Optical and Electronic Properties of Air-Stable Organoboron Compounds with Strongly Electron-Accepting Bis(fluoromesityl)boryl Groups

Electronic Supporting Information

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Contents

Experimental Section

General Information. FMesH (1,3,5-tris(trifluoromethyl)benzene),[1] $(FMes)_2BF$,[2] $[(FMes)Li•Et_2O]_2$,[3] dibromo(4-*tert*-butylphenyl)borane[4] and compound **4**[5] were prepared according to known methods, whereas 4-(dibromoboryl)-*N*,*N*-diphenylaniline was obtained from the reaction of boron tribromide and 4-(trimethylsilyl)-*N*,*N*-diphenylaniline. ***Caution:*** *though safety issues were not found in making* $[(FMes)Li•Et_2O]_2$*, appropriate precautions should be taken as trifluoromethylphenyl Grignard reagents are known to be explosive.*[6] All other starting materials were purchased from commercial sources and used without further purification. Inhibitor-free anhydrous 2-MeTHF was bought from Sigma Aldrich. All other solvents for synthetic reactions and for photophysical and electrochemical measurements were HPLC grade, further treated to remove trace water using an Innovative Technology Inc. Pure-Solv Solvent Purification System and deoxygenated using the freeze-pump-thaw method. All synthetic reactions were performed in an Innovative Technology Inc. glovebox or under an argon atmosphere using standard Schlenk techniques. ^1H, $^{13}C\{^1H\}$ and ^{11}B NMR spectra were measured on a Bruker Avance 500 MHz (^1H, 500 MHz; ^{13}C, 125 MHz; ^{11}B, 160 MHz) or Bruker Avance III 400 MHz (^1H, 400 MHz; ^{13}C, 101 MHz; ^{11}B, 128 MHz) NMR spectrometer. ^{19}F and $^{19}F\{^1H\}$ NMR spectra were measured on a Bruker Avance 200 MHz (^{19}F, 188 MHz) or a Bruker Avance III 400 MHz (^{19}F, 377 MHz) spectrometer. The $^{19}F\{^1H\}$NMR spectra depicted in Figure 2 were processed without exponential line broadening. Mass spectra were recorded on Agilent 7890A/5975C Inert GC/MSD or Varian 320MS-GC/MS systems operating in the EI mode. Elemental analyses were performed on a Leco CHNS-932 Elemental Analyser.

Single-Crystal X-ray Diffraction. Crystals suitable for single-crystal X-ray diffraction were selected, coated in perfluoropolyether oil, and mounted on MiTeGen sample holders. Diffraction data of **1** were collected on a Siemens SMART three-circle diffractometer using graphite monochromated Mo Kα radiation (λ = 0.71073 Å) from an sealed X-ray tube operated at 60 kV and 50 mA, equipped with an Apex II area detector. Diffraction data of $[(FMes)Li•Et_2O]_2$, **2** and **3** were collected on a Bruker D8 Quest three-circle diffractometer utilising mirror-monochromated Mo Kα radiation (λ = 0.71073 Å) from an IμS microfocus sealed X-ray tube (Incoatec, Germany) operated at 50 kV and 1 mA,

equipped with a PHOTON area detector. Both instruments were attached with open-flow N_2 Cryoflex II (Bruker) devices and measurements were performed at 150 K (**1**) or 100 K (([(FMes)Li•Et_2O]$_2$, **2** and **3**). For data reduction, either the Bruker SAINT (**1**) or Apex II ([(FMes)Li•Et_2O]$_2$, **2** and **3**) software suite (Bruker AXS) was used. Subsequently, the structure of **1** was solved by direct methods using XS and refined by full-matrix least-squares on F^2 using XL, as implemented in the SHELXTL suite of programs. The structures of [(FMes)Li•Et_2O]$_2$, **2** and **3** were solved using the Olex2.solve charge-flipping algorithm, and were subsequently refined with Olex2.refine using Gauss-Newton minimisation, as implemented in Olex2.[7] All non-hydrogen atom positions were located from the Fourier maps and refined anisotropically. Hydrogen atom positions were calculated using a riding model in geometric positions and refined isotropically.

General Photophysical Measurements. All measurements were made in standard quartz cuvettes (1 cm x 1 cm cross-section). UV–visible absorption spectra were recorded using an Agilent 8453 diode array UV-visible spectrophotometer. The extinction coefficient of **4** (42 000 M^{-1} cm^{-1} in hexane) was measured twice due to a discrepancy with a literature value (23,000 M^{-1} cm^{-1} in CH_2Cl_2);[8] however, both of our measurements proved to be consistent, and thus the difference is ascribed to a solvent effect. The emission and excitation spectra were recorded using an Edinburgh Instruments FLSP920 spectrometer equipped with a double monochromator for both excitation and emission, operating in right-angle geometry mode. All spectra were fully corrected for the spectral response of the instrument. Unless specially mentioned, the longest-wavelength absorption maximum of the compound in the respective solvent was chosen as the excitation wavelength for the solution-state emission spectra, while the longest-wavelength absorption maximum in hexane was selected for solid-state (powder) emission. All solutions used in photophysical measurements had a concentration lower than 6×10^{-6} M to minimise inner filter effects during photoluminescence measurements.

Variable-Temperature Photoluminescence Spectroscopy. Variable temperature (77–298 K) measurements were performed using an Oxford Instruments Optistat DN N_2 cryostat controlled by an Oxford Instruments Mercury iTC temperature controller. Samples were allowed to equilibrate at each set tempera-ture before measurements were conducted. Both toluene (T_m =178 K, T_g = 117 K) and 2-MeTHF (T_m = 137 K, T_g = 91–95 K) were used as solvents to assess the effect of polarity and because of the different temperatures at which they become rigid. 2-MeTHF solutions were observed to form

clear glasses below T_g if the sample had been cooled quickly to 125 K from 150 K to avoid crystallisation, whereas toluene solutions froze upon cooling below the melting point, irrespective of thermal history.

Time-gated emission spectra of **2** at 77 K were recorded using an Ocean Optics Maya-2000 back-thinned CCD array spectrometer coupled with a 600 μm fibre-optic cable. Spectra were recorded continuously with a 200 ms integration time, allowing the spectral evolution upon closing or opening the shutter to the excitation source to be monitored in real time. Due to the large difference in lifetime of the fluorescence and the phosphorescence (a factor of *ca*. 5 x 10^8), it was possible to record the fluorescence as the first observed spectrum after the shutter to the excitation source was opened, *i.e.* before the phosphorescence signal could be detected, while the phosphorescence spectrum was recorded by first observing the complete decay of the fluorescence signal after closing the shutter before starting the measurement. Estimation of the relative contributions of the short- and long-lived components of **2** was achieved by first scaling the fluorescence spectrum to the normalised non-gated emission spectrum at 400 nm (chosen because there is no spectral overlap of the two components at this wavelength) and calculating the area ratio of the fluorescence and non-gated emission spectra. Spectra were background corrected for the dark noise and spectral sensitivity of the spectrometer.

Fluorescence Quantum Yield Measurements. The fluorescence quantum yields of solutions and powders were measured using a calibrated integrating sphere (inner diameter: 150 mm) from Edinburgh Instruments combined with the FLSP920 spectrometer described above. For solution-state measurements, the longest-wavelength absorption maximum of the compound in the respective solvent was chosen as the excitation wavelength, while for solid-state (powder) measurements, the longest-wavelength absorption maximum in hexane was selected.

Lifetime Measurements. Fluorescence lifetimes were recorded using the time-correlated single-photon counting (TCSPC) method using an Edinburgh Instruments FLS980 spectrometer equipped with a high speed photomultiplier tube positioned after a single emission monochromator. Measurements were made in right-angle geometry mode, and the emission was collected through a polariser set to the magic angle. Solutions were excited with either pulsed diode lasers at wavelengths of 473 (for **3**) or 377 nm (for **4**) or by a pulsed LED at 316 nm (for **2**) at repetition rates of 10 or

20 MHz, as appropriate. The full-width-at-half-maximum (FWHM) of the pulses from both diode lasers was *ca.* 75–90 ps with an instrument response function (IRF) of *ca.* 230 ps FWHM; the pulsed LED had a pulse width of 930 ps FWHM, giving an IRF of a similar magnitude. The IRFs were measured from the scatter from either pure solvent or from the solid sample at the excitation wavelength. Decays were recorded to at least 4 000 counts in the peak channel with a record length of at least 1 000 channels. The band pass of the monochromator was adjusted to give a signal count rate of <60 kHz. Iterative reconvolution of the IRF with one or two decay functions and non-linear least-squares analysis were used to analyze the data. The phosphorescence lifetime of **2** was measured by multi-channel scaling using the FLSP920 spectrometer described above for steady-state measurements. The excitation source was a pulsed xenon flash lamp with a pulse width of <2 μs operating at a repetition rate of 0.1 Hz. The data were analysed by tail fitting, which is appropriate here due to the vastly different timescales of the pulse and the decay in this case. The quality of all decay fits was judged to be satisfactory, based on the calculated values of the reduced χ^2 and Durbin-Watson parameters and visual inspection of the weighted residuals. We note that the lifetimes obtained for solid samples were somewhat dependent on sample preparation and experimental setup; however, the values reported are typical.

Electrochemical Measurements. All cyclic voltammetry experiments were conducted in an argon-filled glovebox using a Gamry Instruments Reference 600 potentiostat. A standard three-electrode cell configuration was employed using a platinum disk working electrode, a platinum wire counter electrode, and a silver wire reference electrode separated by a Vycor frit. Compensation for resistive losses (*IR* drop) was employed for all measurements. A 0.1 M solution of $[NBu_4][PF_6]$was used as the supporting electrolyte. A scan rate of 250 mV s^{-1} was adopted.

Theoretical Studies. All calculations (DFT and TD-DFT) were carried out with the program package Gaussian 09 (Rev. B.01 or Rev. D.01)[9] and were performed on a parallel cluster system. Gaussview 4.1.2 was used to visualise the results, to measure calculated structural parameters, and to plot orbital surfaces. The starting geometries for the calculations were those obtained by X-ray crystallography. The ground-state geometries were optimzed without symmetry contraints using the B3LYP functional[10-12] in combination with the 6-31G(d) basis set.[13] The optimised geometries were confirmed to be local minima by performing frequency calculations and obtaining only positive (real)

frequencies. Based on these optimised structures, the lowest-energy gas-phase vertical transitions were calculated (singlets, six states) by TD-DFT, using the Coulomb-attenuated functional CAM-B3LYP[14] in combination with the 6-31G(d) basis set.[15] The CAM-B3LYP functional has been shown to be effective for the ICT systems, hence its selection here.[16]

Using the optimised ground-state geometries as starting coordinates, TD-DFT geometry optimisations of the S_1 states of **2**, **3** and **4** were performed. Four states, the CAM-B3LYP, B3LYP, BLYP and BHLYP functionals, and the 6-31G(d) basis set were used. Further TD-DFT CAM-B3LYP/6-31G(d) S_1 optimisations of **3** were conducted with inclusion of THF solvation through the polarisable continuum model (PCM) and modified United-Atom Kohn-Sham (UAKS) radii ($a_0 = 0.5$) or inclusion of the D3 dispersion correction of Grimme and coworkers.[17] S_1 optimisation of **2-4** was also performed using TDA CAM-B3LYP/6-31G(d). No symmetry constraint was used in any of the calculations. Frequency calculations were performed at the S_1 optimised geometries to confirm local minima had been found. Dipole moments on the S_1 surface were determined by single point calculations using the density=current option.

Synthesis.

4-(Bis(2,4,6-tris(trifluoromethyl)phenyl)phenylborane (1). The compound $(FMes)_2BF$ (148 mg, 0.25 mmol) was dissolved in toluene (2 mL). The resulting yellow solution was cooled to –35 °C, and PhLi (150 μL, 1.8 M solution in *n*-Bu_2O) was added dropwise to the reaction mixture. The solution was allowed to warm slowly to room temperature (r.t.) over 3 h. The reaction mixture was filtered over celite, and the filtrate was concentrated in vacuum. The crude material was crystallised from pentane at –35 °C, yielding compound **1** (124 mg, 76%). ^{1}H NMR (400 MHz, CD_2Cl_2, r.t., ppm): δ 8.25 (s, 4 H), 7.60 (tt, J = 7 and 1 Hz, 1 H), 7.38 (t, J = 8 Hz, 2 H), 7.19 (dd, J = 8 Hz, J = 1 Hz, 2 H); ^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2, r.t., ppm): δ 145.5 (br), 142.7 (br), 137.2, 137.1 (br), 134.5, 133.5 (q, $^2J_{C\text{-}F}$ = 35 Hz), 128.0, 127.5 (br), 123.6 (q, $^1J_{C\text{-}F}$ = 276 Hz), 123.1 (q, $^1J_{C\text{-}F}$ = 274 Hz); ^{19}F NMR (377 MHz, CD_2Cl_2, r.t., ppm): δ –53.9 (s, br, 12F), –63.9 (s, 6F); ^{11}B NMR (128 MHz, CD_2Cl_2, r.t., ppm): δ 69.5 (br). MS (EI$^+$) *m/z*: 650 $[M]^+$. Elem. Anal. Calcd (%) for $C_{24}H_9BF_{18}$: C 44.34; H 1.40. Found: C 44.31; H 1.81.

(4-(*tert*-Butyl)phenyl)bis(2,4,6-tris(trifluoromethyl)phenyl)borane (2). A solution of $[(FMes)Li•Et_2O]_2$ (1.07 g, 1.48 mmol) in toluene (2 mL) was added to a solution of 4-*tert*-butylphenylboron dibromide (320 mg, 1.05 mmol) in toluene (3 mL) at r.t. over a period of 15 min, and then the reaction mixture was stirred for two days at the same temperature. Hexane (~10 mL) was added to the reaction mixture, and the resultant suspension was filtered. The filtrate was concentrated to dryness in vacuum, and the residue obtained was purified by column chromatography (silica gel, hexane) to afford compound **2** (110 mg, 15%). ^{1}H NMR (500 MHz, CD_2Cl_2, r.t., ppm): δ 8.24 (s, 4 H), 7.39 (d, J = 9 Hz, 2 H), 7.11 (d, J = 9 Hz, 2 H), 1.32 (s, 9 H). ^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2, r.t., ppm): δ 158.9, 143.1 (br), 143.0 (br), 137.5, 137.3 (br), 133.2 (q, $^2J_{C\text{-}F}$ = 35 Hz), 127.5 (br), 124.9, 123.6 (q, $^1J_{C\text{-}F}$ = 275 Hz), 123.1 (q, $^1J_{C\text{-}F}$ = 273 Hz), 35.6, 31.1. ^{19}F{^{1}H} NMR (188 MHz, toluene-d_8, r.t., ppm): δ –53.5 (s, br, 12 F), –63.5 (s, 6 F). ^{19}F{^{1}H} NMR (188 MHz, toluene-d_8, 223 K, ppm): δ –50.6 (s, 6 F), –55.9 (s, 6 F), –62.9 (s, 6 F). ^{11}B NMR (160 MHz, C_6D_6, r.t., ppm): δ 69.0. MS (EI$^+$) *m/z*: 706 $[M]^+$. Elem. Anal. Calcd (%) for $C_{28}H_{17}BF_{18}$: C, 47.62; H, 2.43. Found: C, 48.33; H, 2.72.

4-(Trimethylsilyl)triphenylamine. THF (1 mL) and 1,2-dibromoethane (100 μL, 1.16 mmol) were added sequentially to magnesium turnings (2.20 g, 91.7 mmol) at r.t., and the resulting mixture was stirred for 5 min. A solution of 4-bromotriphenylamine (5.00 g, 15.4 mmol) in THF (15 mL) was prepared. A portion (2 mL) of the 4-bromotriphenylamine solution was added at r.t. to the magnesium turnings, and then the mixture was heated to 55 °C before the remaining solution was added dropwise. After addition, heating was continued for a further 30 min, before the solution was cooled to r.t. and transferred to another flask. Chlorotrimethylsilane (1.68 g, 15.4 mmol) was added dropwise to the prepared Grignard reagent. The mixture was heated to 50 °C for 2 h, and then stirred at r.t. overnight. Water (~100 mL) was added, and the mixture was extracted with hexane (3 × 60 mL). The organic extracts were combined, dried over $MgSO_4$, concentrated and subjected to a short column (silica gel, hexane) to afford 4-(trimethylsilyl)triphenylamine (4.11 g, 84%). ^{1}H NMR (500 MHz, THF-d_8, r.t., ppm): δ 7.38 (d, J = 8 Hz, 2 H), 7.23–7.19 (m, 4 H), 7.06–6.96 (m, 8 H), 0.24 (s, 9 H). ^{13}C{^{1}H} NMR (125 MHz, THF-d_8, r.t., ppm): δ 149.4, 148.6, 134.9, 133.8, 129.8, 125.1, 123.5, 123.5, –1.05. MS (EI$^+$) *m/z*: 317 $[M]^+$. Elem. Anal. Calcd (%) for $C_{21}H_{23}NSi$: C, 79.44; H, 7.30; N, 4.41. Found: C, 79.56; H, 7.20; N, 4.64.

4-(Bis(2,4,6-tris(trifluoromethyl)phenyl)boryl)-*N*,*N*-diphenylaniline (3). To a solution of 4-(trimethylsilyl)triphenylamine (660 mg, 2.08 mmol) in CH_2Cl_2 (5 mL), a CH_2Cl_2 solution of BBr_3 (2 M, 1.15 mL, 2.30 mmol) was added dropwise at r.t. After addition, the mixture was stirred at r.t. for 2 h. The solvent was evaporated, and the residue was dried at 50 °C for 1 h under vacuum. The obtained 4-*N*,*N*-diphenylaminophenylboron dibromide was dissolved in toluene (3 mL) and used directly in the next step of reaction without further purification. A solution of $[(FMes)Li•Et_2O]_2$ (2.10 g, 2.90 mmol) in toluene (3 mL) was added slowly at r.t., and then the mixture was stirred for two days. Hexane (~10 mL) was added to the reaction mixture, and the resultant suspension was filtered. The filtrate was concentrated to dryness under vacuum, and the residue was purified by column chromatography (silica gel, 3:1 hexane/CH_2Cl_2) to afford compound **3** (325 mg, 19% based on 4-(trimethylsilyl)triphenylamine). ^{1}H NMR (500 MHz, CD_2Cl_2, r.t., ppm): δ 8.21 (s, 4 H), 7.36–7.32 (m, 4 H), 7.19–7.15 (m, 6 H), 6.98 (d, J = 9 Hz, 2 H), 6.83 (d, J = 9 Hz, 2 H). ^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2, r.t., ppm): δ 153.6, 146.3, 143.9 (br), 139.6, 139.4 (br), 138.3 (br), 135.0 (br), 132.8 (q, $^2J_{C\text{-}F}$ = 35 Hz), 130.1, 128.5 (br), 126.9, 126.1 (br), 125.7, 123.8 (q, br, $^1J_{C\text{-}F}$ = 273 Hz), 123.2 (q, $^1J_{C\text{-}F}$ = 273 Hz), 118.0. ^{19}F{^{1}H} NMR (188 MHz, toluene-d_8, r.t., ppm): δ –51.0 (s, br, 6 F), –56.4 (s, br, 6 F), –63.4 (s, 6 F). ^{19}F{^{1}H} NMR (188 MHz, toluene-d_8, 223 K, ppm): δ –50.5 (q, J = 12 Hz, 6 F), –56.1 (q, J = 12 Hz, 6 F), –62.8 (6 F). ^{11}B NMR (160 MHz, CD_2Cl_2, r.t., ppm): δ 64.3. MS (EI$^+$) *m/z*: 817 [M]$^+$. Elem. Anal. Calcd (%) for $C_{36}H_{18}BF_{18}N$: C, 52.90; H, 2.22; N, 1.71. Found: C, 53.12; H, 2.02; N, 1.92.

4-(Dimesitylboryl)-*N*,*N*-diphenylaniline (4). This compound was prepared according to literature procedures.[5] The pure compound was obtained as off-white crystalline powder by column chromatography (silica gel, 1:8 hexane/CH_2Cl_2) and subsequent crystallisation from Et_2O and MeOH. ^{1}H NMR (500 MHz, CD_2Cl_2, r.t., ppm): δ 7.33–7.28 (m, 6 H), 7.16–7.14 (m, 4 H), 7.12–7.09 (m, 2 H), 6.90 (d, J = 9 Hz, 2 H), 6.81 (s, 4 H), 2.28 (s, 6 H), 2.04 (s, 12 H). ^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2, r.t., ppm): δ 151.8, 147.2, 142.3 (br), 141.0, 138.9, 138.5, 138.3 (br), 129.9, 128.4, 126.3, 124.6, 120.0, 23.6, 21.3. ^{11}B NMR (160 MHz, CD_2Cl_2, r.t., ppm): δ 71.6. MS (EI$^+$) *m/z*: 493 [M]$^+$. Elem. Anal. Calcd (%) for $C_{36}H_{36}BN$: C, 87.62; H, 7.35; N, 2.84. Found: C, 87.42; H, 7.51; N, 3.02.

Single-Crystal X-ray Diffraction

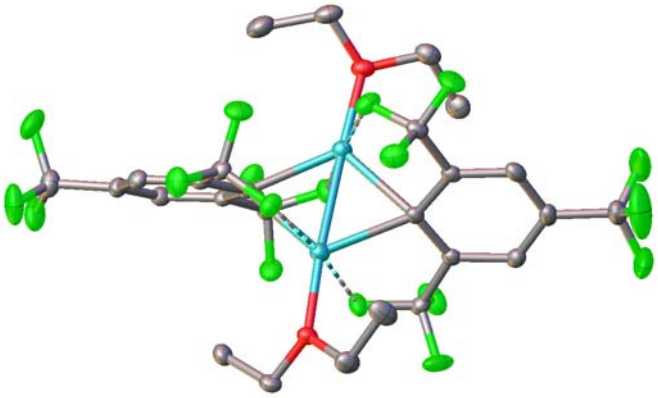

Figure S1. The molecular structure of $[(FMes)Li{\bullet}Et_2O]_2$ as determined by X-ray crystallography. Atom colour code: carbon (grey), lithium (cyan), oxygen (red), fluorine (green). Hydrogen atoms have been omitted for clarity. Short contacts between Li and F atoms are indicated by dashed lines. Atomic displacement ellipsoids are drawn at 50% probability.

Crystal Data. $C_{26}H_{24}F_{18}Li_2O_2$, $M = 724.33$, triclinic, P-1, $a = 9.0486(5)$ Å, $b = 12.7853(7)$ Å, $c = 14.6892(8)$ Å, $V = 1539.05(15)$ Å^3, $\alpha = 84.024(2)°$, $\beta = 74.906(2)°$, $\gamma = 69.739(2)°$, $T = 100$ K, $Z = 2$, μ (Mo Kα) = 0.170 mm^{-1}, 41365 reflections measured, 6046 unique ($R_{int} = 0.0270$) which were used in all calculations. The final wR_2 was 0.1391 (all data) and R_1 was 0.0495 ($I \geq 2\sigma(I)$).

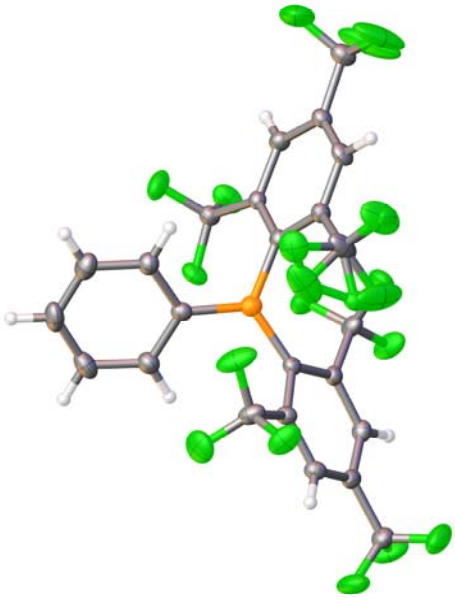

Figure S2. The molecular structure of **1** as determined by X-ray crystallography. Atom colour code: carbon (grey), boron (orange), fluorine (green), hydrogen (white). Atomic displacement ellipsoids are drawn at 50% probability.

Crystal Data. $C_{24}H_9BF_{18}$, $M = 650.12$, orthorhombic, *Pbca*, $a = 15.5600(11)$ Å, $b = 8.7136(6)$ Å, $c = 35.624(3)$ Å, $V = 4830.1(6)$ Å^3, $T = 150$ K, $Z = 8$, μ (Mo Kα) = 0.201 mm^{-1}, 67817 reflections measured, 5438 unique ($R_{int} = 0.0655$) which were used in all calculations. The final wR_2 was 0.1297 (all data) and R_1 was 0.0479 ($I \geq 2\sigma(I)$).

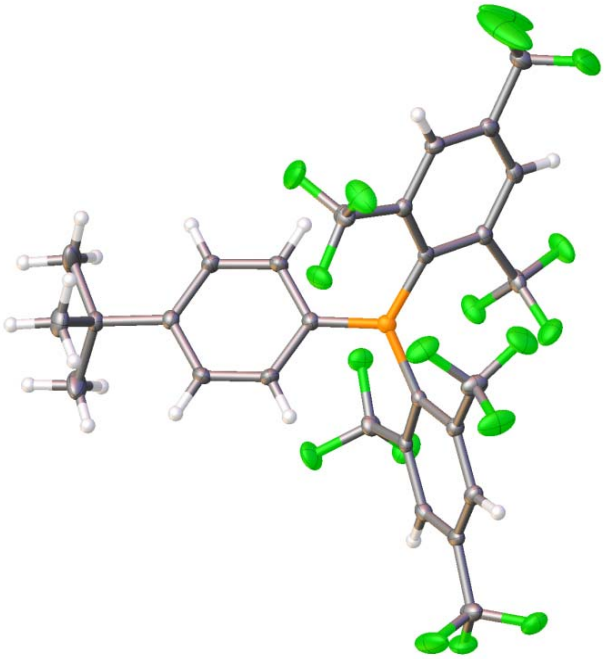

Figure S3. The molecular structure of **2** as determined by X-ray crystallography. Atom colour code: carbon (grey), boron (orange), fluorine (green), hydrogen (white). Atomic displacement ellipsoids are drawn at 50% probability.

Crystal Data. $C_{28}H_{17}BF_{18}$, $M = 706.24$, monoclinic, $P2_1/n$, $a = 9.1239(3)$ Å, $b = 24.4308(8)$ Å, $c = 12.5042(6)$ Å, $\beta = 97.114(1)°$, $V = 2765.8(2)$ Å^3, $T = 100$ K, $Z = 4$, μ(Mo Kα) = 0.183 mm^{-1}, 46204 reflections measured, 5438 unique ($R_{int} = 0.0390$) which were used in all calculations. The final wR_2 was 0.1489 (all data) and R_1 was 0.0543 ($I \geq 2\sigma(I)$).

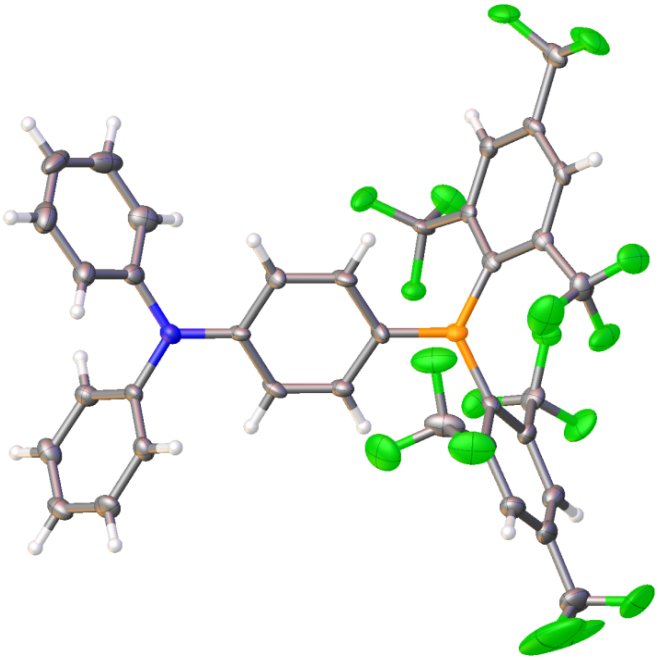

Figure S4. Molecular structure of **3** as determined by X-ray crystallography. Atom colour code: carbon (grey), boron (orange), nitrogen (blue), fluorine (green), hydrogen (white). A second non-symmetry related molecule is omitted for clarity. Atomic displacement ellipsoids are drawn at 50% probability.

Crystal Data. $C_{36}H_{18}BNF_{18}$, $M = 817.35$, tetragonal, $I4_1$, $a = 23.502(1)$ Å, $b = 23.502(1)$ Å, $c = 25.182(1)$ Å, $V = 13909(1)$ Å^3, $T = 100$ K, $Z = 16$, μ (Mo Kα) = 0.159 mm^{-1}, 46880 reflections measured, 13657 unique ($R_{int} = 0.0501$) which were used in all calculations. The final wR_2 was 0.1952 (all data) and R_1 was 0.0628 ($I \geq 2\sigma(I)$).

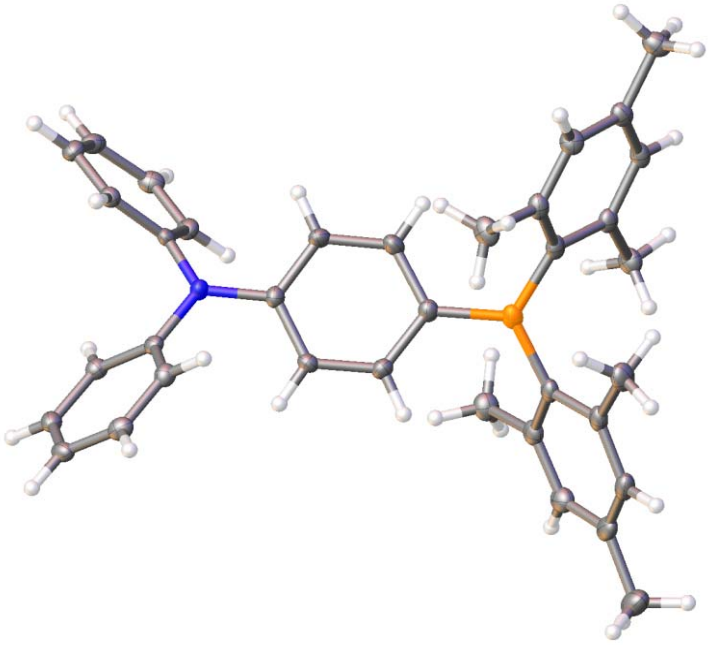

Figure S5. Molecular structure of **4** as determined by X-ray crystallography. Atom colour code: carbon (grey), boron (orange), nitrogen (blue), hydrogen (white). Atomic displacement ellipsoids are drawn at 50% probability.

Crystal Data. $C_{36}H_{36}BN$, $M = 493.52$, monoclinic, $P2_1/n$, $a = 8.8391(3)$ Å, $b = 34.027(1)$ Å, $c = 9.5807(3)$ Å, $\beta = 100.720(1)°$, $V = 2831.3(2)$ Å^3, $T = 100$ K, $Z = 4$, μ (Mo Kα) = 0.065 mm^{-1}, 31666 reflections measured, 5556 unique ($R_{int} = 0.0374$) which were used in all calculations. The final wR_2 was 0.1265 (all data) and R_1 was 0.0460 ($I \geq 2\sigma(I)$).

Variable-Temperature Photoluminescence Spectra

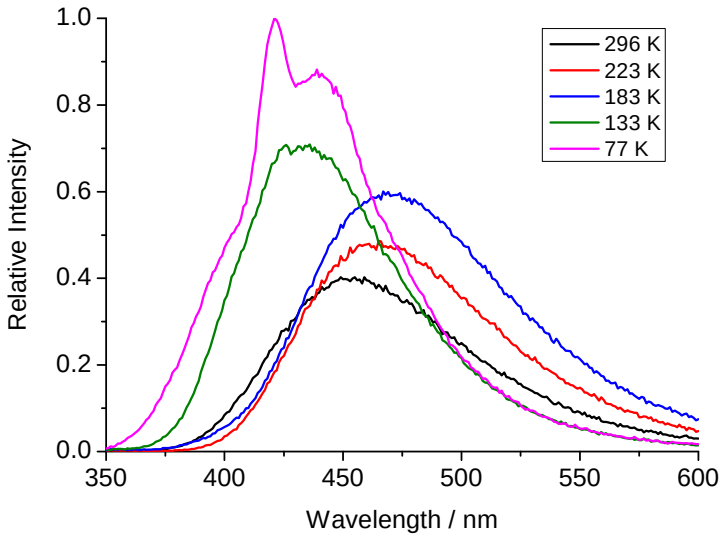

Figure S6. Variable-temperature emission spectra of **2** in toluene. Data are normalised relative to the spectrum recorded at 77 K. All spectra were recorded with identical spectrometer settings.

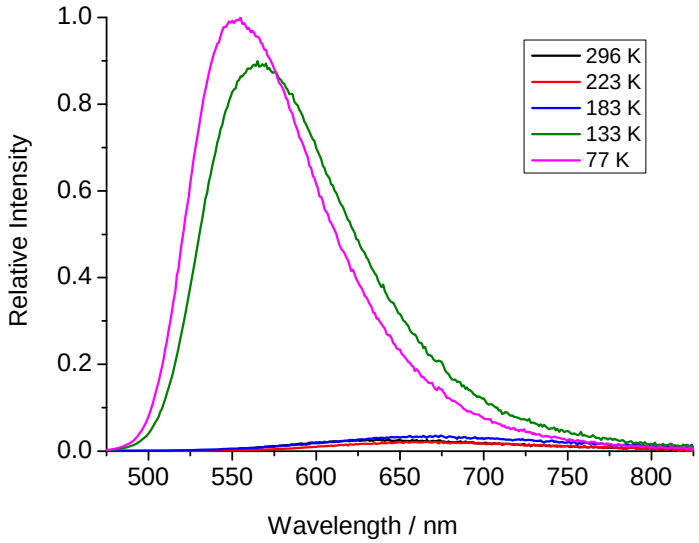

Figure S7. Variable-temperature emission spectra of **3** in toluene. Data are normalised relative to the spectrum recorded at 77 K. All spectra were recorded with identical spectrometer settings.

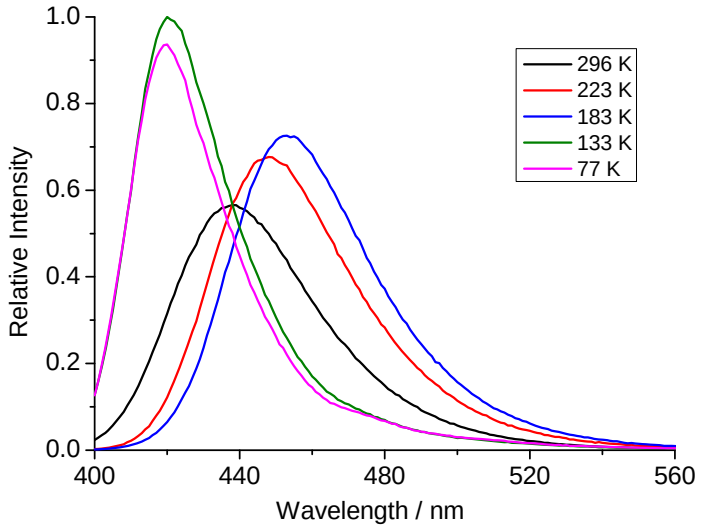

Figure S8. Variable-temperature emission spectra of **4** in toluene. Data are normalised relative to the spectrum recorded at 133 K. All spectra were recorded with identical spectrometer settings.

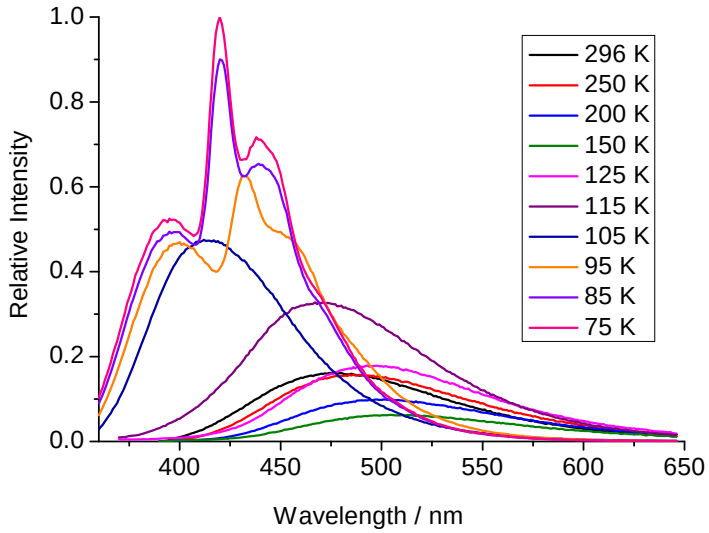

Figure S9. Variable-temperature emission spectra of **2** in 2-MeTHF. Data are normalised relative to the spectrum recorded at 77 K. All spectra were recorded with identical spectrometer settings.

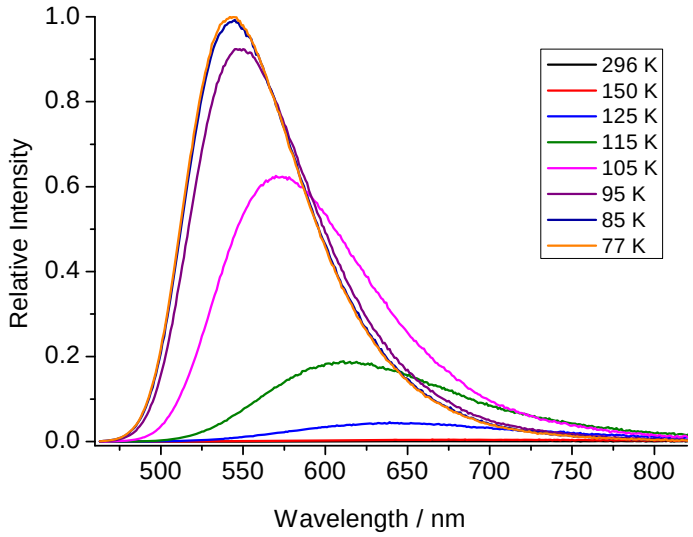

Figure S10. Variable-temperature emission spectra of **3** in 2-MeTHF. Data are normalised relative to the spectrum recorded at 77 K. All spectra were recorded with identical spectrometer settings.

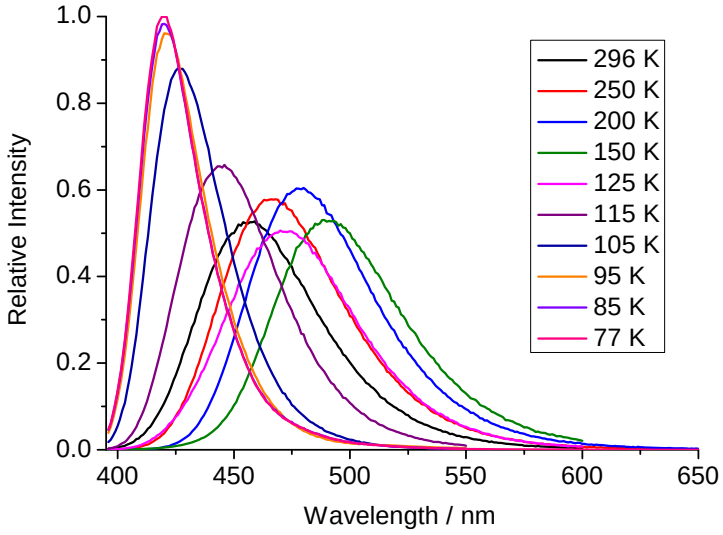

Figure S11. Variable-temperature emission spectra of **4** in 2-MeTHF. Data are normalised relative to the spectrum recorded at 77 K. All spectra were recorded with identical spectrometer settings.

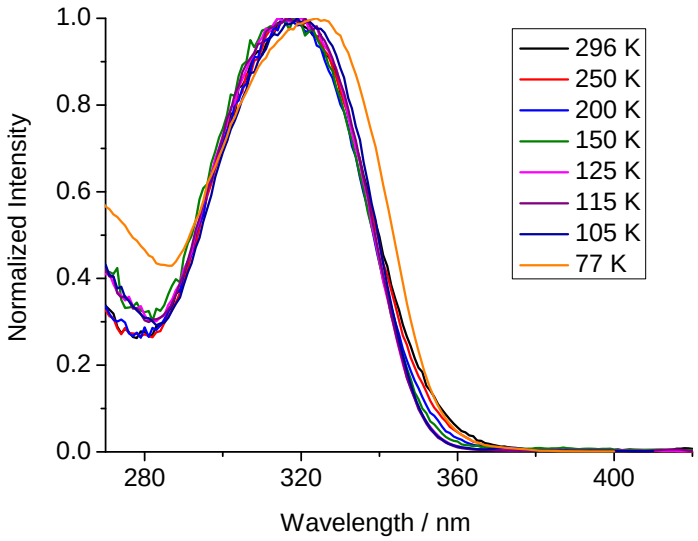

Figure S12. Variable-temperature excitation spectra of **2** in 2-MeTHF. Shift of the maximum is from 318 nm (296 K) to 324 nm (77 K), *i.e.* 6 nm (580 cm^{-1}).

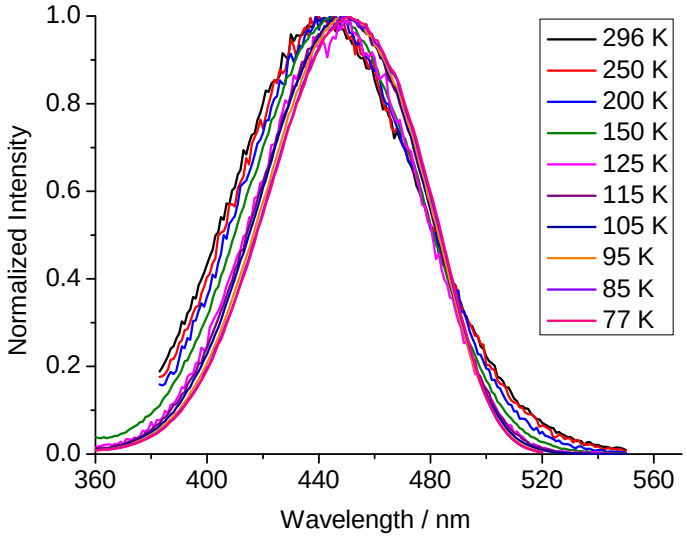

Figure S13. Variable-temperature excitation spectra of **3** in 2-MeTHF. Shift of the maximum is from 442 nm (298 K) to 450 nm (77 K), *i.e.* 8 nm (400 cm^{-1}).

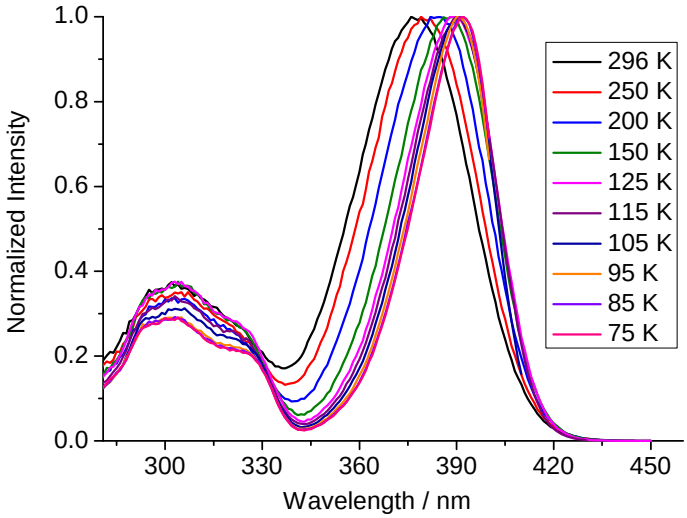

Figure S14. Variable-temperature excitation spectra of **4** in 2-MeTHF. Shift of the maximum is from 377 nm (298 K) to 392 nm (77 K), *i.e.* 15 nm (1000 cm^{-1}).

Cyclic Voltammograms

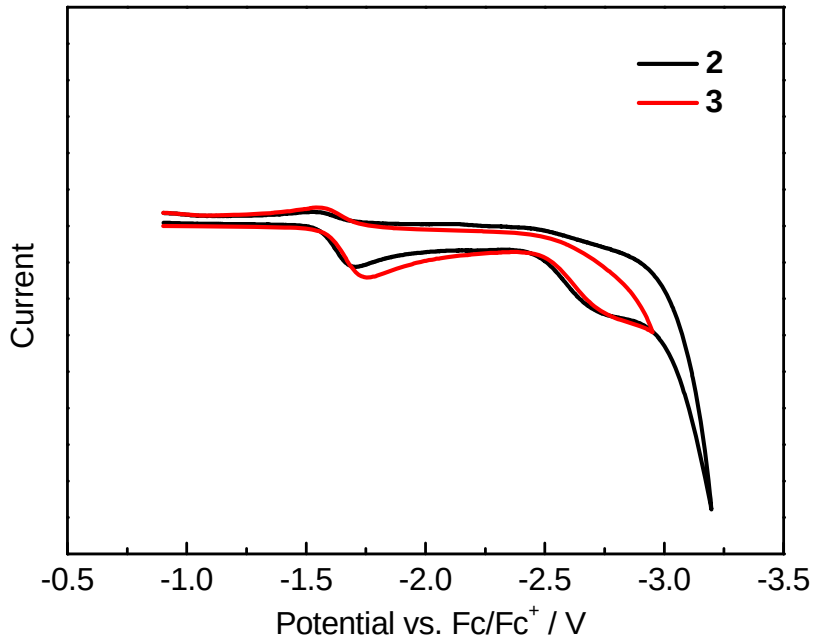

Figure S15. Cyclic voltammograms of **2** and **3** (cathodic scan) measured in THF.

DFT and TD-DFT Calculations

Further optimisations of the S_1 states of **2**–**4** using functionals with varying contributions of Hartree-Fock (HF) exchange (BLYP 0%, B3LYP 20%, BHLYP 50%) resulted in ostensibly the same geometries, with the exception of a greater twist around the C–N bond in **3** and **4** observed in the calculations using functionals with less HF exchange, namely B3LYP in the case of **3** and BLYP and B3LYP for **4** (no stable S_1 geometry of **3** could be located using the BLYP functional). In these calculations, an additional twisting of the phenyl group of the Ph-B(aryl)$_2$ moiety further out of the NC_3 plane is observed, making these groups almost orthogonal to one another. It has been found previously that excited-state optimisation using methods with less HF exchange can artificially lead to more twisted structures,[18,19] and even breakdown of the excited state surface, as observed here for the BLYP calculation of **3**, which can be corrected by the use of a long-range-corrected functional, such as CAM-B3LYP. Crucially, however, the distortion of the (FMes)$_2$B group of **2** and **3** was not substantially affected by method choice. To eliminate the possibility that additional twisting around the C–N bond in the S_1 state of **3** had been missed in the initial CAM-B3LYP/6-31G(d) TD-DFT optimisation calculations, the structures were again optimised following a perturbation of the torsion angle around this bond to a starting value of *ca*. 75°; however, a similar geometry was obtained following optimisation, discounting dual twisting. Furthermore, starting from a perturbed ground state structure, in which the amine dihedral angle was changed to *ca*. 75°, also resulted in the same geometry, and thus a structure with a single twist at the nitrogen atom can also be discounted. Moreover, further S_1 optimisation calculations performed for **3** at the same level of theory modified to include either a dielectric medium (THF solution introduced using the PCM) or dispersion interactions (D3 correction) did not generate substantially perturbed geometries from those described above.

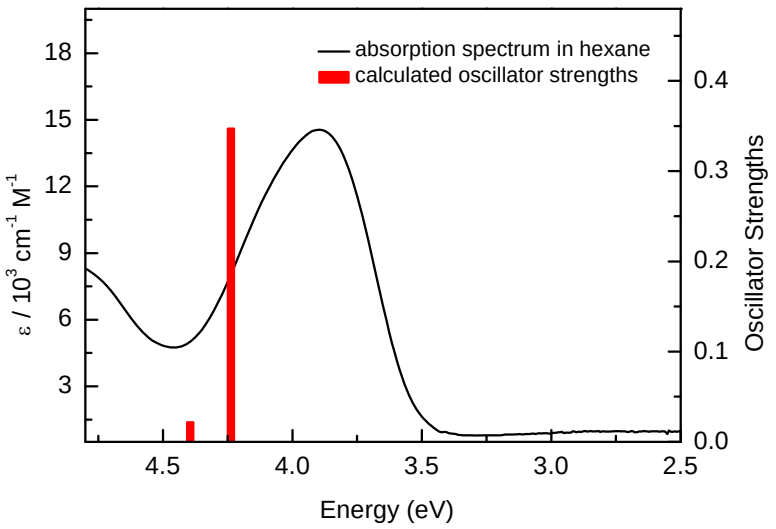

Figure S16. Comparison between the experimental UV-visible absorption spectrum and TD-DFT (CAM-B3LYP/6-31G(d)) calculated transitions of compound **2** from the optimised (B3LYP/6-31G(d)) ground state structure.

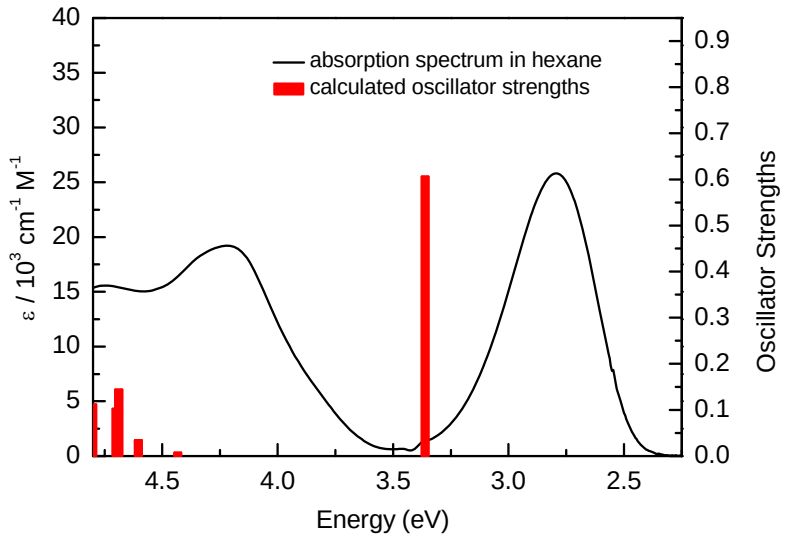

Figure S17. Comparison between the experimental UV-visible absorption spectrum and TD-DFT (CAM-B3LYP/6-31G(d)) calculated transitions of compound **3** from the optimised (B3LYP/6-31G(d)) ground state structure.

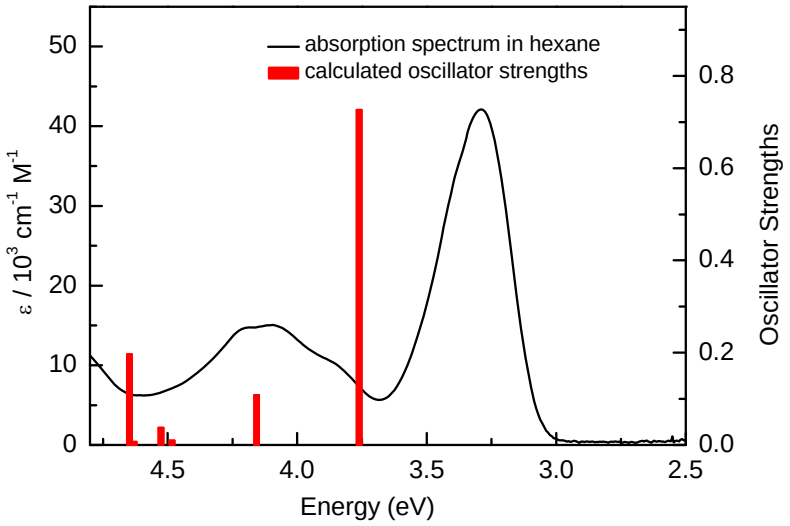

Figure S18. Comparison between the experimental UV-visible absorption spectrum and TD-DFT (CAM-B3LYP/6-31G(d)) calculated transitions of compound **4** from the optimised (B3LYP/6-31G(d)) ground state structure.

NMR Spectra

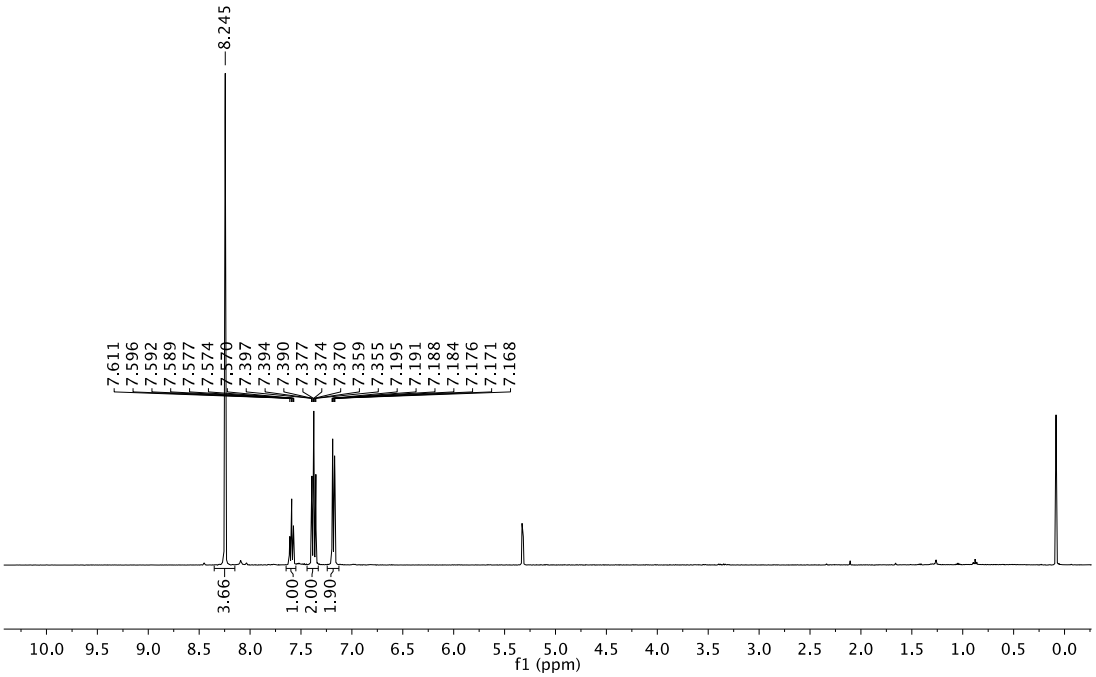

Figure S19. ^{1}H NMR spectrum (r.t.) of compound **1** in CD_2Cl_2 at 400 MHz.

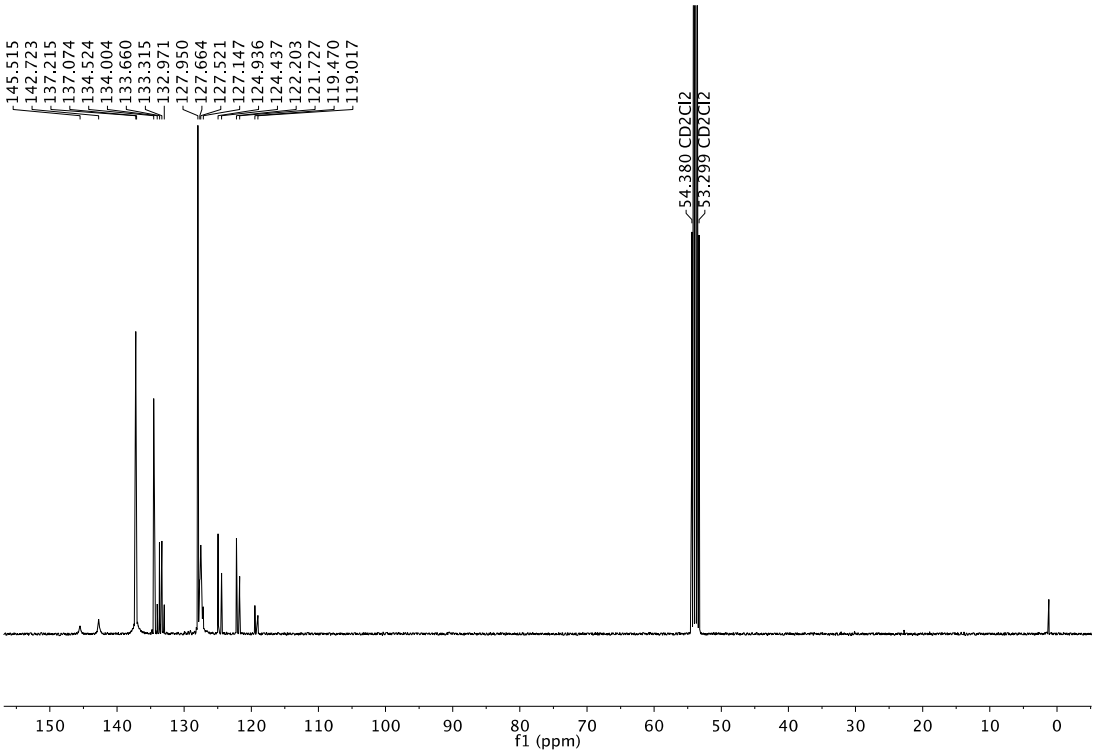

Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum (r.t.) of compound **1** in CD_2Cl_2 at 101 MHz.

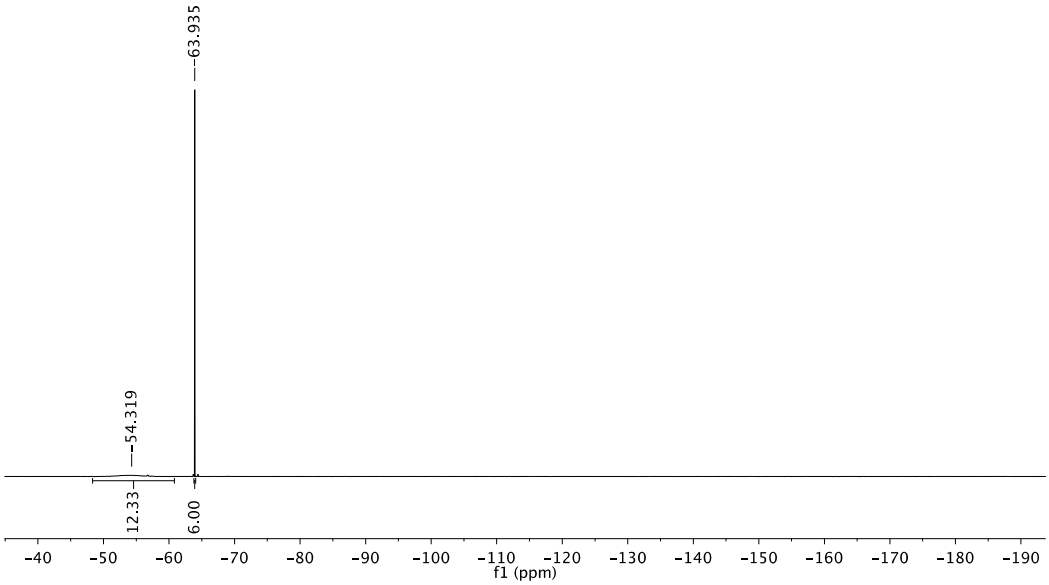

Figure S21. ^{19}F NMR spectrum (r.t.) of compound **1** in CD_2Cl_2 at 377 MHz.

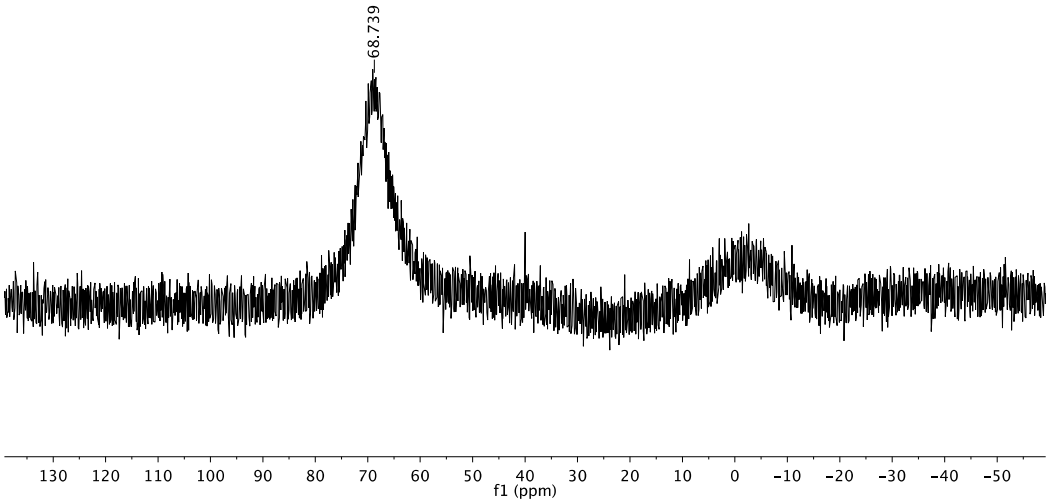

Figure S22. ^{11}B NMR spectrum (r.t.) of compound **1** in CD_2Cl_2 at 128 MHz.

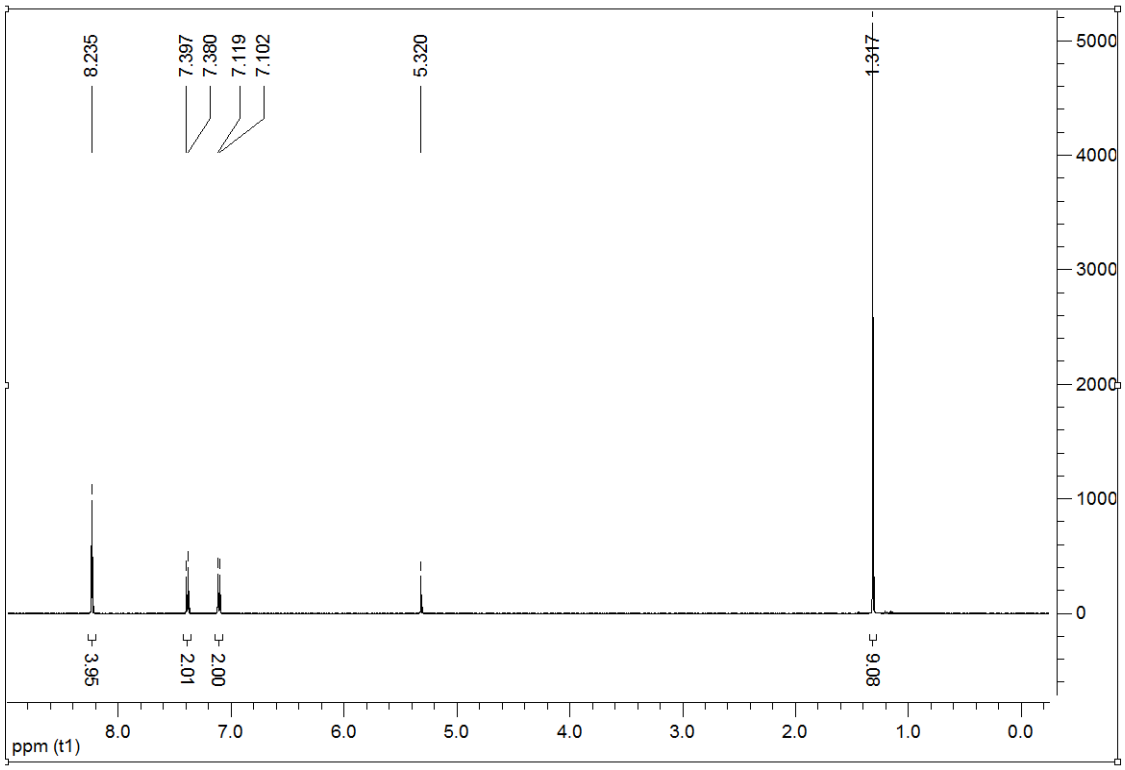

Figure S23. ^{1}H NMR spectrum (r.t.) of compound **2** in CD_2Cl_2 at 500 MHz.

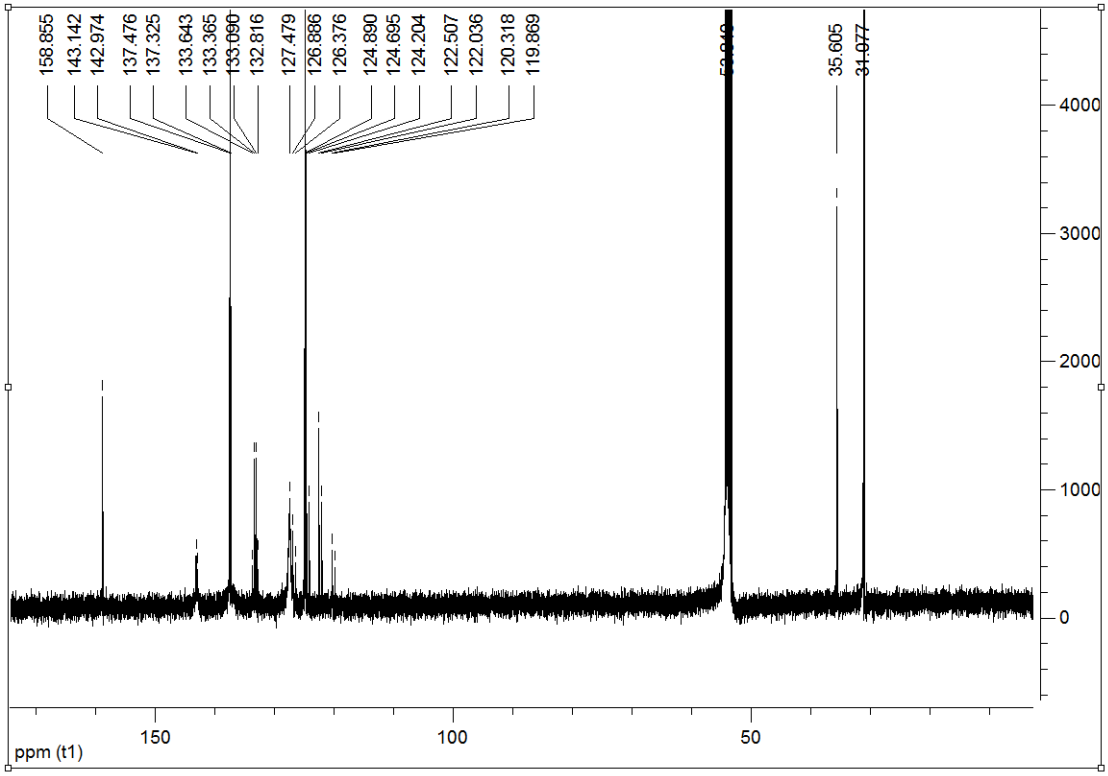

Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum (r.t.) of compound **2** in CD_2Cl_2 at 125 MHz.

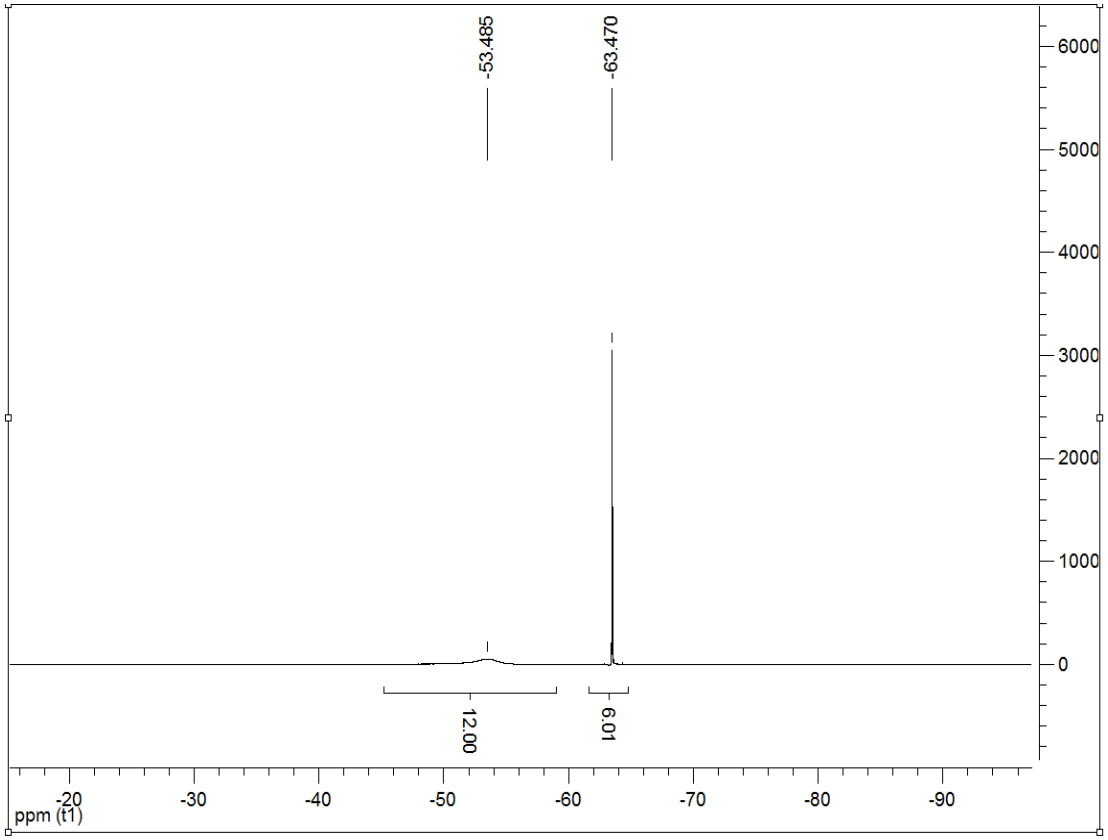

Figure S25. $^{19}F\{^{1}H\}$ NMR spectrum (r.t.) of compound **2** in toluene-d_8 at 188 MHz.

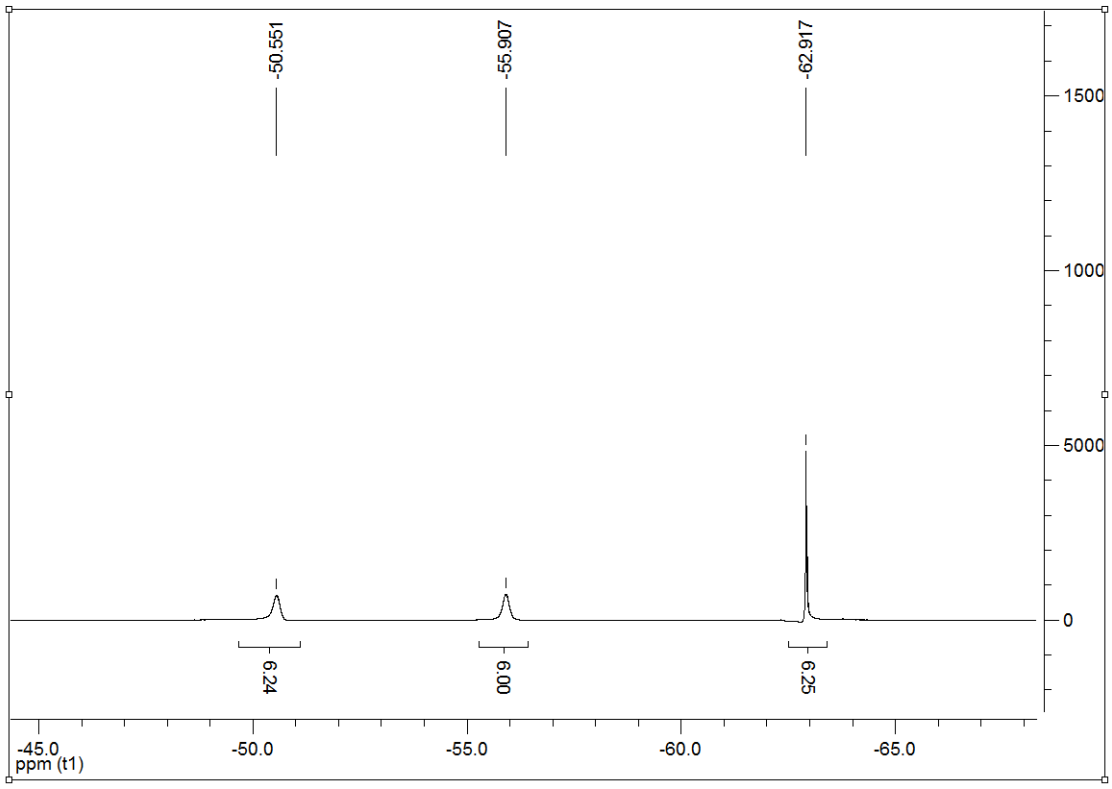

Figure S26. $^{19}F\{^{1}H\}$ NMR spectrum (223 K) of compound **2** in toluene-d_8 at 188 MHz.

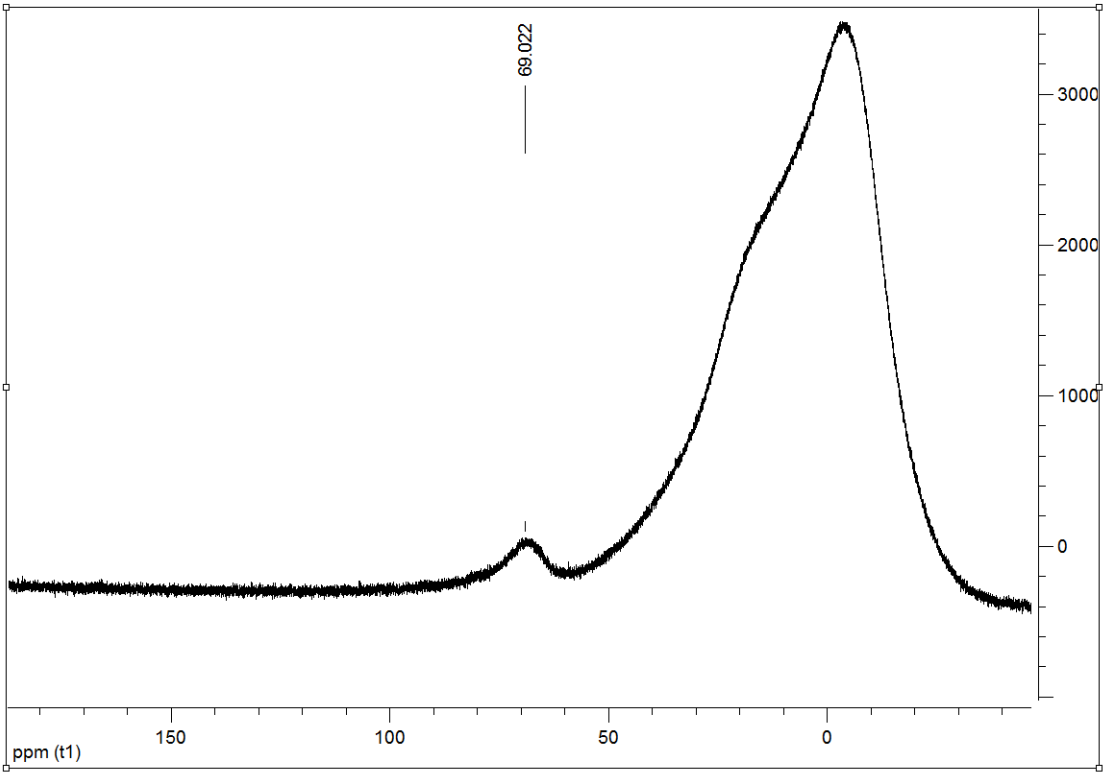

Figure S27. ^{11}B NMR spectrum (r.t.) of compound **2** in C_6D_6 at 160 MHz.

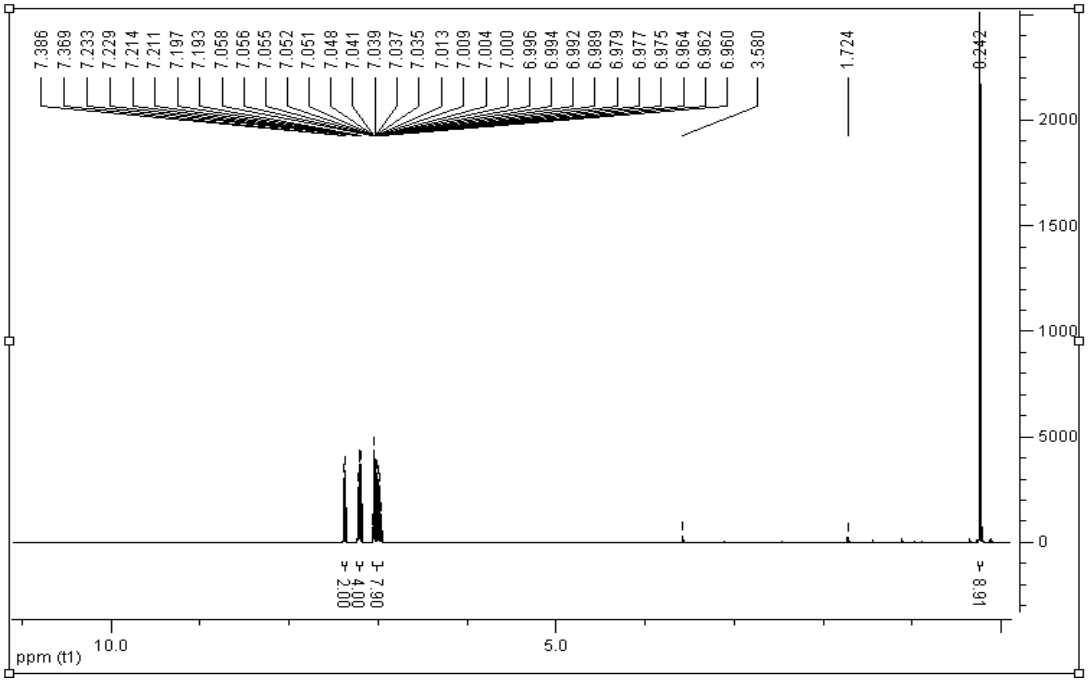

Figure S28. ^{1}H NMR spectrum of 4-(trimethylsilyl)triphenylamine (r.t.) in THF-d_8 at 500 MHz.

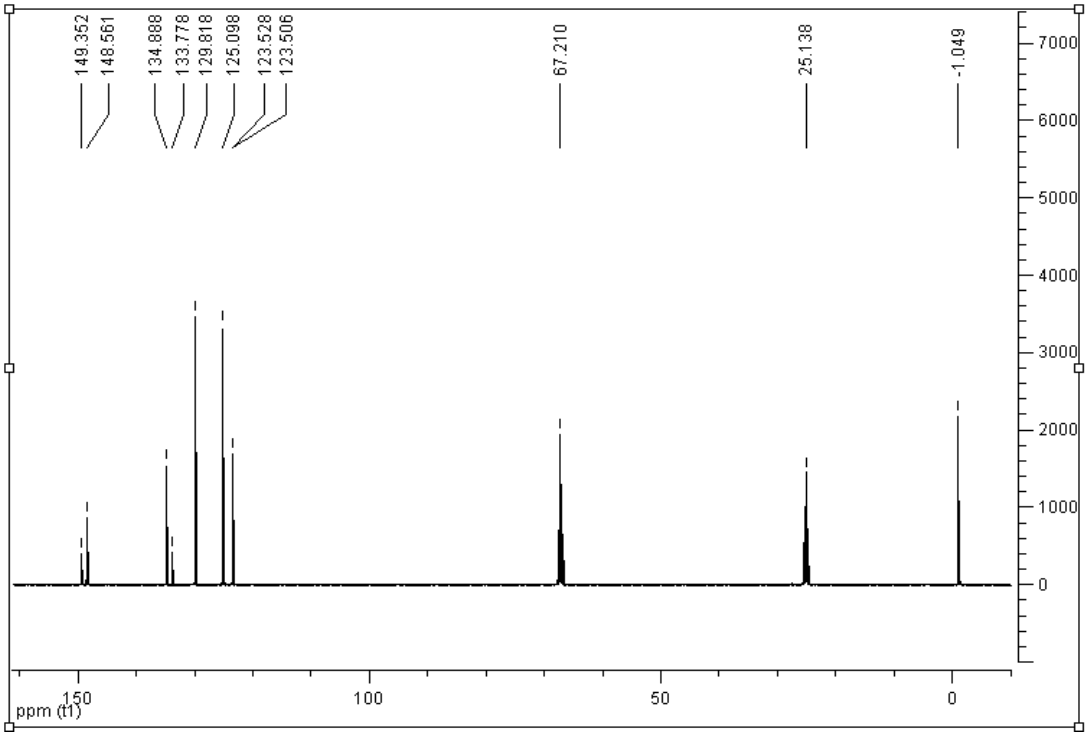

Figure S29. $^{13}C\{^{1}H\}$NMR of 4-(trimethylsilyl)triphenylamine (r.t.) in THF-d_8 at 125 MHz.

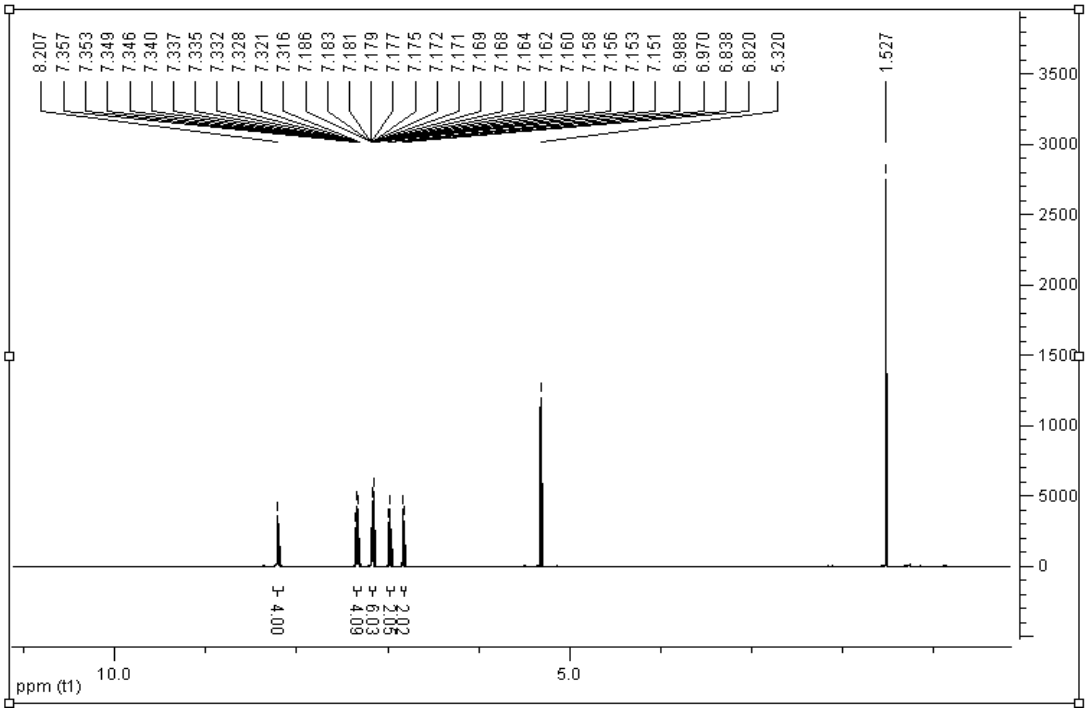

Figure S30. ^{1}H NMR spectrum of compound **3** (r.t.) in CD_2Cl_2 at 500 MHz.

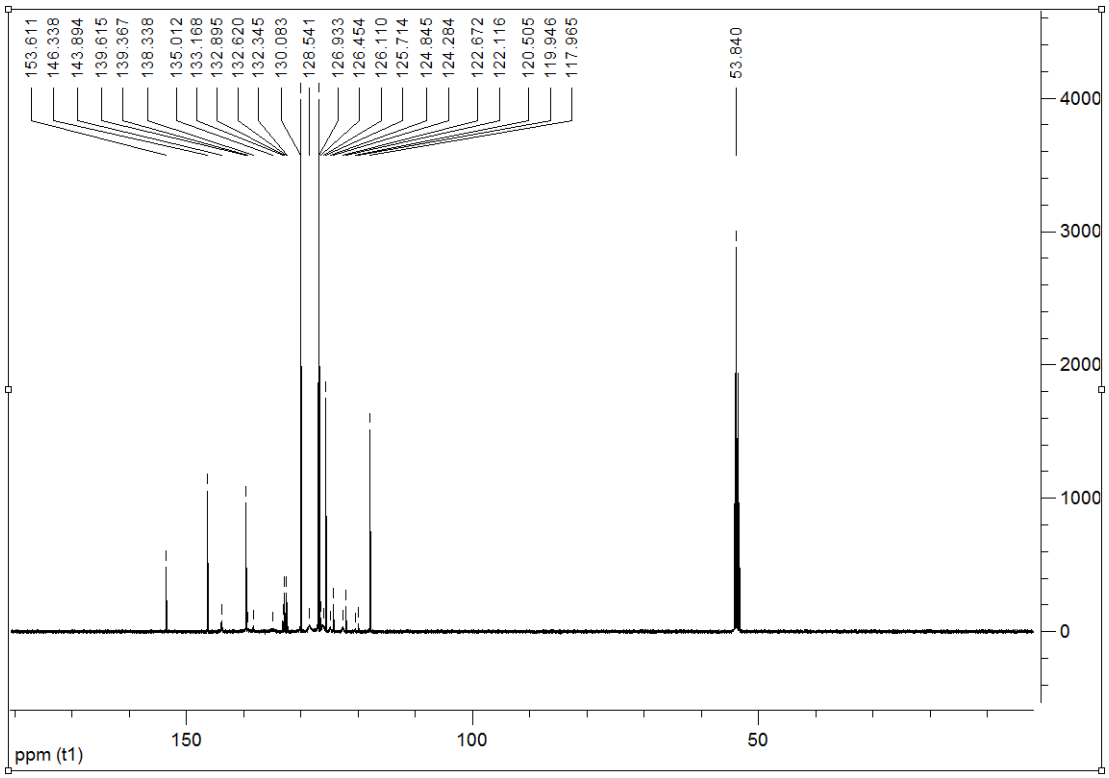

Figure S31. $^{13}C\{^{1}H\}$ NMR spectrum of compound **3** (r.t.) in CD_2Cl_2 at 125 MHz.

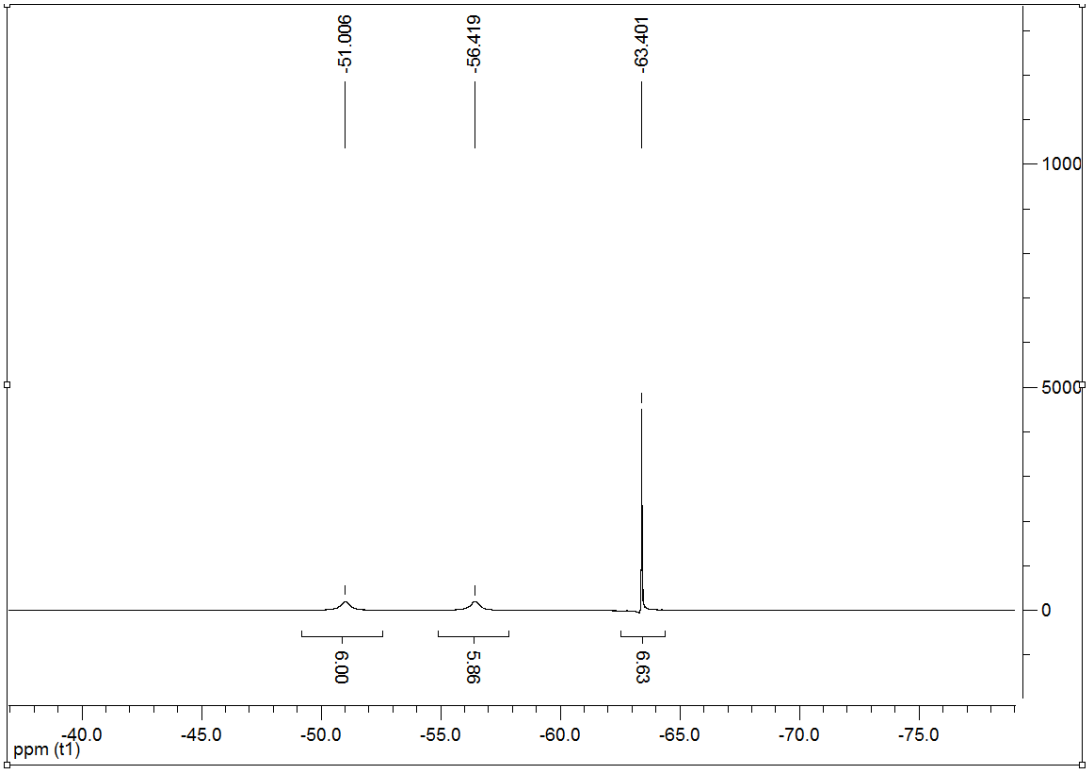

Figure S32. $^{19}F\{^{1}H\}$ NMR spectrum of compound **3** (r.t.) in toluene-d_8 at 188 MHz.

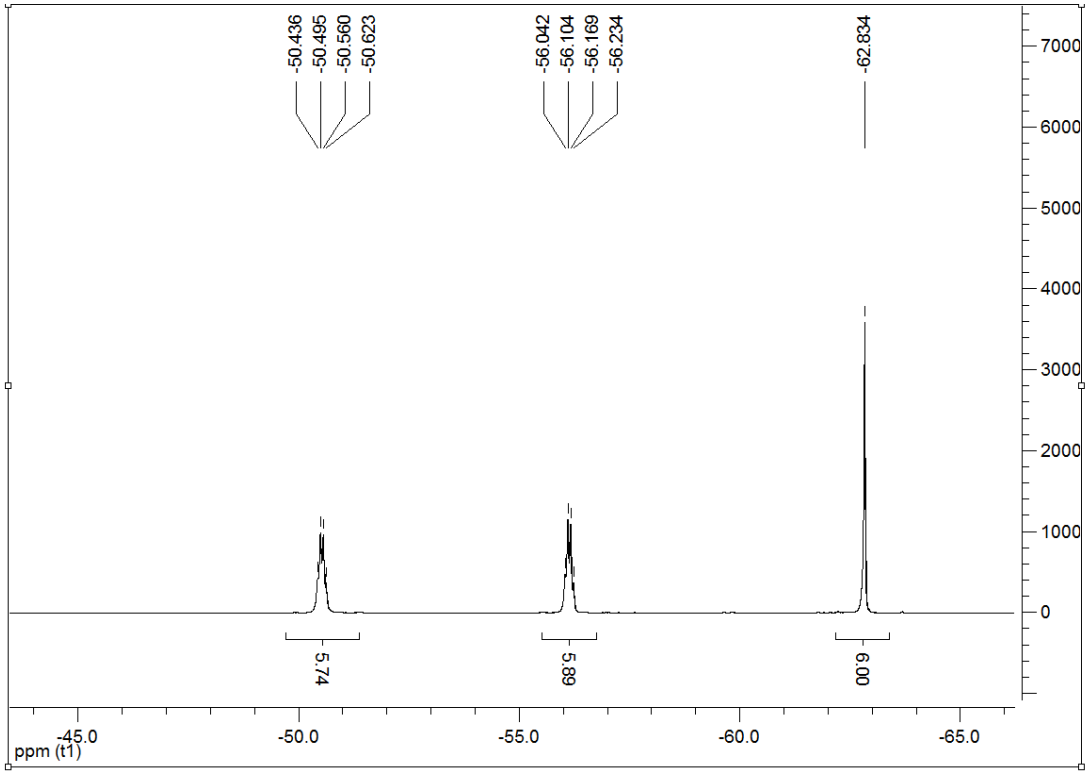

Figure S33. $^{19}F\{^{1}H\}$ NMR spectrum of compound **3** (223K) in toluene-d_8 at 188 MHz.

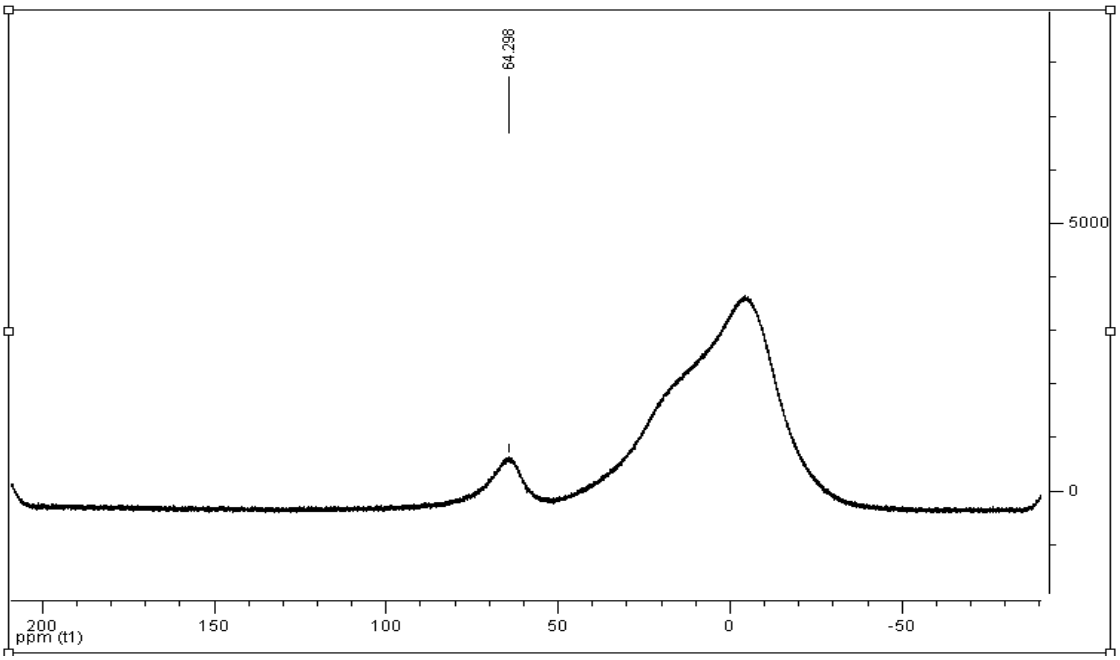

Figure S34. ^{11}B NMR of compound **3** (r.t.) in CD_2Cl_2 at 160 MHz.

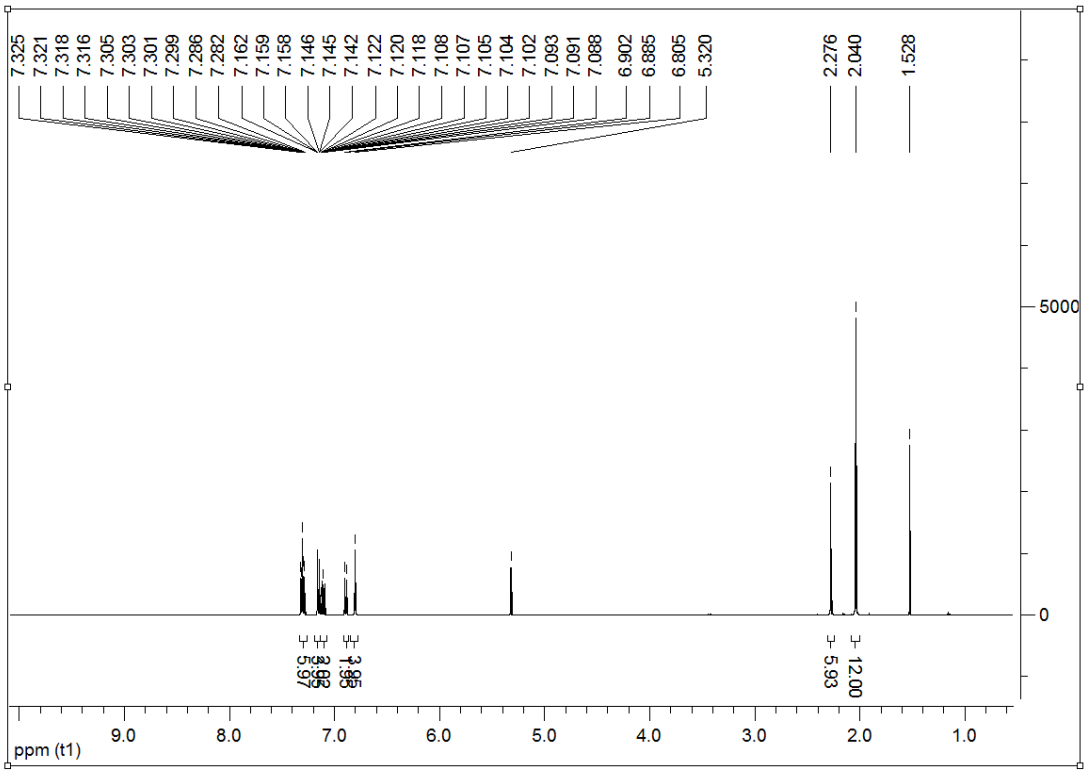

Figure S35. ^{1}H NMR spectrum of compound **4** (r.t.) in CD_2Cl_2 at 500 MHz.

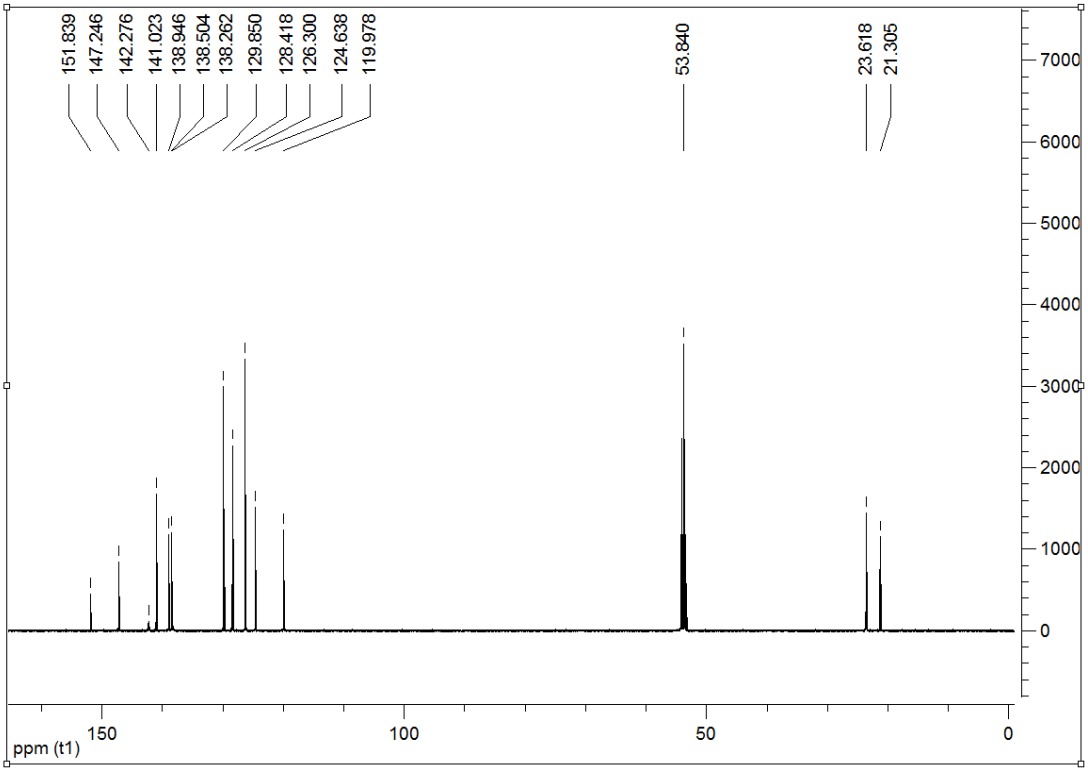

Figure S36. $^{13}C\{^{1}H\}$ NMR spectrum of compound **4** (r.t.) in CD_2Cl_2 at 125 MHz.

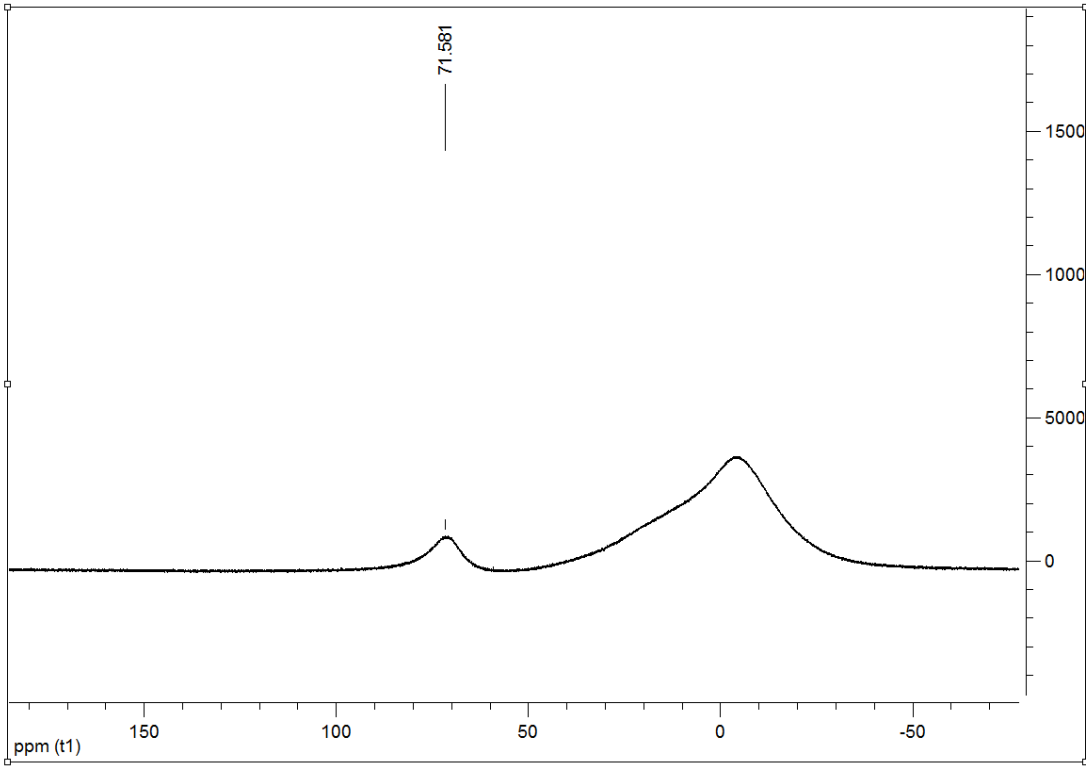

Figure S37. ^{11}B NMR of compound **4** (r.t.) in CD_2Cl_2 at 160 MHz.

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Cartesian coordinates of DFT and TD-DFT optimised structures

Compound **2** S_0
DFT CAM-B3LYP/6-31G(d)

Symbol	X	Y	Z
F	1.249495	8.470366	9.881375
F	1.037836	6.082101	10.755283
F	5.748391	8.265552	12.779115
F	-1.976125	8.853858	16.11697
F	-0.830043	8.776477	10.382301
F	-2.653987	10.05515	14.425702
F	0.558809	10.448987	10.461574
F	0.824979	3.983565	11.256934
F	0.640878	5.481726	12.814299
F	4.062136	7.911646	14.659398
F	2.744974	7.802641	16.37805
F	6.919634	6.643811	13.59568
F	2.819337	6.147733	14.978236
F	-1.219909	10.876936	15.847385
F	6.946703	7.025608	11.454195
F	4.441595	1.350618	13.066059
C	4.997828	10.530949	9.143209
F	5.307374	1.617117	11.08684
C	4.309591	10.993668	10.28214
H	4.250535	12.058912	10.482765
C	-0.431803	9.214145	14.355731
C	5.019089	5.97274	12.347471
C	3.742257	8.717055	10.977308
C	3.338787	3.777435	12.03409
H	2.676729	2.929978	11.909278
C	3.685829	10.117515	11.16063
H	3.161787	10.52827	12.018974
C	1.793502	8.248259	12.824334
C	2.831745	5.072124	11.950911
C	1.729194	8.144893	14.246173
C	4.448549	8.260636	9.845672
H	4.520071	7.194719	9.648503
C	-0.421721	9.333825	12.97664
C	0.663372	8.863544	12.221394
C	0.441123	9.118674	10.72993
C	5.042987	9.141589	8.944314
H	5.554854	8.729255	8.082908
C	5.658507	11.535079	8.183974
F	6.476586	2.111623	12.859012
C	0.651357	8.615553	14.992324
C	3.64483	6.235333	12.098565
C	5.525255	4.66693	12.433176
C	4.693486	3.571289	12.276743
C	6.131495	7.003601	12.545351
C	2.836696	7.502885	15.061259
C	-1.576414	9.748235	15.180716
C	1.338199	5.156789	11.695483
C	5.235085	2.164138	12.328366
B	3.062788	7.737408	11.962688
C	6.71671	12.360019	8.958103
H	7.195222	13.081454	8.28622
H	7.495851	11.71059	9.37114
H	6.27264	12.920159	9.786385
C	4.577006	12.488875	7.618086
H	3.813714	11.932455	7.063861
H	5.035268	13.212161	6.934164
H	4.07306	13.051667	8.40945
C	6.359433	10.843201	6.998649
H	6.811343	11.600575	6.349872
H	5.657234	10.264804	6.388743
H	7.16066	10.174329	7.330612
H	-1.264965	9.789876	12.473075
H	0.657307	8.515608	16.070349
H	6.578864	4.514685	12.631661

Compound **2** S_1
TD-DFT CAM-B3LYP/6-31G(d)

Symbol	X	Y	Z
F	1.288316	8.240296	9.819975
F	1.111032	5.934852	10.817097
F	5.607981	8.418466	12.977566
F	-2.053015	8.995075	16.021722
F	-0.785762	8.717339	10.178685
F	-2.911172	9.673423	14.134891
F	0.710567	10.284507	10.279704
F	1.004194	3.856218	11.414991
F	0.762596	5.413385	12.90168
F	3.879911	7.92896	14.74402
F	2.455754	7.758915	16.366594
F	6.961243	6.883941	13.664729
F	2.655706	6.139782	14.941166
F	-1.591965	10.979371	15.266109
F	6.853864	7.35398	11.549823
F	4.677022	1.394213	12.966971
C	4.968684	10.567988	9.199136
F	5.920939	1.90781	11.261122
C	4.226488	11.017223	10.301403
H	4.118436	12.079332	10.489787
C	-0.606524	9.142145	14.158855
C	5.074823	6.100629	12.474225
C	3.717651	8.72772	11.006658
C	3.534251	3.807901	12.153751
H	2.9255	2.921068	12.035409
C	3.603538	10.12265	11.167701
H	3.031525	10.521977	12.000629
C	1.715756	8.206321	12.770591
C	2.95234	5.068527	12.043569
C	1.578591	8.119117	14.184655
C	4.48255	8.284206	9.905359
H	4.600969	7.218875	9.728045
C	-0.530607	9.223338	12.777854
C	0.602328	8.76921	12.091716
C	0.478968	8.985703	10.585791
C	5.071987	9.175894	9.020222
H	5.632596	8.780195	8.178189
C	5.654157	11.522654	8.207848
F	6.62727	2.32069	13.275047
C	0.453366	8.582267	14.862294
C	3.696132	6.274454	12.18013
C	5.651749	4.830488	12.594262
C	4.891576	3.684514	12.425756
C	6.10315	7.211815	12.668007
C	2.643076	7.48639	15.05797
C	-1.7984	9.695608	14.896733
C	1.457643	5.06959	11.794482
C	5.532131	2.321723	12.48773
B	3.042565	7.734866	11.986969
C	7.177906	11.250171	8.206841
H	7.680875	11.919786	7.498856
H	7.409467	10.220952	7.91407
H	7.608107	11.4203	9.20022
C	5.429994	13.003709	8.567174
H	4.36713	13.270435	8.557571
H	5.936094	13.640316	7.833054
H	5.837395	13.251159	9.553966
C	5.087705	11.278372	6.788247
H	5.572062	11.948516	6.067917
H	4.00896	11.46866	6.757655
H	5.255997	10.250236	6.451659
H	-1.364178	9.632045	12.220311
H	0.400611	8.498349	15.939908
H	6.704004	4.742787	12.834735

Compound **2** S_1
TD-DFT B3LYP/6-31G(d)

Symbol	X	Y	Z
F	1.464607	6.930139	9.734921
F	0.890044	5.284925	11.607616
F	6.122737	7.873559	12.710114
F	-2.04576	9.724419	15.19194
F	-0.632269	7.474189	9.748178
F	-2.916405	9.651019	13.193458
F	0.874456	8.985337	9.353991
F	0.984413	3.627955	12.986704
F	1.001793	5.643021	13.749489
F	3.975417	8.570843	14.352268
F	2.521265	8.95113	15.909147
F	7.518483	6.373812	12.015968
F	2.827644	6.932357	15.1891
F	-1.667546	11.330758	13.779315
F	6.161864	7.293079	10.610317
F	4.808259	1.326847	13.901261
C	4.932228	10.780218	9.480999
F	5.56421	1.317026	11.866365
C	4.943668	10.821344	10.898295
H	5.342677	11.68935	11.407838
C	-0.590243	9.265881	13.38613
C	5.221862	5.735358	12.168268
C	3.882871	8.590695	11.042613
C	3.570143	3.633128	12.907529
H	2.935122	2.805731	13.191988
C	4.450335	9.775611	11.642744
H	4.465646	9.847946	12.719915
C	1.777637	7.997701	12.409072
C	2.998493	4.866649	12.651827
C	1.652907	8.44122	13.757575
C	3.835467	8.590099	9.610827
H	3.425611	7.730046	9.102453
C	-0.50925	8.853558	12.064833
C	0.652041	8.238219	11.58767
C	0.596609	7.888645	10.115271
C	4.364892	9.612288	8.867152
H	4.359433	9.535827	7.785493
C	5.478455	11.898393	8.61214
F	6.802049	2.109332	13.463837
C	0.493391	9.050635	14.233117
C	3.787659	6.040612	12.244596
C	5.756785	4.488868	12.430638
C	4.94761	3.411666	12.802571
C	6.24396	6.795638	11.884419
C	2.740605	8.211136	14.796675
C	-1.811166	9.988669	13.889807
C	1.489791	4.862114	12.750987
C	5.524853	2.054406	13.010749
B	3.197712	7.393703	11.908264
C	6.629749	11.324861	7.737718
H	7.024086	12.123826	7.100564
H	6.293571	10.512647	7.086634
H	7.447754	10.947282	8.359641
C	6.0265	13.081778	9.430707
H	5.251074	13.545963	10.049812
H	6.404494	13.849545	8.748503
H	6.856339	12.782137	10.079717
C	4.344195	12.417784	7.685663
H	4.741989	13.212324	7.045233
H	3.516051	12.83243	8.269802
H	3.943517	11.634569	7.03546
H	-1.356369	8.992994	11.403833
H	0.429837	9.352604	15.270516
H	6.827749	4.345563	12.379555

Compound **2** S_1
TD-DFT BLYP/6-31G(d)

Symbol	X	Y	Z
F	1.809837	6.225354	10.102544
F	0.76378	5.311512	12.760591
F	6.372388	7.596129	12.720002
F	-2.15901	10.315794	14.46792
F	-0.386243	6.327194	10.117998
F	-2.98455	9.496467	12.588439
F	0.781094	7.922063	9.149193
F	1.372152	3.895381	14.314489
F	1.806149	6.027387	14.576371
F	3.836317	8.264407	14.520446
F	3.023239	10.290925	14.786185
F	7.624341	6.0686	11.760519
F	2.167217	8.604883	15.913554
F	-1.822269	11.367443	12.561687
F	6.21188	7.222886	10.548876
F	4.675154	0.938202	13.186511
C	4.92314	10.848995	9.712883
F	4.981836	1.217447	11.024814
C	5.08338	10.790753	11.13422
H	5.561152	11.619295	11.656838
C	-0.625145	9.339396	12.919862
C	5.285939	5.560979	12.050117
C	3.999323	8.559365	11.238656
C	3.583151	3.517906	12.919339
H	2.962009	2.725259	13.333028
C	4.635417	9.700435	11.862558
H	4.772812	9.700144	12.941383
C	1.856746	7.955278	12.429879
C	3.128493	4.831818	12.959656
C	1.64255	8.760046	13.589555
C	3.82189	8.639252	9.812633
H	3.349349	7.809194	9.291235
C	-0.46491	8.551478	11.773342
C	0.747576	7.881122	11.533822
C	0.74971	7.071987	10.24188
C	4.274888	9.719973	9.080448
H	4.144794	9.72195	7.996606
C	5.395186	12.028262	8.865256
F	6.642788	1.607126	12.414309
C	0.430707	9.431433	13.83368
C	3.897547	5.963854	12.384117
C	5.714229	4.240742	12.028126
C	4.852325	3.180648	12.396518
C	6.358615	6.582959	11.778783
C	2.672045	8.955021	14.696752
C	-1.902563	10.124649	13.13899
C	1.792516	5.011687	13.64107
C	5.282465	1.756215	12.263176
B	3.329984	7.325233	12.090701
C	6.443172	11.504146	7.82035
H	6.774961	12.349206	7.194941
H	6.023533	10.734882	7.153818
H	7.325818	11.078445	8.323894
C	6.05378	13.156194	9.703471
H	5.354053	13.586009	10.439184
H	6.37	13.971518	9.033622
H	6.950056	12.802685	10.23917
C	4.165588	12.627452	8.097142
H	4.510862	13.462999	7.466427
H	3.410157	13.014935	8.799779
H	3.678212	11.889638	7.441122
H	-1.293008	8.44178	11.071747
H	0.308242	10.014816	14.747605
H	6.746756	4.012162	11.767971

Compound **2 S_1**
TD-DFT BHandHLYP/6-31G(d)

Symbol	X	Y	Z
F	0.952283	8.609241	9.967476
F	1.761068	6.036352	10.249146
F	5.011337	8.682688	13.867976
F	-2.557518	8.562483	15.710166
F	-0.42576	10.178584	10.407755
F	-3.045245	9.855869	14.056498
F	1.662508	10.508915	10.673246
F	1.759595	3.952474	10.718318
F	0.927221	5.349442	12.101467
F	3.288726	7.29518	15.138168
F	1.560274	6.680863	16.220724
F	6.693116	7.447827	14.328387
F	2.147757	5.598714	14.484829
F	-1.822575	10.572206	15.662671
F	6.488021	8.286868	12.369059
F	5.304408	1.808108	12.834436
C	4.965186	10.349696	9.092214
F	6.749813	2.660977	11.502752
C	4.925966	10.743179	10.443009
H	5.386112	11.665069	10.745379
C	-0.859281	9.030075	14.170901
C	5.073307	6.498562	12.912499
C	3.621656	8.751194	11.04392
C	4.016411	4.124741	12.006599
H	3.59853	3.199776	11.655211
C	4.319235	9.963348	11.383218
H	4.314146	10.280459	12.407523
C	1.573632	8.218239	12.831936
C	3.289869	5.295923	11.894667
C	1.187374	7.748251	14.14785
C	3.69566	8.361521	9.668649
H	3.225156	7.444529	9.371941
C	-0.56621	9.484616	12.898983
C	0.583335	9.096706	12.248334
C	0.687593	9.589219	10.841493
C	4.339285	9.118797	8.743662
H	4.372074	8.78598	7.721382
C	5.644745	11.169111	8.018942
F	6.977823	2.910805	13.619958
C	0.029645	8.149994	14.770811
C	3.779116	6.535394	12.366437
C	5.803709	5.324243	13.021559
C	5.276799	4.134374	12.572505
C	5.800833	7.72871	13.382026
C	2.041885	6.835644	14.983784
C	-2.06727	9.500425	14.894986
C	1.928632	5.163935	11.254426
C	6.078786	2.873495	12.63825
B	2.896466	7.871814	12.157111
C	6.757684	10.320419	7.374526
H	7.246146	10.90398	6.598459
H	6.373417	9.415054	6.914982
H	7.508714	10.036393	8.10688
C	6.266781	12.456546	8.560526
H	5.521957	13.112691	9.003453
H	6.734502	12.9987	7.743959
H	7.03593	12.2561	9.302039
C	4.599567	11.540872	6.949186
H	5.079995	12.129669	6.171933
H	3.795549	12.134358	7.375775
H	4.160867	10.66613	6.479244
H	-1.267107	10.126461	12.399679
H	-0.194504	7.779555	15.752761
H	6.778869	5.339861	13.47316

Compound **2 S_1**
TDA CAM-B3LYP/6-31G(d)

Symbol	X	Y	Z
F	1.263533	7.091105	9.754207
F	0.89187	5.390674	11.59324
F	5.927915	8.087445	12.819323
F	-2.148535	9.356602	15.419868
F	-0.733334	7.896136	9.738735
F	-3.051503	9.371958	13.446799
F	0.961532	9.219315	9.551643
F	1.047099	3.654998	12.84716
F	1.030698	5.604882	13.741419
F	3.844814	8.745066	14.396637
F	2.422856	8.733733	16.013327
F	7.42651	6.689771	12.163315
F	2.960616	6.885865	15.050256
F	-1.902544	11.070099	14.128475
F	6.109094	7.583447	10.721356
F	4.968433	1.467551	13.688185
C	4.955918	10.697127	9.4311
F	5.654103	1.550222	11.644157
C	4.861389	10.836781	10.833931
H	5.260957	11.720134	11.313798
C	-0.715565	9.117572	13.570086
C	5.177407	5.934176	12.171017
C	3.731352	8.662155	11.030426
C	3.625245	3.73588	12.772551
H	3.02127	2.872764	13.015035
C	4.270857	9.868948	11.600239
H	4.202398	10.001068	12.67022
C	1.680439	8.05046	12.469478
C	3.012585	4.956187	12.575363
C	1.559515	8.384761	13.84116
C	3.747928	8.59544	9.592686
H	3.309778	7.733008	9.112774
C	-0.635119	8.828122	12.221522
C	0.540741	8.314828	11.683951
C	0.510684	8.11178	10.19012
C	4.376884	9.541744	8.838999
H	4.431914	9.41239	7.764658
C	5.630539	11.730505	8.549635
F	6.909292	2.324571	13.22086
C	0.386415	8.89385	14.379499
C	3.748365	6.158353	12.229627
C	5.765671	4.698011	12.367076
C	5.003083	3.580072	12.659939
C	6.148812	7.055078	11.975814
C	2.693818	8.173219	14.820484
C	-1.960346	9.725575	14.143559
C	1.51019	4.90984	12.690064
C	5.631234	2.238091	12.805847
B	3.093174	7.500486	11.911549
C	6.801314	11.047567	7.809152
H	7.298889	11.782158	7.168877
H	6.465707	10.223824	7.17437
H	7.539427	10.654155	8.513977
C	6.182348	12.920344	9.342798
H	5.392041	13.463805	9.869553
H	6.659151	13.622565	8.653826
H	6.9377	12.611755	10.071654
C	4.608444	12.256834	7.519761
H	5.094696	12.995175	6.875254
H	3.762584	12.742906	8.014764
H	4.216489	11.463005	6.879232
H	-1.49613	8.986585	11.584888
H	0.328802	9.113676	15.437169
H	6.842162	4.605204	12.323358

Compound **3 S_0**
DFT CAM-B3LYP/6-31G(d)

Symbol	X	Y	Z
F	18.56329	20.136792	8.477987
F	17.559746	21.007423	10.728388
F	19.251511	19.279604	6.596653
F	16.062044	22.524066	11.135645
F	16.316664	21.787092	9.118377
F	16.671804	22.49069	3.094942
F	15.710382	20.674815	2.386346
C	15.659149	21.632889	3.338935
N	19.881878	14.438183	8.660997
F	19.115541	21.426998	6.834854
F	13.184431	20.399087	8.412359
C	13.645703	19.511578	12.269341
C	19.991995	13.589993	9.805805
F	13.318875	20.564114	14.359917
C	20.220141	11.896476	12.030359
H	20.308415	11.240764	12.891827
F	14.500178	22.302478	3.16568
C	15.945341	19.736117	7.266149
C	18.420277	15.967993	7.431979
H	18.67682	15.471438	6.502861
F	13.004206	16.233386	10.015298
C	17.69296	17.202392	9.81327
H	17.431285	17.677434	10.754555
C	15.266338	19.107121	9.947914
C	18.843259	13.062316	10.413857
H	17.864565	13.310285	10.01488
C	14.608887	20.616029	5.383092
H	13.638862	20.781827	4.934111
C	18.978973	15.50982	8.644299
C	17.545316	17.04022	7.423762
H	17.133335	17.355288	6.469456
C	16.98443	20.884367	5.340359
H	17.877458	21.273394	4.866639
C	14.395005	18.103746	10.447257
C	18.601982	16.159224	9.839417
H	19.031061	15.838129	10.781958
F	11.58625	20.349912	13.066801
C	13.595976	18.311846	11.577245
H	12.935218	17.524276	11.917438
C	13.367016	19.676355	7.2841
B	16.127102	18.859562	8.610044
C	21.666213	12.585115	5.96174
H	21.747971	11.566133	5.59322
C	17.078883	20.260118	6.587512
C	18.961365	12.228898	11.524936
H	18.063934	11.827247	11.987593
C	17.136794	17.697021	8.608918
C	21.364241	12.412656	11.418373
H	22.348959	12.164957	11.805401
F	14.624331	16.521448	8.615926
C	18.49656	20.261096	7.142301
F	12.40705	18.604421	14.0686
C	15.30758	20.307433	10.708915
C	14.697971	19.998361	6.630768
C	14.52079	20.503548	11.842083
H	14.596963	21.429578	12.39673
C	14.276289	16.684892	9.902094
F	12.321493	19.956415	6.476139
C	20.832955	12.856002	7.045895
H	20.27087	12.058044	7.520845
F	13.253967	18.37412	7.616461
C	20.716091	14.165339	7.533272
C	21.255086	13.260245	10.317136
H	22.144012	13.669351	9.847365
C	15.754758	21.036041	4.718745
F	15.047225	15.844023	10.634869
C	12.738659	19.755796	13.447
C	22.37961	13.613801	5.343041
H	23.023798	13.400303	4.494912
C	21.4415	15.196711	6.918596
H	21.358288	16.209927	7.299369
C	16.30714	21.408405	10.415254
C	22.25945	14.91927	5.824532
H	22.815738	15.726959	5.356607

Compound **3 S_1**
TD-DFT CAM-B3LYP/6-31G(d)

Symbol	X	Y	Z
F	18.847331	19.711917	8.546647
F	17.263258	20.38965	10.579428
F	18.974861	18.248602	6.951696
F	16.010204	21.658021	11.789865
F	15.885831	21.767897	9.644687
F	17.744327	22.668873	3.507157
F	16.215648	21.420683	2.63285
C	16.503517	22.184063	3.71128
N	19.828941	14.486921	8.794673
F	19.769855	20.222677	6.673626
F	13.548925	21.07672	8.581969
C	13.096525	18.920999	11.912066
C	20.474359	14.059951	9.991659
F	12.661298	19.552582	14.135679
C	21.722183	13.206293	12.321665
H	22.210316	12.873684	13.23151
F	15.65031	23.22526	3.670564
C	16.149482	19.806532	7.382299
C	17.845608	15.457022	7.805486
H	17.828231	14.669655	7.062059
F	12.502562	16.157153	9.042923
C	17.896182	17.4432	9.757743
H	17.929467	18.231697	10.497788
C	14.890176	18.839161	9.702858
C	19.705251	13.698764	11.099008
H	18.623129	13.739443	11.037638
C	15.184476	21.317284	5.656009
H	14.32293	21.835328	5.259062
C	18.835317	15.432388	8.821101
C	16.913606	16.457318	7.78567
H	16.155419	16.450567	7.014701
C	17.508023	20.803669	5.540219
H	18.476086	20.948408	5.080224
C	13.892847	17.864084	9.905155
C	18.794192	16.415211	9.844734
H	19.532305	16.394004	10.63671
F	11.043947	19.750582	12.718688
C	13.009585	17.905511	10.977786
H	12.250053	17.14131	11.081989
C	13.649156	20.533946	7.352563
B	15.982105	18.801783	8.523888
C	20.992018	12.090611	6.215973
H	21.169304	11.025475	6.111584
C	17.405348	20.042797	6.690514
C	20.334246	13.277192	12.261902
H	19.735227	12.993002	13.120432
C	16.953346	17.543838	8.69937
C	22.484027	13.559291	11.211376
H	23.566819	13.510604	11.255701
F	14.025546	16.906878	7.717012
C	18.726389	19.565747	7.213866
F	11.650917	17.786642	13.381899
C	14.960232	19.84008	10.700912
C	15.051493	20.562295	6.801006
C	14.08211	19.884852	11.774517
H	14.174197	20.668211	12.514812
C	13.745779	16.664124	9.00637
F	12.779993	21.220627	6.584661
C	20.527463	12.591364	7.422886
H	20.3389	11.930469	8.261607
F	13.147595	19.284964	7.436782
C	20.288063	13.959918	7.551895
C	21.866745	13.98536	10.044772
H	22.454164	14.272161	9.17982
C	16.402739	21.430737	4.988689

F	14.573631	15.666124	9.397304
C	12.112848	19.001961	13.038795
C	21.2206	12.946528	5.142073
H	21.584113	12.549921	4.200092
C	20.523717	14.826337	6.481153
H	20.347761	15.890819	6.597758
C	16.019969	20.91737	10.665073
C	20.985518	14.311016	5.278552
H	21.171564	14.983064	4.447823

Compound **3** S_1
TD-DFT B3LYP/6-31G(d)

Symbol	X	Y	Z
F	18.816219	19.969208	7.980995
F	17.595038	20.734728	10.22734
F	18.941124	18.430419	6.44076
F	16.436451	22.072426	11.478581
F	16.017053	21.953362	9.360621
F	16.698018	22.1095	2.7441
F	15.224801	20.574232	2.316283
C	15.557803	21.543773	3.216264
N	19.919358	14.451054	8.762544
F	19.412924	20.482195	5.969607
F	13.550303	21.068095	8.697299
C	13.789858	19.169277	12.311566
C	19.87585	13.576036	9.859519
F	13.683953	19.974543	14.532954
C	19.753453	11.870297	12.075844
H	19.704448	11.210142	12.935898
F	14.579061	22.478366	3.133146
C	15.982268	19.773826	7.226644
C	17.950596	15.522808	7.750928
H	17.882911	14.701512	7.042863
F	12.859344	16.17876	9.745734
C	18.157815	17.643824	9.547496
H	18.258166	18.465448	10.247819
C	15.194655	19.000326	9.820932
C	18.634008	13.301631	10.475663
H	17.7304	13.752161	10.083058
C	14.632767	20.94908	5.47807
H	13.681317	21.352614	5.160603
C	18.95068	15.538741	8.717757
C	17.052058	16.590042	7.701405
H	16.285131	16.584611	6.935316
C	16.961253	20.566181	5.057295
H	17.833438	20.714976	4.433879
C	14.308546	17.988248	10.268591
C	19.060153	16.582215	9.632167
H	19.843989	16.573271	10.384502
F	11.832757	19.943633	13.397773
C	13.615873	18.072608	11.477618
H	12.936852	17.279833	11.766415
C	13.458483	20.38761	7.527763
B	16.079303	18.896564	8.477035
C	22.356476	13.012789	6.371033
H	22.793123	12.05144	6.119894
C	17.105246	19.994617	6.309321
C	18.582577	12.444925	11.564811
H	17.623612	12.223078	12.021565
C	17.142386	17.679241	8.580231
C	20.988243	12.166757	11.489849
H	21.902365	11.754006	11.904826
F	14.19473	16.823405	8.168941
C	18.540776	19.722475	6.681592
F	12.694786	18.078665	14.102721
C	15.360615	20.089538	10.721007
C	14.745043	20.385362	6.736494
C	14.673008	20.174203	11.930888
H	14.834749	21.021583	12.583998
C	14.08418	16.701985	9.505019
F	12.430587	20.963559	6.856066
C	21.442107	13.095523	7.408274
H	21.142872	12.201986	7.942519
F	13.027961	19.136947	7.840257
C	20.844475	14.343184	7.730672
C	21.058596	13.012963	10.391253
H	22.020355	13.283118	9.970455
C	15.720917	21.018455	4.5984
F	14.97995	15.746082	9.886741
C	13.002518	19.291012	13.585325
C	22.693216	14.152858	5.630173
H	23.407824	14.080862	4.816763
C	21.160828	15.486834	6.949701
H	20.682295	16.434896	7.160174
C	16.338342	21.213853	10.433555
C	22.084267	15.381454	5.923936
H	22.332702	16.26336	5.343198

Compound **3** S_1
TD-DFT CAM-BHandHLYP/6-31G(d)

Symbol	X	Y	Z
F	18.841173	19.828177	8.418417
F	17.309803	20.482699	10.508655
F	19.008431	18.408942	6.812207
F	16.061168	21.70117	11.743559
F	15.873526	21.805158	9.620099
F	17.496872	22.690763	3.387032
F	15.996798	21.393132	2.579792
C	16.288849	22.172175	3.634141
N	19.840639	14.492622	8.794636
F	19.689074	20.408838	6.549845
F	13.522457	21.026139	8.588578
C	13.265276	18.875168	11.9716
C	20.360623	14.008121	10.016075
F	12.902268	19.469187	14.207105
C	21.3677	13.048248	12.413388
H	21.759833	12.675851	13.344816
F	15.408068	23.177437	3.603838
C	16.122906	19.842066	7.335088
C	17.923595	15.522579	7.7455
H	17.904738	14.740055	7.007783
F	12.632241	16.148032	9.095971
C	17.968903	17.507703	9.683715
H	18.00942	18.293141	10.41563
C	14.973409	18.853477	9.70292
C	19.493324	13.712122	11.066602
H	18.43262	13.840575	10.934193
C	15.060286	21.29043	5.622591
H	14.177025	21.769124	5.245657
C	18.880734	15.47763	8.780266
C	17.013712	16.541165	7.703639
H	16.284197	16.550193	6.915676
C	17.390781	20.857744	5.449167
H	18.333434	21.03163	4.965168
C	14.02039	17.848288	9.941255
C	18.854123	16.47111	9.78234
H	19.581287	16.446737	10.574423
F	11.238221	19.64372	12.869231
C	13.179476	17.860984	11.043121
H	12.4551	17.077572	11.172881
C	13.604843	20.484638	7.368594
B	16.024421	18.842189	8.485277
C	21.102526	12.135864	6.249416
H	21.273394	11.078425	6.136423
C	17.348668	20.113136	6.605905
C	20.001882	13.236468	12.260398
H	19.328601	13.001768	13.06756
C	17.034086	17.605588	8.629549
C	22.228433	13.338062	11.363495
H	23.290297	13.201518	11.481384
F	14.142163	16.877228	7.770894
C	18.699913	19.695232	7.097126
F	11.91053	17.702684	13.480633
C	15.044124	19.855865	10.695142
C	14.985655	20.552663	6.778121
C	14.207444	19.869941	11.796505

H	14.297581	20.651754	12.527262
C	13.86851	16.645972	9.051524
F	12.700152	21.134667	6.628551
C	20.591083	12.619662	7.43755
H	20.35798	11.949975	8.247366
F	13.146919	19.230904	7.473058
C	20.354571	13.986069	7.579779
C	21.732827	13.815664	10.165797
H	22.397632	14.057116	9.354525
C	16.250863	21.435766	4.919846
F	14.685236	15.653489	9.443519
C	12.327936	18.921901	13.134475
C	21.382923	13.003345	5.20216
H	21.78196	12.620722	4.277833
C	20.640898	14.862068	6.531703
H	20.472245	15.918721	6.654202
C	16.063859	20.965515	10.627247
C	21.150658	14.363317	5.348123
H	21.376903	15.041397	4.542761

Compound **3** S_1
TD-DFT CAM-B3LYP-D3/6-31G(d)

Symbol	X	Y	Z
F	18.849457	19.583407	8.626133
F	17.281982	20.341484	10.605551
F	18.957991	18.100225	7.047437
F	16.063331	21.707237	11.745922
F	15.973017	21.734863	9.595613
F	17.879343	22.517498	3.543825
F	16.324032	21.298933	2.672429
C	16.623731	22.068976	3.743113
N	19.793419	14.467496	8.762893
F	19.811847	20.049047	6.760901
F	13.602154	21.107662	8.597256
C	13.059232	19.059264	11.924951
C	20.459251	14.009805	9.933747
F	12.600747	19.793645	14.11192
C	21.747382	13.098312	12.218342
H	22.251461	12.742971	13.110703
F	15.798314	23.131768	3.683203
C	16.173808	19.74575	7.4312
C	17.772793	15.411099	7.833232
H	17.75991	14.637023	7.075737
F	12.469501	16.164845	9.17658
C	17.828831	17.364207	9.820094
H	17.862066	18.14527	10.567993
C	14.874157	18.856791	9.748696
C	19.708795	13.611223	11.041155
H	18.625796	13.648391	10.995308
C	15.265211	21.265229	5.685563
H	14.424531	21.805744	5.27369
C	18.77611	15.385341	8.834169
C	16.834212	16.404775	7.837949
H	16.068282	16.410544	7.07494
C	17.575092	20.680246	5.591497
H	18.548629	20.793487	5.133854
C	13.853779	17.911848	9.970695
C	18.734175	16.341237	9.882251
H	19.481454	16.310434	10.665308
F	11.012096	19.962881	12.65764
C	12.958114	18.011701	11.027608
H	12.178583	17.27096	11.151426
C	13.697251	20.535329	7.380569
B	15.962947	18.761245	8.579758
C	21.017204	12.242115	6.065508
H	21.230842	11.190365	5.907561
C	17.441582	19.935366	6.749046
C	20.357923	13.161497	12.181886
H	19.774009	12.848948	13.040913
C	16.889637	17.47909	8.762761
C	22.490287	13.488315	11.107192
H	23.573873	13.445662	11.133887
F	13.9636	16.898993	7.80856
C	18.742625	19.428574	7.293854
F	11.566435	18.016575	13.414924
C	14.962093	19.886031	10.713005
C	15.102649	20.525338	6.835905
C	14.071879	19.991724	11.771708
H	14.173203	20.795589	12.488582
C	13.705296	16.686485	9.108564
F	12.843284	21.219406	6.593302
C	20.545217	12.66681	7.298306
H	20.387097	11.961933	8.107026
F	13.17498	19.296852	7.490821
C	20.260206	14.018265	7.494354
C	21.852831	13.944159	9.963131
H	22.42335	14.260102	9.097099
C	16.492216	21.334332	5.028147
F	14.553503	15.711209	9.513553
C	12.059462	19.207289	13.0297
C	21.20672	13.15769	5.033543
H	21.575661	12.820533	4.070744
C	20.457204	14.945473	6.467468
H	20.244924	15.995948	6.638303
C	16.059734	20.922	10.651746
C	20.92607	14.505287	5.238193
H	21.081795	15.223044	4.440158

Compound **3** S_1
TD-DFT CAM-B3LYP/6-31G(d) with THF from PCM model

Symbol	X	Y	Z
F	18.765887	19.901701	8.565499
F	17.209014	20.730159	10.485542
F	19.117744	18.595829	6.874461
F	15.833647	22.001436	11.55195
F	15.720794	21.872649	9.408375
F	17.482306	22.765446	3.441147
F	16.027357	21.417168	2.588422
C	16.278703	22.202855	3.661669
N	19.826756	14.496988	8.73688
F	19.653944	20.672311	6.767542
F	13.366597	20.891553	8.469571
C	13.27309	18.95985	12.018846
C	20.327323	13.979248	9.97069
F	12.79252	19.766043	14.178963
C	21.295263	12.94341	12.35582
H	21.675471	12.53758	13.290458
F	15.361192	23.189599	3.620444
C	16.105117	19.849326	7.347239
C	18.034273	15.649747	7.590454
H	18.080528	14.930874	6.778566
F	12.96944	15.861423	9.477529
C	17.895701	17.443739	9.725984
H	17.864221	18.167283	10.536507
C	15.009122	18.892011	9.75672
C	19.432528	13.588577	10.967741
H	18.361791	13.676663	10.797806
C	15.018704	21.221658	5.584741
H	14.112576	21.638703	5.160304
C	18.894559	15.491878	8.713935
C	17.129376	16.672669	7.563461
H	16.462524	16.761197	6.710562
C	17.387996	20.942129	5.515845
H	18.346897	21.167651	5.062213
C	14.147556	17.820442	10.089777
C	18.774723	16.400284	9.804811
H	19.433945	16.297412	10.660862
F	11.13598	19.574868	12.807804
C	13.295288	17.85386	11.187236
H	12.641971	17.011861	11.393045
C	13.556253	20.285028	7.279866
B	16.032385	18.853888	8.529216
C	21.010103	12.063997	6.202292
H	21.094389	10.986826	6.078964

C	17.338821	20.189577	6.679445
C	19.923147	13.074217	12.160649
H	19.22723	12.76419	12.936671
C	17.043194	17.640722	8.603121
C	22.181444	13.327624	11.351796
H	23.254005	13.230092	11.50255
F	14.268674	16.697069	7.980276
C	18.695851	19.837226	7.224342
F	12.033711	17.803531	13.654536
C	14.974195	19.981898	10.662504
C	14.949453	20.467522	6.738451
C	14.126591	20.021144	11.75984
H	14.140736	20.875908	12.427646
C	14.122515	16.534537	9.304762
F	12.614694	20.798714	6.460718
C	20.476007	12.577925	7.375382
H	20.139833	11.916796	8.170275
F	13.22374	18.990098	7.445843
C	20.357634	13.960086	7.525144
C	21.703467	13.844158	10.155691
H	22.388119	14.15412	9.370057
C	16.234184	21.450519	4.943738
F	15.107732	15.697075	9.70266
C	12.313667	19.024503	13.164355
C	21.428907	12.920199	5.186065
H	21.848367	12.511879	4.269495
C	20.783506	14.825644	6.515335
H	20.704459	15.901628	6.655384
C	15.924432	21.143364	10.517167
C	21.314873	14.298462	5.346088
H	21.651467	14.970942	4.560554

Compound **3** S_1
TDA CAM-B3LYP/6-31G(d)

Symbol	X	Y	Z
F	18.869521	19.706342	8.545045
F	17.266941	20.370077	10.578648
F	18.959375	18.238021	6.951404
F	16.022768	21.614197	11.822171
F	15.88392	21.765934	9.680452
F	17.773621	22.730872	3.558723
F	16.241191	21.501959	2.664112
C	16.530466	22.248268	3.754154
N	19.823617	14.477922	8.79195
F	19.786529	20.197379	6.6642
F	13.559306	21.086265	8.602984
C	13.089854	18.898098	11.90169
C	20.488354	14.06423	9.983157
F	12.65823	19.500168	14.134099
C	21.773702	13.235881	12.301756
H	22.276496	12.91315	13.20716
F	15.681606	23.293505	3.727227
C	16.162292	19.821253	7.393111
C	17.827982	15.442395	7.822563
H	17.797186	14.647179	7.088016
F	12.467873	16.193267	8.983408
C	17.915121	17.451645	9.748373
H	17.9611	18.246694	10.480138
C	14.886154	18.832245	9.693829
C	19.737319	13.716756	11.107097
H	18.654368	13.758114	11.063157
C	15.206026	21.360507	5.685758
H	14.347657	21.888733	5.295589
C	18.833324	15.42642	8.822794
C	16.897644	16.444423	7.806013
H	16.128503	16.429712	7.046452
C	17.525841	20.833858	5.561816
H	18.494326	20.977151	5.102446
C	13.879743	17.863716	9.880404
C	18.809607	16.420669	9.835619
H	19.557233	16.405138	10.618709
F	11.043972	19.733706	12.719031
C	12.995498	17.897287	10.952669
H	12.229101	17.138353	11.044642
C	13.663033	20.561601	7.366016
B	15.987234	18.804459	8.522034
C	20.936163	12.046515	6.223735
H	21.10706	10.979444	6.128949
C	17.418743	20.057437	6.700885
C	20.385045	13.307821	12.264215
H	19.800068	13.034297	13.135788
C	16.956886	17.543959	8.702885
C	22.517404	13.575069	11.175004
H	23.600721	13.525474	11.20191
F	14.015733	16.932743	7.68084
C	18.735867	19.559672	7.213114
F	11.632922	17.754731	13.353201
C	14.962132	19.819614	10.705313
C	15.067798	20.590331	6.819962
C	14.082652	19.856367	11.778163
H	14.179044	20.629338	12.528742
C	13.720055	16.67846	8.964426
F	12.800365	21.264338	6.605202
C	20.492292	12.563275	7.431709
H	20.313638	11.913036	8.280873
F	13.154064	19.314317	7.429028
C	20.261097	13.934256	7.54838
C	21.881286	13.988453	10.013955
H	22.454535	14.264422	9.136065
C	16.424875	21.477167	5.020293
F	14.526509	15.660862	9.349608
C	12.105848	18.970902	13.028711
C	21.152287	12.888998	5.136727
H	21.499654	12.479907	4.193997
C	20.484497	14.787268	6.46442
H	20.315344	15.853833	6.571767
C	16.024165	20.895621	10.683034
C	20.925626	14.256079	5.260962
H	21.102195	14.917639	4.41982

Compound **4** S_0
DFT CAM-B3LYP/6-31G(d)

Symbol	X	Y	Z
N	5.223168	9.599242	-2.247702
C	9.34527	14.280163	0.320125
C	3.855235	9.770502	-2.61166
C	5.900942	8.415786	-2.663969
C	5.89357	10.581913	-1.489925
C	1.615931	8.870896	-2.848155
C	7.26842	10.825368	-1.679107
C	7.252889	12.573734	0.046069
C	5.204824	11.343916	-0.525415
H	4.147191	11.166868	-0.359852
C	11.768701	15.39002	-0.712722
C	5.877185	12.302356	0.220767
H	5.322477	12.861347	0.970406
C	10.558992	14.213475	1.057268
C	3.402075	10.994521	-3.127417
C	7.21283	6.071101	-3.483686
C	1.164317	10.093016	-3.350547
C	9.381139	14.915589	-0.950019
C	2.948455	8.708958	-2.472798
C	7.916182	11.801173	-0.933689
C	7.376434	14.115266	2.276293
C	6.694215	7.69268	-1.759899
H	6.791607	8.043418	-0.737297
C	7.128405	13.169764	3.307215
C	6.254453	14.915151	4.780878
C	5.768582	7.951459	-3.981249
C	6.483077	15.841715	3.760917
H	6.223473	16.886136	3.926454
C	7.351054	6.535201	-2.173695
C	10.641696	13.529713	2.407174
C	6.41486	6.783188	-4.381531
C	11.736536	14.750501	0.528653
C	2.063998	11.152947	-3.483567

C	10.575604	15.464242	-1.431737
C	6.590597	13.584492	4.531413
H	6.429499	12.842449	5.312135
C	7.235938	16.558272	1.494281
H	6.588542	16.404228	0.621463
H	8.26563	16.594595	1.126897
H	6.989124	17.540965	1.908945
C	7.043512	15.473048	2.534401
C	7.438167	11.690538	3.156541
H	6.605565	11.151068	2.689153
H	7.615056	11.234856	4.136934
H	8.31925	11.501784	2.537671
C	8.154619	15.05082	-1.83554
H	8.017376	14.166707	-2.469771
C	13.042447	16.007267	-1.240362
C	5.694443	15.346096	6.115984
H	5.204055	14.514146	6.632664
H	4.96272	16.153807	6.002493
H	6.486699	15.719801	6.778935
B	7.994697	13.660954	0.884437
H	0.925471	8.039345	-2.734344
H	7.815175	10.253911	-2.42197
H	4.102404	11.815398	-3.245326
H	7.720411	5.164543	-3.800688
H	0.123701	10.21791	-3.636012
H	3.294786	7.761662	-2.071692
H	8.973363	11.978396	-1.115608
H	5.158035	8.509746	-4.683932
H	7.962264	5.986233	-1.462205
H	11.638543	13.651429	2.843095
H	10.453135	12.451276	2.328709
H	9.911095	13.931989	3.114926
H	6.302901	6.436301	-5.405394
H	12.655211	14.672335	1.107905
H	1.727931	12.106993	-3.881082
H	10.570866	15.963839	-2.39947
H	8.254817	15.917388	-2.498214
H	7.229989	15.172598	-1.265371
H	13.027386	16.0863	-2.332674
H	13.921797	15.41929	-0.954602
H	13.189095	17.020707	-0.842504

Compound **4** S_1
TD-DFT CAM-B3LYP/6-31G(d)

Symbol	X	Y	Z
N	5.204073	9.569984	-2.270024
C	9.27316	14.293386	0.265638
C	3.908754	9.83137	-2.744037
C	5.845942	8.349955	-2.535302
C	5.873137	10.551467	-1.513371
C	1.66733	9.095181	-3.255147
C	7.217011	10.898223	-1.811623
C	7.230843	12.543126	0.021891
C	5.213259	11.208152	-0.441699
H	4.192681	10.929695	-0.197231
C	11.651665	15.475027	-0.783111
C	5.876644	12.158012	0.289301
H	5.358835	12.647531	1.108726
C	10.480679	14.318768	1.012115
C	3.548325	11.144861	-3.088901
C	7.199853	5.966881	-3.068969
C	1.315847	10.396642	-3.612466
C	9.296033	14.904432	-1.012516
C	2.948676	8.807281	-2.820995
C	7.85517	11.857743	-1.07087
C	7.394879	14.027147	2.272533
C	6.737502	7.815406	-1.590064
H	6.882583	8.331199	-0.648796
C	7.134862	13.067615	3.282001
C	6.339766	14.782862	4.815984
C	5.655342	7.686121	-3.759815
C	6.606752	15.733134	3.832494
H	6.400115	16.781146	4.040995
C	7.398856	6.629148	-1.860635
C	10.573705	13.709923	2.391384
C	6.327515	6.504483	-4.015028
C	11.631991	14.888828	0.480751
C	2.262019	11.414226	-3.525556
C	10.467431	15.478001	-1.507444
C	6.620702	13.456241	4.51931
H	6.445001	12.696284	5.27831
C	7.379799	16.496877	1.601062
H	6.881242	16.304642	0.645955
H	8.444205	16.615474	1.381637
H	7.005501	17.449753	1.986689
C	7.130852	15.385038	2.592828
C	7.423107	11.596737	3.089127
H	6.603581	11.087846	2.568751
H	7.557104	11.100133	4.05516
H	8.321105	11.429886	2.489765
C	8.065226	14.994283	-1.884774
H	7.910389	14.076312	-2.463334
C	12.91586	16.07458	-1.339841
C	5.76187	15.186332	6.146718
H	5.834885	14.374434	6.875932
H	4.702075	15.454013	6.057092
H	6.278342	16.058886	6.560277
B	7.962033	13.615227	0.848655
H	0.929413	8.300825	-3.301012
H	7.717273	10.413438	-2.64445
H	4.290793	11.930935	-3.026377
H	7.726458	5.041589	-3.277504
H	0.307899	10.615725	-3.948636
H	3.211744	7.801951	-2.513605
H	8.881635	12.114523	-1.315084
H	5.002154	8.119338	-4.508176
H	8.074677	6.216599	-1.118731
H	11.607233	13.721021	2.749822
H	10.229472	12.671101	2.397908
H	9.958474	14.249335	3.116454
H	6.182986	6.004433	-4.967229
H	12.545787	14.877621	1.071801
H	1.996914	12.429099	-3.80323
H	10.448271	15.951689	-2.487113
H	8.157023	15.819888	-2.597329
H	7.156705	15.14688	-1.297594
H	12.708803	16.707295	-2.20766
H	13.619128	15.296427	-1.660537
H	13.433142	16.685157	-0.592451

Compound **4** S_1
TD-DFT B3LYP/6-31G(d)

Symbol	X	Y	Z
N	5.176779	9.530756	-2.299699
C	9.161325	14.447609	0.186592
C	4.202824	9.933019	-3.214407
C	5.510197	8.18861	-2.109659
C	5.872051	10.54896	-1.514253
C	2.132506	9.528699	-4.426194
C	7.107498	11.054111	-1.957298
C	7.232549	12.542476	0.022389
C	5.303671	11.021289	-0.31772
H	4.33821	10.643712	0.012857
C	11.315181	15.942548	-0.997528
C	5.973075	11.983745	0.419181
H	5.508644	12.353904	1.329119
C	10.458719	14.492077	0.776768
C	4.263912	11.232245	-3.777432
C	6.246526	5.508188	-1.714274
C	2.226628	10.795066	-5.013232
C	8.986603	15.1899	-1.015371
C	3.103786	9.09415	-3.536605
C	7.754987	12.021129	-1.206906
C	7.519474	13.888455	2.363705
C	6.044437	7.768484	-0.866229
H	6.164287	8.492627	-0.071594

C	7.493036	12.851816	3.338763
C	6.722328	14.385993	5.082753
C	5.398026	7.245748	-3.164717
C	6.749605	15.411537	4.132642
H	6.457646	16.417916	4.432118
C	6.385856	6.440106	-0.675772
C	10.776579	13.728547	2.046012
C	5.764372	5.923709	-2.959981
C	11.494706	15.220088	0.186045
C	3.294763	11.639768	-4.678458
C	10.048023	15.914883	-1.57599
C	7.104056	13.114506	4.660257
H	7.112112	12.298352	5.382574
C	7.105688	16.370618	1.86262
H	6.425738	16.190514	1.020646
H	8.089421	16.578232	1.43034
H	6.762478	17.274518	2.378429
C	7.137986	15.188343	2.809245
C	7.902934	11.427571	3.017063
H	7.081613	10.859102	2.560746
H	8.205455	10.896187	3.92705
H	8.732156	11.392362	2.304471
C	7.654182	15.260727	-1.736178
H	7.494863	14.390633	-2.386908
C	12.45438	16.714743	-1.622062
C	6.291107	14.65151	6.506713
H	6.482192	13.785327	7.149702
H	5.217683	14.877491	6.570232
H	6.821757	15.510392	6.936792
B	7.966866	13.619661	0.852613
H	1.284154	8.887654	-4.644955
H	7.554912	10.672955	-2.872997
H	5.08138	11.886808	-3.506444
H	6.533626	4.472952	-1.559225
H	1.463135	11.131492	-5.707536
H	2.994281	8.137931	-3.039095
H	8.71933	12.383705	-1.55233
H	5.082743	7.574848	-4.14768
H	6.772222	6.124388	0.287984
H	11.827001	13.861191	2.328697
H	10.599808	12.653027	1.920812
H	10.154642	14.051194	2.886746
H	5.697417	5.218016	-3.782187
H	12.474094	15.222988	0.664059
H	3.364011	12.628051	-5.121482
H	9.871422	16.484596	-2.488223
H	7.60098	16.156838	-2.365552
H	6.812444	15.27855	-1.037737
H	12.100538	17.364875	-2.42977
H	13.213218	16.044354	-2.048965
H	12.967262	17.345731	-0.885289

Compound **4** S_1
TD-DFT BLYP/6-31G(d)

Symbol	X	Y	Z
N	5.161357	9.507387	-2.317783
C	9.140669	14.508163	0.179491
C	4.264159	9.913867	-3.326965
C	5.406066	8.145957	-2.045201
C	5.868091	10.542895	-1.519388
C	2.237812	9.539935	-4.654614
C	7.11258	11.037351	-1.959332
C	7.236552	12.547646	0.026363
C	5.289333	11.023566	-0.32741
H	4.310769	10.655447	-0.001252
C	11.250788	16.070994	-1.059118
C	5.964964	12.000029	0.414782
H	5.490194	12.381171	1.323402
C	10.459971	14.591745	0.748278
C	4.43076	11.180214	-3.961382
C	5.958519	5.426223	-1.498899
C	2.438136	10.769242	-5.31038
C	8.926037	15.249601	-1.032983
C	3.134542	9.108891	-3.672945
C	7.768708	12.011859	-1.197293
C	7.568127	13.867571	2.40128
C	5.832853	7.74458	-0.744809
H	5.94373	8.494949	0.035683
C	7.557215	12.796717	3.359896
C	6.811794	14.293734	5.171821
C	5.311156	7.161525	-3.077695
C	6.822284	15.351415	4.242195
H	6.528361	16.35487	4.575228
C	6.083046	6.39839	-0.481392
C	10.829127	13.833379	2.018657
C	5.585806	5.819996	-2.797934
C	11.471719	15.351212	0.130844
C	3.535968	11.582999	-4.952088
C	9.965435	16.002425	-1.620412
C	7.185058	13.024093	4.702293
H	7.201692	12.181827	5.405797
C	7.135994	16.382434	1.979722
H	6.461749	16.212868	1.121273
H	8.12286	16.626941	1.554814
H	6.768979	17.269084	2.524403
C	7.1904	15.165038	2.896348
C	7.9712	11.374873	2.990815
H	7.157121	10.82149	2.48705
H	8.252095	10.802085	3.891531
H	8.824981	11.365339	2.293884
C	7.568772	15.287316	-1.729788
H	7.390906	14.38544	-2.344311
C	12.352246	16.909255	-1.689878
C	6.439334	14.527332	6.627998
H	6.242984	13.576493	7.15184
H	5.536385	15.1569	6.722911
H	7.246191	15.04485	7.181366
B	7.98367	13.643427	0.871022
H	1.365595	8.925608	-4.891298
H	7.571357	10.643815	-2.872642
H	5.267525	11.814583	-3.675155
H	6.174424	4.376901	-1.284077
H	1.734154	11.104157	-6.075945
H	2.939885	8.186965	-3.124222
H	8.745423	12.366155	-1.539068
H	5.085058	7.469863	-4.098825
H	6.385789	6.099236	0.524745
H	11.89506	13.975268	2.266006
H	10.651663	12.748599	1.908418
H	10.231199	14.158527	2.885221
H	5.532889	5.082562	-3.602648
H	12.467645	15.377451	0.590906
H	3.687373	12.544314	-5.44849
H	9.757145	16.564371	-2.539892
H	7.495503	16.162586	-2.398219
H	6.738571	15.333494	-1.006311
H	12.100941	17.192063	-2.726196
H	13.315274	16.368265	-1.712366
H	12.528388	17.846998	-1.128875

Compound **4** S_1
TD-DFT CAM-BHandHLYP/6-31G(d)

Symbol	X	Y	Z
N	5.206151	9.57359	-2.2676
C	9.267862	14.29237	0.260607
C	3.923601	9.838656	-2.749083
C	5.839652	8.356323	-2.52043
C	5.873671	10.5528	-1.512738
C	1.688146	9.113974	-3.27589
C	7.210809	10.900488	-1.810373
C	7.227726	12.538746	0.01835
C	5.218489	11.205467	-0.444032
H	4.205225	10.929549	-0.19952
C	11.634718	15.482841	-0.785
C	5.878678	12.153679	0.285653
H	5.362012	12.637875	1.098327

C	10.474283	14.319803	1.002391
C	3.572182	11.148765	-3.104424
C	7.175779	5.965318	-3.028859
C	1.348128	10.411209	-3.643334
C	9.2886	14.904194	-1.012679
C	2.959178	8.822945	-2.829743
C	7.849072	11.856807	-1.071842
C	7.39487	14.019679	2.27132
C	6.718755	7.820047	-1.568723
H	6.860448	8.335007	-0.635535
C	7.138556	13.062151	3.278094
C	6.353855	14.769629	4.814251
C	5.655074	7.686558	-3.739302
C	6.614861	15.718249	3.833644
H	6.409419	16.758322	4.042965
C	7.370083	6.631518	-1.826349
C	10.575593	13.705849	2.374947
C	6.317608	6.50272	-3.981852
C	11.618848	14.894062	0.47311
C	2.296502	11.421215	-3.553442
C	10.453688	15.482417	-1.505548
C	6.632294	13.447906	4.514807
H	6.461616	12.692001	5.267955
C	7.369842	16.485992	1.607034
H	6.868496	16.295914	0.661062
H	8.425356	16.610035	1.3832
H	6.9958	17.429528	1.99596
C	7.131275	15.37323	2.594964
C	7.424094	11.59417	3.086257
H	6.604039	11.085872	2.581126
H	7.568619	11.104777	4.046539
H	8.310231	11.426814	2.482481
C	8.061692	14.993519	-1.884484
H	7.915115	14.086837	-2.469682
C	12.892359	16.090167	-1.338172
C	5.784375	15.170342	6.145269
H	5.852388	14.359204	6.865196
H	4.733347	15.445977	6.060533
H	6.306856	16.030349	6.55934
B	7.960119	13.612228	0.846425
H	0.951138	8.329322	-3.322366
H	7.708685	10.420571	-2.637668
H	4.31183	11.926572	-3.040854
H	7.693157	5.041417	-3.226507
H	0.351739	10.63227	-3.987834
H	3.210004	7.825237	-2.514655
H	8.867947	12.109382	-1.316625
H	5.017522	8.11717	-4.49144
H	8.031572	6.220375	-1.081977
H	11.604426	13.719913	2.725285
H	10.239341	12.67181	2.37692
H	9.96628	14.235134	3.101729
H	6.178684	6.002514	-4.926052
H	12.527375	14.883587	1.058146
H	2.041465	12.428387	-3.8385
H	10.431509	15.955022	-2.477089
H	8.149683	15.821855	-2.583519
H	7.15712	15.134929	-1.301768
H	12.687809	16.685978	-2.223606
H	13.613628	15.322822	-1.618673
H	13.379152	16.732865	-0.607317

Compound **4** S_1
TDA CAM-B3LYP/6-31G(d)

Symbol	X	Y	Z
N	5.199232	9.563186	-2.275516
C	9.254926	14.309505	0.25085
C	3.940696	9.859976	-2.813477
C	5.811402	8.318446	-2.468387
C	5.872383	10.550477	-1.514469
C	1.703092	9.194841	-3.432628
C	7.197949	10.924575	-1.841766
C	7.22815	12.538922	0.018406
C	5.226001	11.172503	-0.419275
H	4.214069	10.875527	-0.159862
C	11.604559	15.53282	-0.816588
C	5.890848	12.12401	0.312185
H	5.381491	12.593095	1.14885
C	10.475038	14.333512	0.976755
C	3.637486	11.185355	-3.172808
C	7.11731	5.879898	-2.854476
C	1.412581	10.505832	-3.809675
C	9.250884	14.9425	-1.016715
C	2.951203	8.866703	-2.936164
C	7.836809	11.885232	-1.099195
C	7.408263	14.003221	2.281252
C	6.672378	7.810706	-1.479124
H	6.814137	8.371851	-0.564009
C	7.18312	13.032994	3.288839
C	6.386855	14.724188	4.849046
C	5.633321	7.599657	-3.665217
C	6.618816	15.685236	3.867028
H	6.397918	16.728178	4.086217
C	7.306809	6.596297	-1.675388
C	10.596844	13.700114	2.342558
C	6.281814	6.392033	-3.846912
C	11.611744	14.924219	0.436905
C	2.385164	11.493469	-3.675382
C	10.408548	15.536191	-1.520896
C	6.685056	13.404799	4.538104
H	6.53619	12.636869	5.294869
C	7.335339	16.475637	1.626087
H	6.813842	16.283467	0.683223
H	8.392017	16.608513	1.379455
H	6.959766	17.421304	2.027942
C	7.125641	15.353964	2.615727
C	7.491008	11.567897	3.081707
H	6.664532	11.04668	2.585164
H	7.663668	11.071051	4.041525
H	8.371919	11.418724	2.453385
C	8.00604	15.034509	-1.868839
H	7.859131	14.13009	-2.470269
C	12.853102	16.156123	-1.382504
C	5.82795	15.109303	6.193272
H	5.916172	14.289269	6.911627
H	4.765749	15.373286	6.123474
H	6.346962	15.979329	6.609161
B	7.958503	13.60971	0.844266
H	0.942063	8.425343	-3.511377
H	7.68875	10.457179	-2.690381
H	4.398651	11.948203	-3.067436
H	7.625381	4.933384	-3.005627
H	0.429992	10.75634	-4.195212
H	3.163401	7.855268	-2.610605
H	8.853974	12.16088	-1.361651
H	5.012966	8.012832	-4.451639
H	7.956645	6.205146	-0.899604
H	11.634523	13.722769	2.688301
H	10.271432	12.655208	2.332379
H	9.981186	14.213804	3.085628
H	6.149117	5.85107	-4.778173
H	12.535349	14.911726	1.012546
H	2.165945	12.515848	-3.964884
H	10.368455	16.026092	-2.491959
H	8.073463	15.881102	-2.559235
H	7.103669	15.153627	-1.265034
H	12.627834	16.783708	-2.249503
H	13.569536	15.391598	-1.706712
H	13.363343	16.777884	-0.639356