	-0.261480	-0.018120
3	C	-3.702444	-1.192350	0.044724
4	C	-2.359916	-0.837669	0.058061
5	C	-2.046954	0.558871	0.009746
6	C	-3.110746	1.505387	-0.027630
7	C	-0.725312	1.081655	0.011402
8	C	0.484365	0.333036	-0.295928
9	C	1.653863	0.612934	0.285796
10	C	2.952090	-0.079526	0.007589
11	Cl	3.517674	-0.832628	1.546587
12	O	-0.609999	2.359505	0.282349
13	Cl	2.857771	-1.331741	-1.260586
14	Cl	4.133389	1.189428	-0.498810
15	H	-2.871603	2.555771	-0.069511
16	H	-3.953991	-2.242291	0.098716
17	H	-5.207620	1.845148	-0.100397
18	H	0.401607	-0.467904	-1.010689
19	H	0.277563	2.702030	0.097076
20	H	1.742536	1.365347	1.059186
21	C	-1.350012	-1.946870	0.171463
22	H	-1.847020	-2.861892	0.483231
23	H	-0.877135	-2.152568	-0.790910
24	H	-0.564241	-1.727457	0.890473
25	C	-6.171858	-0.701452	-0.048668
26	H	-6.637951	-0.396931	-0.988124
27	H	-6.266998	-1.779499	0.051196
28	H	-6.736340	-0.220851	0.751979





Summary of Natural Population Analysis:

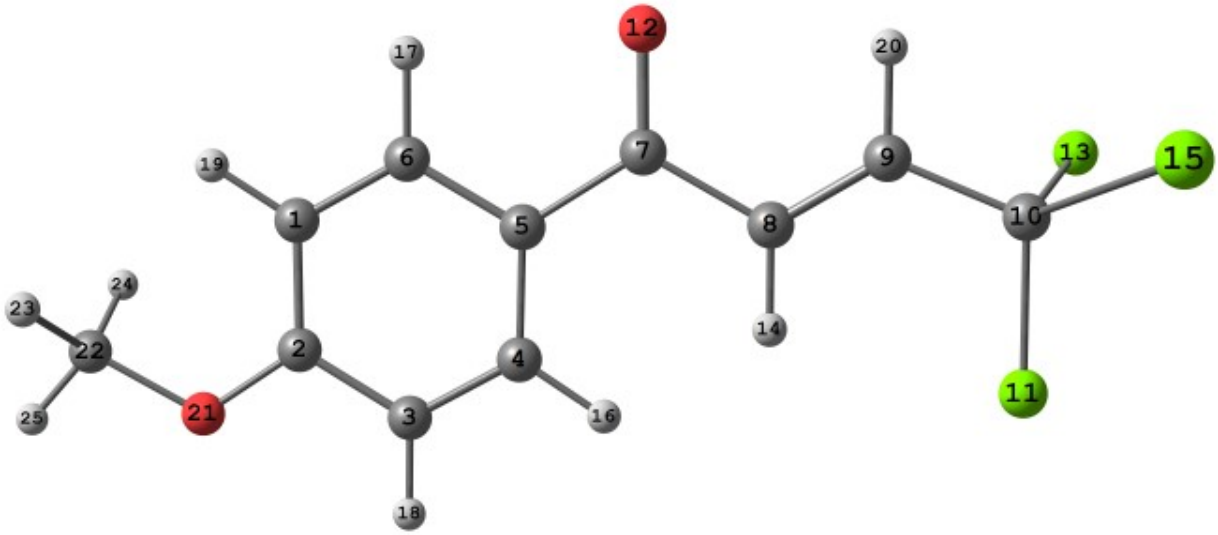
		Natural Population				
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.21134	1.99902	4.19303	0.01929	6.21134
C	2	0.10206	1.99906	3.88196	0.01693	5.89794
C	3	-0.21953	1.99893	4.20108	0.01951	6.21953
C	4	0.09929	1.99901	3.88612	0.01558	5.90071
C	5	-0.17537	1.99885	4.15529	0.02123	6.17537
C	6	-0.08843	1.99909	4.07117	0.01818	6.08843
C	7	0.57142	1.99896	3.40444	0.02518	5.42858
C	8	-0.26683	1.99891	4.24639	0.02154	6.26683
C	9	-0.13512	1.99881	4.10955	0.02676	6.13512
C	10	-0.18080	1.99905	4.11676	0.06499	6.18080
Cl	11	0.06049	9.99951	6.92093	0.01907	16.93951
O	12	-0.58898	1.99970	6.56572	0.02355	8.58898
Cl	13	0.06797	9.99948	6.91258	0.01996	16.93203
Cl	14	0.06175	9.99951	6.91983	0.01890	16.93825
H	15	0.23650	0.00000	0.76142	0.00207	0.76350
H	16	0.22545	0.00000	0.77243	0.00212	0.77455
H	17	0.22981	0.00000	0.76841	0.00178	0.77019
H	18	0.26589	0.00000	0.73153	0.00258	0.73411
H	19	0.52538	0.00000	0.47171	0.00292	0.47462
H	20	0.25034	0.00000	0.74687	0.00279	0.74966
C	21	-0.60895	1.99926	4.59578	0.01390	6.60895
H	22	0.22995	0.00000	0.76852	0.00153	0.77005
H	23	0.23372	0.00000	0.76474	0.00153	0.76628
H	24	0.23006	0.00000	0.76823	0.00171	0.76994
C	25	-0.60726	1.99927	4.59564	0.01235	6.60726
H	26	0.23750	0.00000	0.76101	0.00149	0.76250
H	27	0.22042	0.00000	0.77810	0.00148	0.77958
H	28	0.23459	0.00000	0.76390	0.00151	0.76541
* Total *		1.00000	55.98641	85.63315	0.38044	142.00000

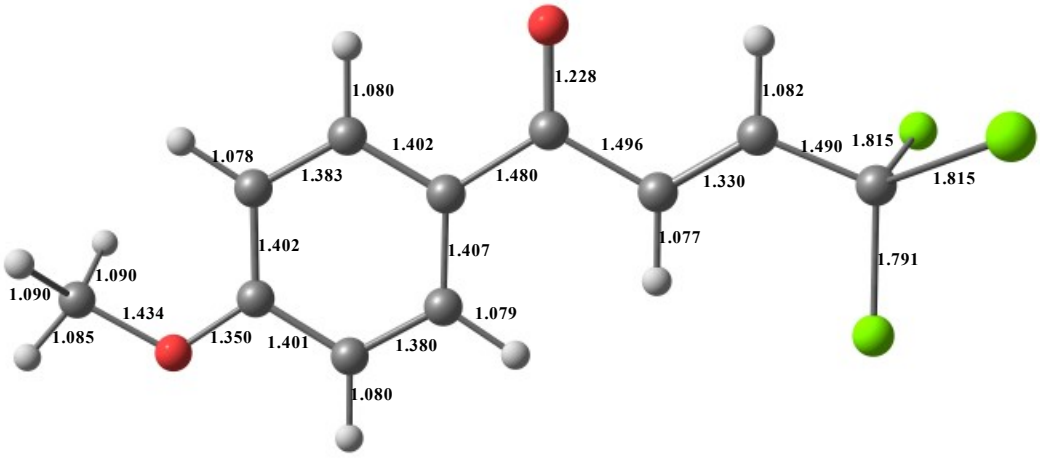
2o

Energy E(B3LYP) = -1955.85996284 h, G^{298} = -1955.731756 h, μ=6.50 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.164704	-0.912959	-0.000344
2	C	-4.407812	0.467467	-0.000013
3	C	-3.328257	1.360491	0.000465
4	C	-2.032194	0.885383	0.000621
5	C	-1.766898	-0.496085	0.000348
6	C	-2.860408	-1.373570	-0.000138
7	C	-0.404895	-1.074474	0.000594
8	C	0.773209	-0.152248	0.000519
9	C	2.005628	-0.651458	0.000359
10	C	3.276176	0.127152	-0.000027
11	Cl	3.059656	1.904817	0.000986
12	O	-0.228151	-2.289972	0.000759
13	Cl	4.236168	-0.338024	1.468092
14	H	0.617133	0.913080	0.000583
15	Cl	4.234193	-0.336592	-1.470004
16	H	-1.230669	1.607314	0.001001
17	H	-2.670144	-2.436528	-0.000372
18	H	-3.529231	2.422025	0.000709
19	H	-4.978627	-1.620099	-0.000757
20	H	2.152704	-1.723549	0.000375
21	O	-5.637091	1.026123	-0.000141
22	C	-6.787838	0.171215	-0.000529
23	H	-6.808405	-0.453077	-0.893558
24	H	-6.808549	-0.453692	0.892064
25	H	-7.644603	0.836412	-0.000366





Summary of Natural Population Analysis:

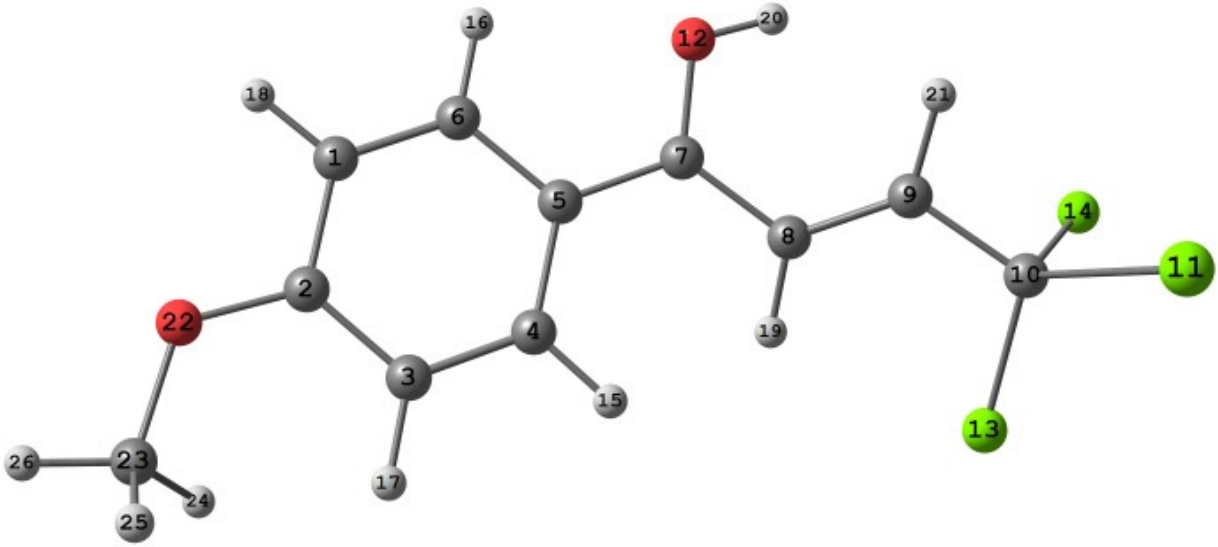
Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
C	1	-0.28577	1.99904	4.26894	0.01779	6.28577
C	2	0.36682	1.99882	3.61236	0.02201	5.63318
C	3	-0.25168	1.99906	4.23180	0.02082	6.25168
C	4	-0.14403	1.99910	4.12807	0.01687	6.14403
C	5	-0.19054	1.99894	4.17055	0.02106	6.19054
C	6	-0.12464	1.99909	4.10555	0.02000	6.12464
C	7	0.53966	1.99899	3.42613	0.03522	5.46034
C	8	-0.23433	1.99881	4.21428	0.02125	6.23433
C	9	-0.19296	1.99882	4.16480	0.02935	6.19296
C	10	-0.15933	1.99902	4.09721	0.06310	6.15933
Cl	11	0.04699	9.99948	6.93350	0.02002	16.95301
O	12	-0.62473	1.99977	6.60047	0.02449	8.62473
Cl	13	0.03184	9.99952	6.94981	0.01884	16.96816
H	14	0.22387	0.00000	0.77361	0.00252	0.77613
Cl	15	0.03178	9.99952	6.94988	0.01883	16.96822
H	16	0.21659	0.00000	0.78161	0.00180	0.78341
H	17	0.22898	0.00000	0.76866	0.00236	0.77102
H	18	0.22788	0.00000	0.76998	0.00214	0.77212
H	19	0.22865	0.00000	0.76921	0.00213	0.77135
H	20	0.24874	0.00000	0.74791	0.00334	0.75126
O	21	-0.53917	1.99970	6.51428	0.02518	8.53917
C	22	-0.20978	1.99923	4.19713	0.01342	6.20978
H	23	0.18291	0.00000	0.81492	0.00217	0.81709
H	24	0.18291	0.00000	0.81492	0.00217	0.81709
H	25	0.19937	0.00000	0.79939	0.00124	0.80063
* Total *		0.00003	55.98689	85.60495	0.40812	141.99997

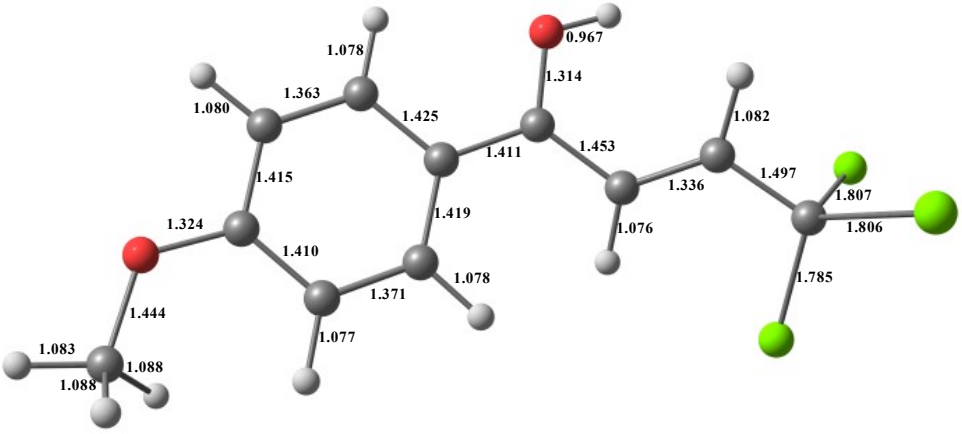
Bo

Energy E(B3LYP) = -1956.27568178 h, G^{298} = -1956.133538 h, μ=3.64 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.091334	1.307526	0.059374
2	C	-4.402335	-0.073015	0.028754
3	C	-3.369178	-1.029613	-0.041795
4	C	-2.063621	-0.611637	-0.082430
5	C	-1.730521	0.767460	-0.053321
6	C	-2.791300	1.716464	0.019812
7	C	-0.389559	1.207264	-0.072488
8	C	0.741450	0.305726	-0.207495
9	C	1.986116	0.634987	0.148454
10	C	3.185517	-0.252693	0.028897
11	Cl	3.880746	-0.465692	1.682043
12	O	-0.198139	2.502296	0.045191
13	Cl	2.845832	-1.858010	-0.674226
14	Cl	4.390331	0.604431	-1.009958
15	H	-1.292490	-1.363834	-0.126955
16	H	-2.560936	2.769847	0.038647
17	H	-3.591191	-2.083600	-0.063767
18	H	-4.902846	2.017790	0.109883
19	H	0.540963	-0.677009	-0.597868
20	H	0.720667	2.768538	-0.098619
21	H	2.232865	1.590745	0.592124
22	O	-5.692408	-0.368967	0.067846
23	C	-6.121138	-1.747302	0.036840
24	H	-5.800200	-2.221058	-0.888227
25	H	-5.731581	-2.283443	0.899374
26	H	-7.202909	-1.707995	0.079887





Summary of Natural Population Analysis:

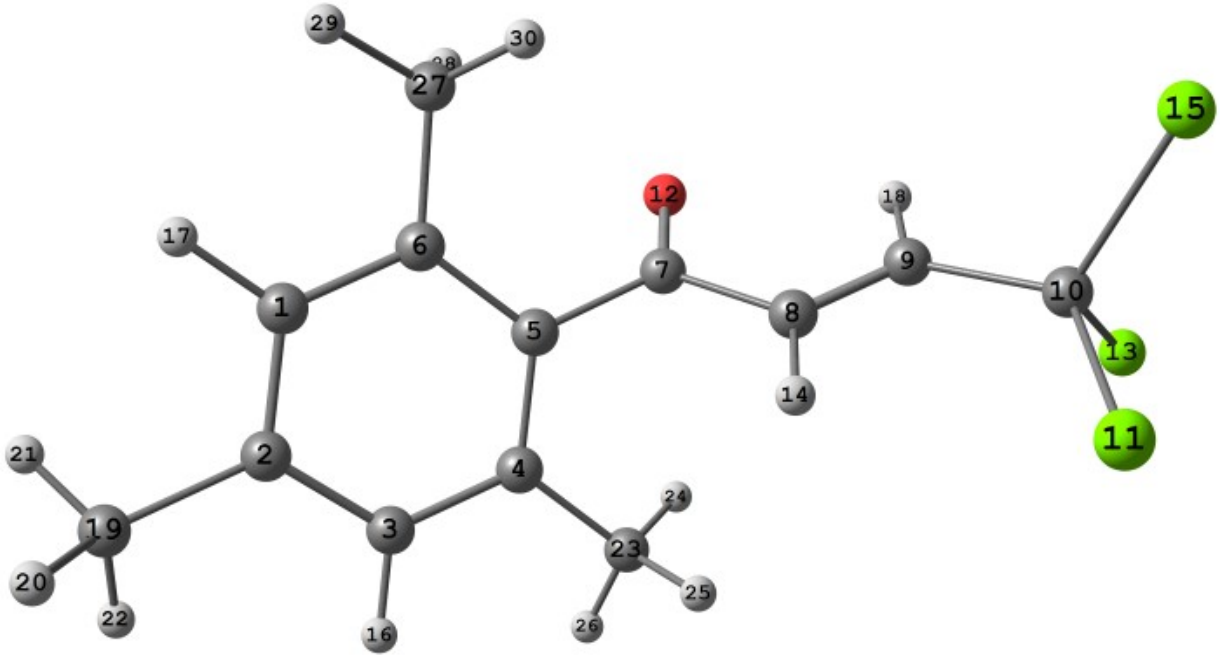
		Natural Population				
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.23160	1.99905	4.21215	0.02039	6.23160
C	2	0.44024	1.99890	3.53864	0.02222	5.55976
C	3	-0.28136	1.99905	4.26423	0.01809	6.28136
C	4	-0.07482	1.99911	4.05892	0.01679	6.07482
C	5	-0.17337	1.99893	4.15561	0.01883	6.17337
C	6	-0.09667	1.99909	4.07897	0.01861	6.09667
C	7	0.54025	1.99892	3.43581	0.02502	5.45975
C	8	-0.25591	1.99891	4.23645	0.02056	6.25591
C	9	-0.13520	1.99882	4.10977	0.02661	6.13520
C	10	-0.17861	1.99906	4.11450	0.06505	6.17861
Cl	11	0.05773	9.99951	6.92375	0.01901	16.94227
O	12	-0.60104	1.99970	6.57782	0.02352	8.60104
Cl	13	0.06645	9.99948	6.91407	0.02000	16.93355
Cl	14	0.05865	9.99951	6.92291	0.01893	16.94135
H	15	0.23047	0.00000	0.76770	0.00183	0.76953
H	16	0.24076	0.00000	0.75721	0.00203	0.75924
H	17	0.24308	0.00000	0.75491	0.00201	0.75692
H	18	0.24168	0.00000	0.75626	0.00206	0.75832
H	19	0.25505	0.00000	0.74241	0.00254	0.74495
H	20	0.52147	0.00000	0.47566	0.00287	0.47853
H	21	0.24167	0.00000	0.75537	0.00296	0.75833
O	22	-0.49228	1.99968	6.46762	0.02498	8.49228
C	23	-0.21348	1.99921	4.20158	0.01269	6.21348
H	24	0.19436	0.00000	0.80377	0.00187	0.80564
H	25	0.19428	0.00000	0.80384	0.00187	0.80572
H	26	0.20818	0.00000	0.79066	0.00116	0.79182
==========						
* Total *		1.00000	55.98693	85.62058	0.39249	142.00000

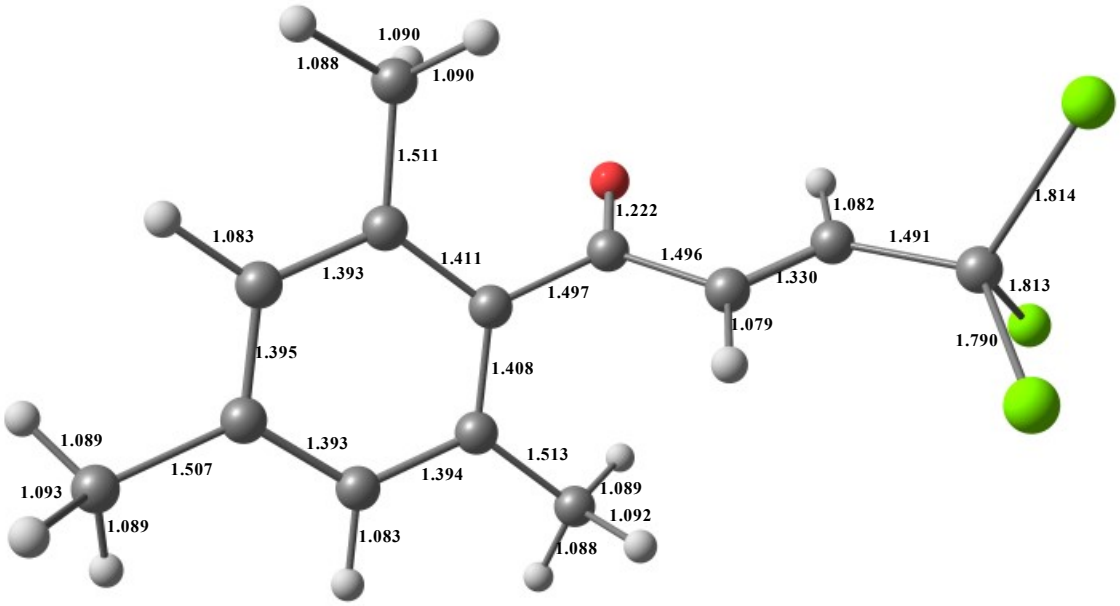
2p

Energy E(B3LYP) = -1959.27344965 h, G^{298} = -1959.099317 h, μ=4.38 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	4.139777	0.834292	-0.471121
2	C	4.533935	-0.501216	-0.393907
3	C	3.616230	-1.429316	0.092625
4	C	2.324510	-1.064461	0.468883
5	C	1.953154	0.291335	0.382894
6	C	2.873165	1.257316	-0.075884
7	C	0.586608	0.734407	0.803312
8	C	-0.584096	0.095243	0.125786
9	C	-1.825313	0.443989	0.451129
10	C	-3.080740	-0.071443	-0.165756
11	Cl	-2.828468	-1.286957	-1.455808
12	O	0.425963	1.620400	1.629083
13	Cl	-4.097232	-0.814499	1.139250
14	H	-0.388057	-0.624849	-0.653007
15	Cl	-3.992280	1.333064	-0.863843
16	H	3.913056	-2.466218	0.189430
17	H	4.840625	1.570647	-0.844414
18	H	-1.993813	1.173576	1.232773
19	C	5.907709	-0.929209	-0.841446
20	H	5.917836	-1.132209	-1.914963
21	H	6.646989	-0.151874	-0.651492
22	H	6.224495	-1.839176	-0.333923
23	C	1.395530	-2.134288	0.998997
24	H	0.789185	-1.784216	1.833086
25	H	0.714216	-2.496015	0.226530
26	H	1.970705	-2.991113	1.344829
27	C	2.530728	2.725567	-0.175189
28	H	2.528485	3.198099	0.806958
29	H	3.262496	3.239830	-0.795174
30	H	1.544568	2.889683	-0.608424





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.21983	1.99894	4.20220	0.01869	6.21983
C	2	0.00467	1.99903	3.97938	0.01692	5.99533
C	3	-0.21895	1.99894	4.20129	0.01872	6.21895
C	4	0.00915	1.99898	3.97598	0.01589	5.99085
C	5	-0.15531	1.99867	4.13242	0.02422	6.15531
C	6	0.01964	1.99898	3.96461	0.01678	5.98036
C	7	0.55800	1.99919	3.40671	0.03610	5.44200

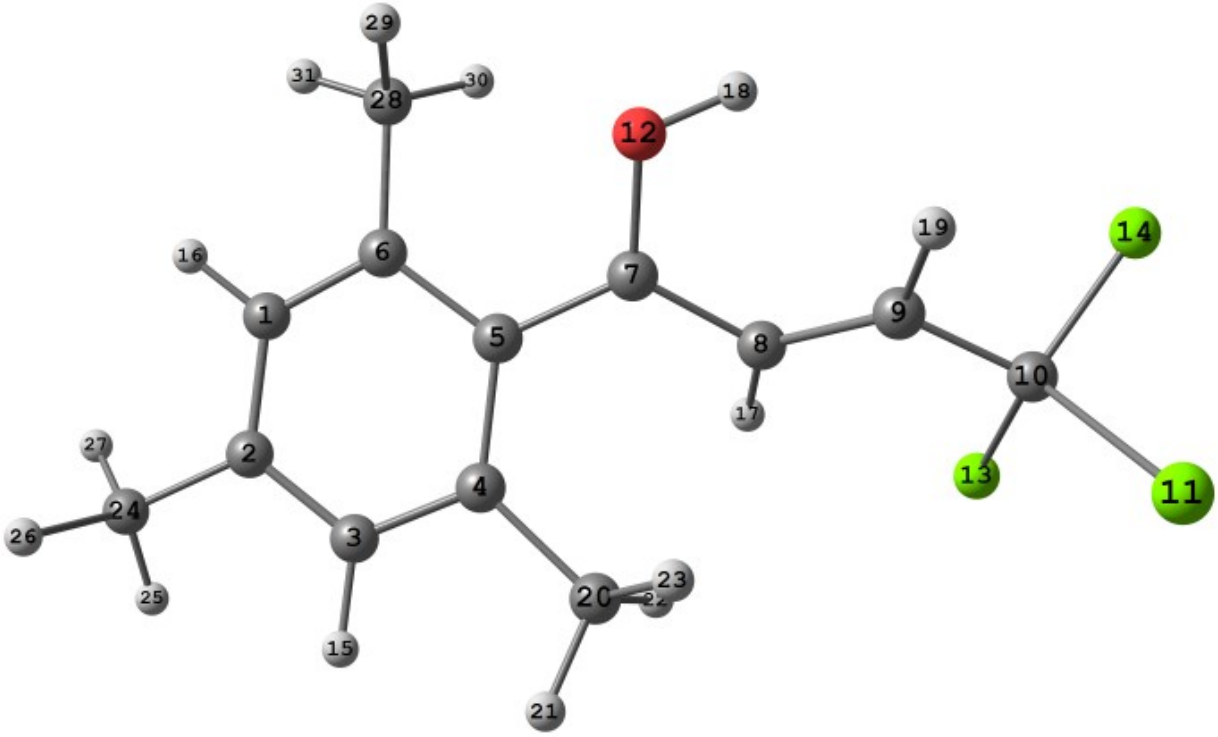
C	8	-0.25078	1.99890	4.23010	0.02179	6.25078
C	9	-0.17756	1.99880	4.15122	0.02754	6.17756
C	10	-0.16126	1.99902	4.09940	0.06284	6.16126
Cl	11	0.04900	9.99948	6.93162	0.01990	16.95100
O	12	-0.58799	1.99976	6.56325	0.02499	8.58799
Cl	13	0.03512	9.99952	6.94663	0.01873	16.96488
H	14	0.23238	0.00000	0.76532	0.00229	0.76762
Cl	15	0.03451	9.99952	6.94727	0.01870	16.96549
H	16	0.21014	0.00000	0.78782	0.00204	0.78986
H	17	0.20985	0.00000	0.78814	0.00201	0.79015
H	18	0.24829	0.00000	0.74848	0.00323	0.75171
C	19	-0.59227	1.99929	4.58122	0.01176	6.59227
H	20	0.21932	0.00000	0.77912	0.00156	0.78068
H	21	0.21326	0.00000	0.78521	0.00153	0.78674
H	22	0.21234	0.00000	0.78615	0.00151	0.78766
C	23	-0.59917	1.99928	4.58811	0.01178	6.59917
H	24	0.21515	0.00000	0.78339	0.00146	0.78485
H	25	0.21954	0.00000	0.77867	0.00179	0.78046
H	26	0.21907	0.00000	0.77942	0.00151	0.78093
C	27	-0.59193	1.99928	4.58070	0.01195	6.59193
H	28	0.22257	0.00000	0.77564	0.00178	0.77743
H	29	0.20932	0.00000	0.78914	0.00154	0.79068
H	30	0.21374	0.00000	0.78461	0.00165	0.78626
* Total *		0.00000	57.98558	91.61321	0.40121	150.00000

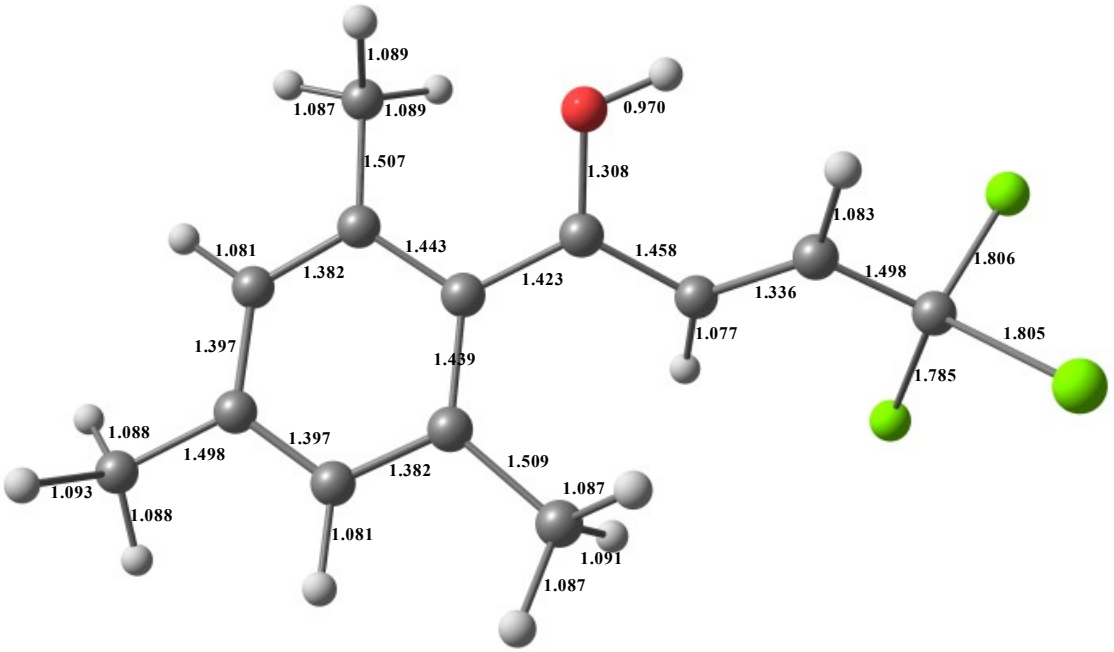
Bp

Energy E(B3LYP) = -1959.68345906 h, G^{298} = -1959.493602 h, μ=7.24 D

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-4.315293	0.642028	-0.177385
2	C	-4.507752	-0.740152	-0.120441
3	C	-3.394514	-1.560500	0.074504
4	C	-2.112273	-1.057810	0.188179
5	C	-1.924595	0.367948	0.124158
6	C	-3.071382	1.229059	-0.038420
7	C	-0.618925	0.927201	0.211432
8	C	0.604881	0.247835	-0.196645
9	C	1.790439	0.515008	0.357540
10	C	3.096404	-0.097078	-0.045420
11	Cl	3.750891	-0.988161	1.381756
12	O	-0.520123	2.159054	0.640634
13	Cl	2.986722	-1.211145	-1.435232
14	Cl	4.216816	1.257877	-0.459799
15	H	-3.539827	-2.629195	0.149961
16	H	-5.171845	1.280931	-0.341040
17	H	0.519670	-0.479267	-0.986434
18	H	0.362912	2.535288	0.503672
19	H	1.893326	1.187141	1.200201
20	C	-1.014696	-2.059066	0.450578
21	H	-1.454904	-2.984353	0.814031
22	H	-0.469408	-2.306346	-0.461511
23	H	-0.295470	-1.718715	1.190995
24	C	-5.881566	-1.326790	-0.229468
25	H	-5.854037	-2.331741	-0.646218
26	H	-6.330354	-1.397125	0.765140
27	H	-6.533620	-0.702601	-0.837361
28	C	-3.013369	2.731467	-0.141145
29	H	-2.798106	3.187726	0.824122
30	H	-2.243484	3.070329	-0.832160
31	H	-3.973311	3.104883	-0.487621





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.29266	1.99891	4.20915	0.08460	6.29266
C	2	-0.30116	1.99907	4.09469	0.20740	6.30116
C	3	0.13375	1.99886	2.70298	1.16441	5.86625
C	4	-0.43334	1.99905	4.13039	0.30390	6.43334
C	5	-0.19069	1.99870	4.15158	0.04041	6.19069

C	6	0.04571	1.99901	3.88578	0.06951	5.95429
C	7	0.54667	1.99895	3.40840	0.04599	5.45333
C	8	-0.27441	1.99883	4.24185	0.03373	6.27441
C	9	-0.13987	1.99867	4.11120	0.03000	6.13987
C	10	-0.18686	1.99906	4.11750	0.07030	6.18686
Cl	11	0.05569	9.99951	6.92171	0.02309	16.94431
O	12	-0.58407	1.99970	6.55754	0.02683	8.58407
Cl	13	0.06643	9.99948	6.91272	0.02137	16.93357
Cl	14	0.05734	9.99951	6.92091	0.02224	16.94266
H	15	0.01103	0.00000	0.86093	0.12804	0.98897
H	16	0.22239	0.00000	0.77531	0.00231	0.77761
H	17	0.26280	0.00000	0.73397	0.00323	0.73720
H	18	0.52381	0.00000	0.47260	0.00359	0.47619
H	19	0.25353	0.00000	0.74420	0.00227	0.74647
C	20	-0.62566	1.99925	4.59591	0.03050	6.62566
H	21	0.22277	0.00000	0.76799	0.00924	0.77723
H	22	0.22477	0.00000	0.76757	0.00766	0.77523
H	23	0.22355	0.00000	0.77173	0.00473	0.77645
C	24	-0.62407	1.99926	4.59560	0.02920	6.62407
H	25	0.22021	0.00000	0.77277	0.00702	0.77979
H	26	0.23356	0.00000	0.75846	0.00799	0.76644
H	27	0.22106	0.00000	0.77413	0.00481	0.77894
C	28	-0.60891	1.99926	4.58419	0.02546	6.60891
H	29	0.23246	0.00000	0.76344	0.00410	0.76754
H	30	0.22909	0.00000	0.76938	0.00153	0.77091
H	31	0.21512	0.00000	0.78262	0.00226	0.78488
* Total *		-0.05999	57.98509	90.65720	2.41770	151.05999