Electronic Supplementary Material (ESI) for Chemical Science.

Tuning the π-Bridge of Quadrupolar Triarylborane Chromophores for One- and Two-Photon Excited Fluorescence Imaging of Lysosomes in Live Cells

Electronic Supporting Information

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Experimental Section

General information. Unless otherwise noted, the following conditions apply. Reactions were performed using standard Schlenk or glovebox (Innovative Technology Inc.) techniques under an atmosphere of argon. Only oven-dried glassware was used. Solvents used for reactions were HPLC grade, dried using an Innovative Technology Inc. Solvent Purification System, and further deoxygenated. Tris(dibenzylideneacetone)-dipalladium(0),[1] bis[4-(*N*,*N*-dimethyl-amino)-2,6-xylyl]-2,6-dimethyl-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborlan-2-yl)-phenyl-borane,[2] 2,7-dibromopyrene,[3] *N*-*tert*-butoxycarbonyl-3,6-dibromo-9*H*-carbazole,[4] di-*tert*-butyl-3,6-bis-(5-bromothiophen-2-yl)-1,4-dioxopyrrolo[3,4-c]pyrrole-2,5-(1H,4H)-dicarboxylate[5] and 2-(3,5-dimethylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane[6] were synthesized according to literature procedures. All other starting materials were purchased from commercial sources and were used without further purification.

Reaction progress was monitored using thin layer chromatography (TLC) plates pre-coated with a layer of silica (Polygram® Sil G/UV254) with fluorescent indicator UV254 from Marchery-Nagel. Automated flash column chromatography was performed using a Biotage® Isolera Four system with silica gel (Biotage SNAP cartridge KP-Sil 50g or KP-Sil 100g obtained from Biotage) as the stationary phase and the solvent system indicated. Solvents were generally removed *in vacuo* using a rotary evaporator at a maximum temperature of 50 °C.

^{1}H, and ^{13}C{^{1}H} solution NMR spectroscopic data were obtained at ambient temperature using a Bruker Avance 500 NMR spectrometer (operating at 500 MHz for ^{1}H and 125 MHz for ^{13}C{^{1}H}). Chemical shifts (δ) were referenced to solvent peaks as follows: ^{1}H NMR spectra were referenced to residual protiated solvent in CD_2Cl_2 (5.32 ppm), CD_3OD (3.31 ppm) or DMSO (2.50 ppm); and ^{13}C{^{1}H} spectra were referenced to CD_2Cl_2 (53.84 ppm), CD_3OD (49.00 ppm) or DMSO (39.52 ppm). The solid-state magic-angle spinning (MAS) NMR spectra were recorded using a Bruker DSX-400 or a Bruker Avance Neo 400 WB spectrometer operating at 128.38 MHz for ^{11}B and a 4 mm rotor. Spectra are referenced to external BF_3•Et_2O. Isotropic chemical shifts were estimated by simulating the observed spectrum using the Solid Line Shape Analysis 2.2.4 (SOLA) in Bruker TopSpin. Due to the very small amount of sample of **4M** and **5M**, a residual boron signal of the boron nitride stator is observable at -30 to 15 ppm.

Elemental analyses were performed on an Elementar vario MICRO cube elemental analyser. As is common for related organo-$BMes_2$ compounds, carbon analyses of **1M**, **2**, **2M**, **4M** and **5M** were up to 3.6% below the calculated value, while hydrogen, nitrogen and sulphur analyses were satisfactory. This has been ascribed previously to the formation of boron carbide.[7] High resolution mass spectrometry (MS) was performed with a Thermo Fisher Scientific Exactive Plus Orbitrap MS System with either an atmospheric-pressure chemical ionization (APCI),

liquid injection field desorption ionization (LIFDI) or a heated-electrospray ionization (HESI) probe.

General photophysical measurements. All measurements were performed in standard quartz cuvettes (1 cm x 1 cm cross-section), except for **5M** in DMSO (plastic or silylated cuvettes were used). UV-visible absorption spectra were recorded using an Agilent 8453 diode array UV-visible spectrophotometer. The molar extinction coefficients were calculated from three independently prepared samples in MeCN (**1M**-**5M**) and hexane (**1**-**5**) solution.
The emission 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, and all spectra were fully corrected for the spectral response of the instrument. All solutions used in photophysical measurements had a concentration lower than 5×10^{-6} M to minimize inner filter effects during fluorescence measurements.

Fluorescence quantum yield measurements. The fluorescence quantum yields 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, unless stated otherwise.

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 polarizer set to the magic angle. Solutions were excited with a pulsed diode laser at a wavelength of 376 nm (**1**-**4**, **1M**-**4M**) and 509 nm (**5**, **5M**) at repetition rates of 10 or 20 MHz, as appropriate. The full-width-at-half-maximum (FWHM) of the pulse from the diode laser was *ca.* 80 ps with an instrument response function (IRF) of *ca.* 230 ps FWHM and *ca.* 200 ps with an instrument response function (IRF) of *ca.* 1120 ps FWHM, respectively. The IRFs were measured from the scatter of an aqueous suspension of Ludox at the excitation wavelength. Decays were recorded to 10 000 counts in the peak channel with a record length of 8 192 channels. The band pass of the emission monochromator and a variable neutral density filter on the excitation side were adjusted to give a signal count rate of <60 kHz. Iterative reconvolution of the IRF with one decay function and non-linear least-squares analysis were used to analyse the data. 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.

Two-photon induced fluorescence spectroscopy. The two-photon absorption cross-section of the compounds was determined by the relative two-photon induced fluorescence technique.

In detail, the fundamental laser source used is an amplified Ti: sapphire laser (Solstice, Spectra Physics) operating at 1 KHz repetition rate with 100 fs pulses at 800 nm. 70% of the available energy seeds a computer-controlled optical parametric amplifier (TOPAS-C, Light Conversion), which produces pulses in the range of 290 - 2600 nm. Excitation of the samples was achieved using a protected silver parabolic mirror, and vertically polarized light with the excitation energy varying in the 0.2 – 3 μJ range. The latter conditions established by using a series of three thin broadband polarizers and a mechanical rotational mount. Maintenance of identical excitation conditions for both reference and samples was achieved using a high precision motorized rotational stage to ensure that the unknown compounds and the secondary reference standard are subjected to the same excitation conditions. Perylene in CH_2Cl_2, Coumarin 540A in CCl_4, Rhodamine 6G in CH_3OH and Styryl 9M in $CHCl_3$ were used as reference compounds.[8, 9] The emitted fluorescence signal was detected at 90° with respect to the excitation beam, and recorded using a compact CCD spectrometer. Two-photon excitation was verified by log-log plots of fluorescence intensities *vs*. excitation power at various wavelengths, all giving slopes of 2 (see Figure S5).

Theoretical studies. All calculations (DFT and TD-DFT) were carried out with the Gaussian 09 (Rev. D.01) program package[10] and were performed on a parallel cluster system. GaussView 5.0.9 was used to visualize the results, to measure calculated structural parameters, and to plot orbital surfaces (isovalue: ±0.03 [e a_0^{-3}]$^{1/2}$). The ground-state geometries were optimized using the B3LYP functional[11-13] in combination with the 6-31G(d) basis set.[14, 15] The optimized geometries were confirmed to be local minima by performing frequency calculations and obtaining only positive (real) frequencies. Stability analysis showed the wavefunction to be stable in each case. Based on these optimized structures, the lowest-energy gas-phase vertical transitions were calculated (singlets, 10 states) by TD-DFT, using the Coulomb-attenuated functional CAM-B3LYP[16] in combination with the 6-31G(d) basis set.[11, 12] The CAM-B3LYP functional has been shown to be effective for the ICT systems, hence its selection here.[17-21] The optimizations were conducted with inclusion of hexane (**1**-**5**) or water (**1M**-**5M**) solvation through the polarizable continuum model (PCM). The ultrafine integration grid was used throughout.

Cell culture. HeLa and HepG2 cells (RIKEN Cell Bank, Japan) were cultured in Dulbecco's modified Eagle's medium (DMEM, Wako) containing 10% fetal bovine serum (FBS, Biosera) and 1% Antibiotic-Antimycotic (AA, Wako) at 37 °C in a 5% CO_2/95% air incubator. Cells (5 × 10^4) were seeded in poly-lysine coated glass-bottom dishes three days before imaging. In order to facilitate the generation of lipid droplets, the HepG2 cells were treated with fatty acids (oleic acid:palmitic acid = 2:1, 1 mM) in DMEM for 24 h before staining with dyes.

Staining Experiments. The incubation medium was removed from the HeLa cells, and the cells were further incubated with 5 μM **1**-**3** in DMEM containing 0.5% DMSO for 1 h in a CO_2 incubator. Afterwards, the cells were rinsed with DMEM three times and the dish was filled with 1.5 mL of DMEM. Fluorescence images before and after washing were obtained with a FV10i-DOC confocal laser-scanning microscope (OLYMPUS), with a 405 nm LD laser for excitation. The fluorescence signals were collected between 570-670 nm.

The incubation medium was removed from the HepG2 cells and the cells were further incubated with 5 μM of **1** or 5 μM of **1** premixed with 0.04% Pluronic F-127 in DMEM containing 0.5% DMSO for 24 h in a CO_2 incubator. Fluorescence images before and after washing were obtained with a FV10i-DOC confocal laser-scanning microscope (OLYMPUS), with a 405 nm LD laser for excitation. The fluorescence signals were collected between 570-670 nm.

Co-staining experiments. The incubation medium was removed from the cells, and the cells were further incubated with 0.5 μM **1M**-**5M** in DMEM containing 0.5% DMSO for 2 h in a CO_2 incubator. Then the cells were rinsed with DMEM three times and the dish was filled with 2.0 mL of DMEM containing 0.1 μM LysoTracker™ Green or LysoTracker™ Red (Invitrogen) and further incubated for 20 min in a CO_2 incubator. Fluorescence images were obtained with a confocal microscope (TCS SP8 STED 3X; Leica), including an inverted DMI6000 CS microscope equipped with a laser diode (405 nm), a tuneable (470 – 670 nm) pulsed white light laser (WLL; repetition rate of 78 MHz) for excitation. For confocal imaging, a HyD detector and 100 × oil-immersion objective (NA 1.4) were used. The dyes were excited with the 405 nm diode laser (**1M**, **2M**, **3M, 4M**), and the 561 nm wavelength of the WLL (LysoTracker™ Red). The fluorescence signals were collected between 450 and 550 nm (**1M**, **2M**, **3M**), 500 and 605 nm (**4M**), 600 and 750 nm (LysoTracker™ Red in the co-staining experiment with **1M**-**3M**) and 607 and 786 nm (LysoTracker™ Red in the co-staining experiment with **4M**) with a time gating interval of 0.1 − 12 ns. Each image was recorded with a line average of 4. To avoid crosstalk among the channels, the emission signals were collected independently in the sequential scanning mode. Fluorescence images (**5M**) were obtained with an FV10i-DOC confocal laser-scanning microscope (OLYMPUS), using LD lasers of 473 nm and 559 nm were used for the excitation of LysoTracker™ Green and **5M**, respectively. The fluorescence signals were collected between 490 and 540 nm (LysoTracker™ Green) and 570 and 670 nm (**5M**). Images were processed with Fiji software.

Cytotoxicity evaluation. HeLa cells were seeded into a flat-bottomed 96-well plate (1×10^4 cells/well) and incubated in DMEM at 37 °C in a 5% CO_2/95% air incubator for 24 h. The medium was then replaced with culture medium (100 μL/well) containing various concentrations of **1M**-**5M** (0, 0.5, 1, 5, and 10 μM) in DMEM (0.5% DMSO). Then the cells were incubated for 24 h at 37 °C, MTT reagent (10 μL/well, 0.5 mg/mL) in PBS was added to each

well, and the plates were incubated for another 4 h in a CO_2 incubator. The medium was then removed, the formazan crystals were solubilized in DMSO (100 μL/well) for 10 min at room temperature, and the absorbance of each well was measured using a SpectraMax i3 (Molecular Devices) with an excitation at 535 nm.

Uptake pathway. The incubation medium was removed from the cells, and the cells were incubated with 0.5 μM **5M** in 1.5 mL DMEM. Fluorescence images (**5M**) were obtained with a FV10i-DOC confocal laser-scanning microscope (OLYMPUS), and a 559 nm LD laser was used for the excitation of **5M**. The fluorescence signals were collected between 570 and 670 nm every 10 min over a period of 2 hours. Images were processed with Fiji software.
In the cellular uptake control experiment, cells were stained at 37 °C with 500 nM of **5M** in DMEM, washed with fresh DMEM and subsequent imaging. In the cellular uptake experiment at 4 °C experiment, cells were incubated at 4 °C for 30 min, then grown in DMEM containing **5M** (500 nM) for 2 h at 4 °C, washed with fresh DMEM and subsequent imaging. In the cellular uptake experiment in the presence of NaN_3 cells were first pretreated at 37 °C for 30 min with DMEM containing 0.1% NaN_3 and then incubated with DMEM containing **5M** (500 nM) and 0.1% NaN_3 for 2 h at 37 °C. Afterwards, the cells were washed with fresh DMEM followed by imaging. Fluorescence images were obtained with a FV10i-DOC confocal laser-scanning microscope (OLYMPUS), and a 559 nm LD laser was used for the excitation of **5M**. The fluorescence signals were collected between 570 and 670 nm.

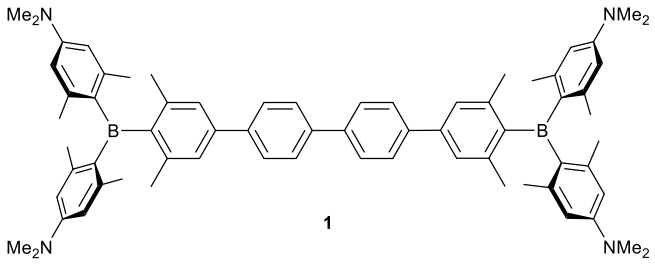
Photostability. The incubation medium was removed from the cells, and the cells were further incubated with 0.5 μM **5M** or 0.1 μM LysoTracker™ Red (Invitrogen) in DMEM in a CO_2 incubator for 2 h or 20 min, respectively. Then cells stained with **5M** were rinsed with DMEM three times and the dish was filled with 1.5 mL of DMEM. Imaging experiments were conducted using a Leica TCS SP8 STED 3X system (Leica Microsystems), including an inverted DMI6000 CS microscope equipped with a tuneable (470 − 670 nm) pulsed white light laser (WLL; repetition rate of 78 MHz) for excitation. For confocal imaging, a HyD detector and 100 × oil-immersion objective (NA 1.4) were used. For the evaluation of photostability under confocal conditions, dye-stained cells prepared above were irradiated with a WLL at 561 nm, the fluorescence signals were collected between 570 and 770 nm and images were acquired at the following setting: 1024 × 1024 pixels; scan speed of 100 Hz; bidirectional model; zoom factor of 5; line average of 4; frame average of 1. The total signal intensity of each image was normalized to the value of the first image and plotted as a function of the number of recorded confocal images.

TPA imaging. The incubation medium was removed from the cells, and the cells were further incubated with 0.5 μM **5M** in DMEM in a CO_2 incubator for 2 h. Then the cells were rinsed with DMEM three times and the dish was filled with 15 mL of DMEM containing 20 mM HEPES (pH

= 7.4). Imaging experiments were conducted using a Leica SP8-MP system (Leica Microsystems), equipped with a tuneable (680 − 1300 nm) for laser two-photon excitation. For TPA imaging, a HyD detector with a 650/50 bandpass filter and a Lens HC Fluotar L 25 × 0.95 W VisIR objective were used. The dye was excited with the 720 nm wavelength of the laser and fluorescence signals were collected between 600 and 700 nm.

Synthesis

4,4´-Bis[4-[bis[4-(*N*,*N*-dimethylamino)-2,6-xylyl]boryl]-3,5-xylyl]-1,1´-biphenyl 1



1

Compound **6** (500 mg, 0.93 mmol, 2.1 eq.), 4,4´-dibromobiphenyl (138 mg, 0.44 mmol, 1.0 eq.) and KOH (149 mg, 2.66 mmol, 6.0 eq.) were dissolved in a degassed mixture of H_2O (5 mL) and toluene (10 mL). The reaction mixture was degassed for 15 min and SPhos (36.4 mg, 88.7 μmol, 20 mol%) and $Pd_2(dba)_3$ (24.3 mg, 23.5 μmol, 5 mol%) were added. After heating to 85 °C for 3 d, the aqueous layer was extracted with hexane (3 x 30 mL). The solvent was evaporated and the crude product was purified by automated flash column chromatography (KP-Sil 50g, hexane:ethylacetate 5:1) to obtain compound **1** as a yellow solid (310 mg, 72%).

^{1}H NMR (500 MHz, CD_2Cl_2): δ = 7.77 – 7.73 (m, 8H), 7.25 (s, 4H), 6.33 (s, 4H), 6.33 (s,4H), 2.96 (s, 24H), 2.12 (s, 12H), 2.03 (s, 12H), 1.99 (s, 12H) ppm.

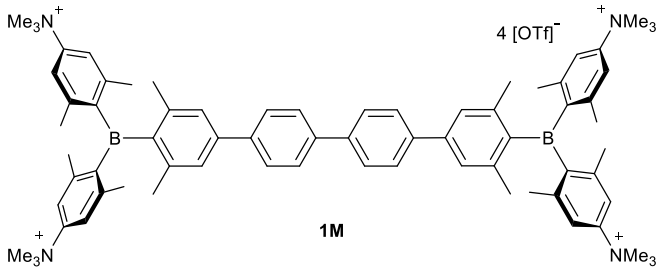
^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2): δ = 151.7, 149.0, 143.2, 142.9, 141.1, 140.4, 140.2, 139.6, 136.2, 127.5, 127.4, 126.0, 111.9, 111.8, 40.2, 24.0, 23.8, 23.1 ppm.

Solid-State ^{11}B{^{1}H} NMR (128 MHz): Isotropic chemical shift δ_{iso} = 72.8 ppm, quadrupole coupling constant C_Q = 4.49 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

HRMS (ESI$^+$): *m/z* found: $[M]^+$ 975.6637; calc. for $[C_{68}H_{80}B_2N_4]^+$ 975.6642 ($|\Delta|$ = 0.51 ppm).

Elem. Anal. Calc. (%) for $C_{68}H_{80}B_2N_4$: C 83.77, H 8.27, N 5.75; found: C 83.83, H 8.28, N 5.49.

4,4´-Bis[4-[bis[4-(*N*,*N*,*N*-trimethylammonio)-2,6-xylyl]-boryl]-3,5-xylyl]-1,1´-biphenyl tetratriflate 1M



In a soda-lime glass vial, compound **1** (15.0 mg, 15.4 μmol, 1.0 eq.) was dissolved in degassed DCM (2.0 mL). After the addition of MeOTf (7.74 μL, 69.2 μmol, 4.5 eq.), the reaction mixture was stirred at r.t. for 2 d. The white precipitate was collected by filtration and washed with Et_2O (6.0 mL) to obtain compound **1M** as a pale yellow solid (19.6 mg, 78%).

^{1}H NMR (500 MHz, CD_3OD): δ = 7.80 (s, 8H), 7.58 (s, 4H), 7.58 (s, 4H), 7.40 (s, 4H), 3.67 (s, 36H), 2.26 (s, 12H), 2.18 (s, 12H), 2.13 (s, 12H) ppm.

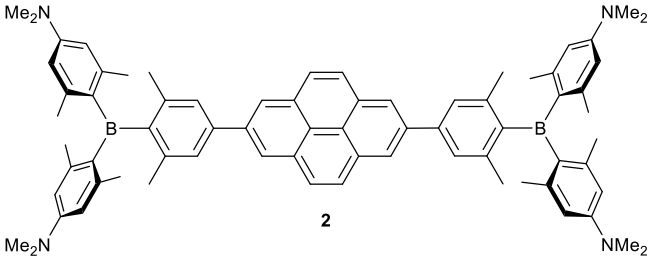
^{13}C{^{1}H} NMR (125 MHz, CD_3OD): δ = 149.7, 149.5, 145.2, 145.0, 144.5, 144.4, 142.9, 141.2, 140.5, 128.4, 128.3, 127.8, 121.8 (q, J = 319 Hz), 120.1, 57.5, 23.6, 23.6, 23.4 ppm.

Solid-State ^{11}B{^{1}H} NMR (128 MHz): Isotropic chemical shift δ_{iso} = 79.2 ppm, quadrupole coupling constant C_Q = 4.86 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

HRMS (ESI$^+$): *m/z* found: $[M\text{-}2OTf]^{2+}$ 666.3266; calc. for $[C_{74}H_{92}B_2F_6N_4O_6S_2]^{2+}$ 666.3269 ($|\Delta|$ = 0.45 ppm).

Elem. Anal. Calc. (%) for $C_{76}H_{92}B_2F_{12}N_4O_{12}S_4$: C 55.95, H 5.68, N 3.43, S 7.86; found: C 54.76, H 5.88, N 3.53, S 7.62.

2,7-Bis[4-[bis[4-(*N*,*N*-dimethylamino)-2,6-xylyl]boryl]-3,5-xylyl]-pyrene 2



2

Compound **6** (1.00 g, 1.86 mmol, 2.2 eq.), 2,7-dibromopyrene (304 mg, 0.85 mmol, 1.0 eq.) and KOH (285 mg, 5.07 mmol, 6.0 eq.) were dissolved in a degassed mixture of H_2O (5 mL) and toluene (10 mL). The reaction mixture was degassed for 15 min and SPhos (104 mg, 254 μmol, 30 mol%) and $Pd_2(dba)_3$ (52.5 mg, 50.7 μmol, 6 mol%) were added. After heating to 85 °C for 16 h, the aqueous layer was extracted with hexane (3 x 30 mL). The solvent was evaporated and the crude product was purified by automated flash column chromatography (KP-Sil 100g, hexane:ethylacetate 9:1). The yellow solid obtained was dissolved in DCM and crystallized by adding MeOH to afford **2** as a yellow solid (399 mg, 46%).

^{1}H NMR (500 MHz, CD_2Cl_2): δ = 8.49 (s, 4H), 8.15 (s, 4H), 7.51 (s, 4H), 6.36 (s, 8H), 2.97 (s, 24H), 2.21 (s, 12H), 2.07 (s, 12H), 2.05 (s, 12H) ppm.

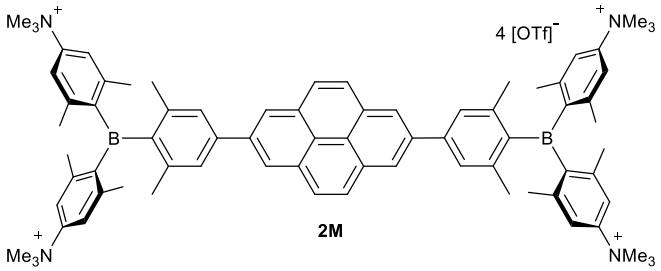
^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2): δ = 151.7, 149.1, 143.3, 143.0, 141.4, 141.0, 139.3, 136.2, 131.9, 128.2, 127.0, 124.1, 123.9, 111.9, 111.9, 40.2, 24.1, 23.9, 23.2 ppm.

Solid-State ^{11}B{^{1}H} NMR (128 MHz): Isotropic chemical shift δ_{iso} = 71.9 ppm, quadrupole coupling constant C_Q = 4.51 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

HRMS (ESI$^+$): *m/z* found: $[M]^+$ 987.6623; calc. for $[C_{69}H_{80}B_2N_4]^+$ 987.6642 ($|\Delta|$ = 1.92 ppm).

Elem. Anal. Calc. (%) for $C_{72}H_{82}B_2N_4$: C 84.36, H 8.06, N 5.47; found: C 82.87, H 8.05, N 5.33.

2,7-Bis[4-[bis[4-(*N*,*N*,*N*-trimethylammonio)-2,6-xylyl]-boryl]-3,5-xylyl]-pyrene tetratriflate 2M



In a soda-lime glass vial, compound **2** (15.0 mg, 146 μmol, 1.0 eq.) was dissolved in degassed DCM (3.0 mL). After the addition of MeOTf (7.47 μL, 65.7 μmol, 4.5 eq.), the reaction mixture was stirred at r.t. for 2 d. The precipitate was collected by filtration and washed with Et_2O (6.0 mL) to obtain compound **2M** as a brown solid (21.4 mg, 91%).

^{1}H NMR (500 MHz, CD_3OD): δ = 8.55 (s, 4H), 8.23 (s, 4H), 7.69 (s, 4H), 7.62 (br s, 4H), 7.62 (br s, 4H), 3.67 (s, 36H), 2.33 (s, 12H), 2.23 (s, 12H), 2.22 (s, 12H) ppm.

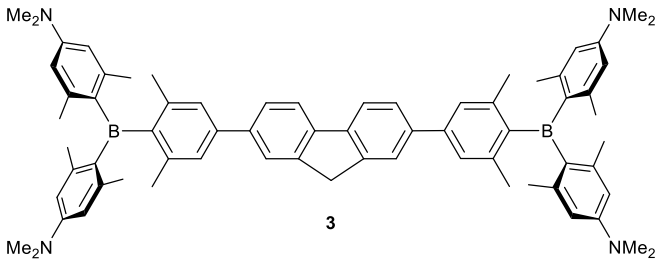
^{13}C{^{1}H} NMR (125 MHz, CD_3OD): δ = 149.7, 149.5, 145.3, 145.2, 145.0, 144.5, 143.0, 139.4, 133.1, 129.1, 128.8, 125.1, 124.7, 121.8 (q, *J* = 319 Hz), 120.1, 57.5, 23.6, 23.5 ppm.

Solid-State ^{11}B{^{1}H} NMR (128 MHz): Isotropic chemical shift δ_{iso} = 77.2 ppm, quadrupole coupling constant C_Q = 4.78 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

HRMS (ESI^+): *m/z* found: $[M\text{-}4OTf]^{4+}$ 270.6869; calc. for $[C_{76}H_{92}B_2N_4]^{4+}$ 270.6872 ($|\Delta|$ = 1.11 ppm).

Elem. Anal. Calc. (%) for $C_{80}H_{92}B_2F_{12}N_4O_{12}S_4$: C 57.21, H 5.52, N 3.34 S 7.64; found: C 56.17, H 5.75, N 3.39, S 7.37.

2,7-Bis[4-[bis[4-(*N*,*N*-dimethylamino)-2,6-xylyl]-boryl]-3,5-xylyl]-fluorene 3



3

Compound **6** (1.00 g, 1.86 mmol, 2.2 eq.), 2,7-dibromofluorene (274 mg, 0.85 mmol, 1.0 eq.) and KOH (285 mg, 5.08 mmol, 6.0 eq.) were dissolved in a degassed mixture of H_2O (5 mL) and toluene (10 mL). The reaction mixture was degassed for 15 min and SPhos (104 mg, 253 μmol, 30 mol%) and $Pd_2(dba)_3$ (52.5 mg, 50.7 μmol, 6 mol%) were added. After heating to 85 °C for 16 h, the aqueous layer was extracted with hexane (3 x 30 mL). The solvent was evaporated and the crude product was purified by automated flash column chromatography (KP-Sil 100g, hexane:ethylacetate 98:2). The yellow solid obtained was dissolved in Et_2O and crystallized by adding MeOH to afford **3** as a yellow solid (511 mg, 61%).

^{1}H NMR (500 MHz, CD_2Cl_2): δ = 7.88 – 7.85 (m, 4H), 7.72 – 7.70 (m, 2H), 7.28 (s, 4H), 6.35 (s, 4H), 6.35 (s, 4H), 4.03 (s, 2H), 2.97 (s, 24H), 2.14 (s, 12H), 2.06 (s, 12H), 2.02 (s, 12H) ppm.

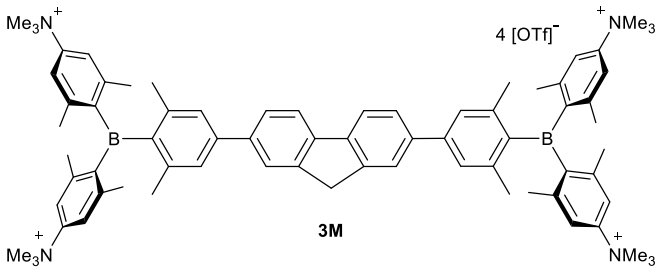
^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2): δ = 151.7, 148.8, 144.7, 143.2, 142.9, 141.1, 141.1, 140.9, 140.1, 136.3, 126.2, 126.0, 123.8, 120.4, 111.9, 111.8, 40.2, 37.4, 24.0, 23.8, 23.2 ppm.

Solid-State ^{11}B{^{1}H} NMR (128 MHz): Isotropic chemical shift δ_{iso} = 73.0 ppm, quadrupole coupling constant C_Q = 4.53 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

HRMS (ESI$^+$): *m/z* found: $[M]^+$ 987.6623; calc. for $[C_{69}H_{80}B_2N_4]^+$ 987.6642 ($|\Delta|$ = 1.92 ppm).

Elem. Anal. Calc. (%) for $C_{69}H_{80}B_2N_4$: C 83.96, H 8.17, N 5.68; found: C 83.94, H 8.38, N 5.71.

2,7-Bis[4-[bis[4-(*N*,*N*,*N*-trimethylammonio)-2,6-xylyl]-boryl]-3,5-xylyl]-fluorene tetratriflate 3M



In a soda-lime glass vial, compound **3** (15.0 mg, 15.2 μmol, 1.0 eq.) was dissolved in degassed DCM (2.0 mL). After the addition of MeOTf (7.74 μL, 68.4 μmol, 4.5 eq.), the reaction mixture was stirred at r.t. for 2 d. The yellow precipitate was collected by filtration and washed with Et_2O (6.0 mL) to obtain compound **3M** as a yellow solid (22.8 mg, 91%).

^{1}H NMR (500 MHz, CD_3OD): δ = 7.93 – 7.92 (m, 2H), 7.91 - 7.90 (m, 2H), 7.73 - 7.72 (m, 2H), 7.58 (s, 8H), 7.41 (s, 4H), 4.06 (s, 2H), 3.67 (s, 36H), 2.27 (s, 12H), 2.18 (s, 12H), 2.13 (s, 12H) ppm.

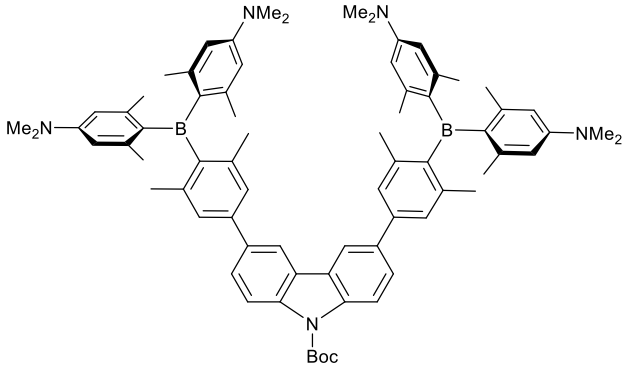
^{13}C{^{1}H} NMR (125 MHz, CD_3OD): δ = 149.6, 149.5, 145.8, 145.3, 144.9, 144.5, 142.9, 142.4, 140.3, 127.9, 127.0, 124.6, 121.8 (q, *J* = 319 Hz), 121.4, 120.1, 57.5, 37.8, 23.6, 23.4 ppm.

Solid-State ^{11}B{^{1}H} NMR (128 MHz): Isotropic chemical shift δ_{iso} = 77.1 ppm, quadrupole coupling constant C_Q = 4.76 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

HRMS (ESI^+): *m/z* found: $[M\text{-}4OTf]^{4+}$ 261.6870; calc. for $[C_{73}H_{92}B_2N_4]^{4+}$ 261.6872 (|Δ| = 0.76 ppm).

Elem. Anal. Calc. (%) for $C_{77}H_{92}B_2F_{12}N_4O_{12}S_4$: C 56.28, H 5.64, N 3.41 S 7.80; found: C 56.38, H 5.94, N 3.56 S 7.63.

3,6-Bis[4-[bis[4-(*N*,*N*-dimethylamino)-2,6-xylyl]boryl]-3,5-xylyl]-*N*-*Boc*-carbazole 4



4

Compound **6** (1.00 g, 1.86 mmol, 2.2 eq.), 3,6-dibromo-*N*-*Boc*-carbazole (359 mg, 0.84 mol, 1.0 eq.) and KOH (283 mg, 5.04 mmol, 6.0 eq.) were dissolved in a degassed mixture of H_2O (10 mL) and toluene (20 mL). The reaction mixture was degassed for 15 min and SPhos (103 mg, 252 μmol, 30 mol%) and $Pd_2(dba)_3$ (52.2 mg, 50.4 μmol, 6 mol%) were added. After heating to 85 °C for 3 d, the aqueous layer was extracted with hexane (3 x 30 mL). The solvent was evaporated and the crude product was purified by automated flash column chromatography (KP-Sil 100g, hexane:ethylacetate 97:3 → 95:5 → 90:10) to obtain compound **4** as a yellow solid (757 mg, 83%).

^{1}H NMR (500 MHz, CD_2Cl_2): δ = 8.42 - 8.41 (m, 2H), 8.40 - 8.39 (m, 2H), 7.87 - 7.85 (m, 2H), 7.40 (s, 4H), 6.39 - 6.38 (m, 8H), 3.00 (s, 24H), 2.21 (s, 12H), 2.10 (s, 12H), 2.08 (s, 12H), 1.84 (s, 9H) ppm.

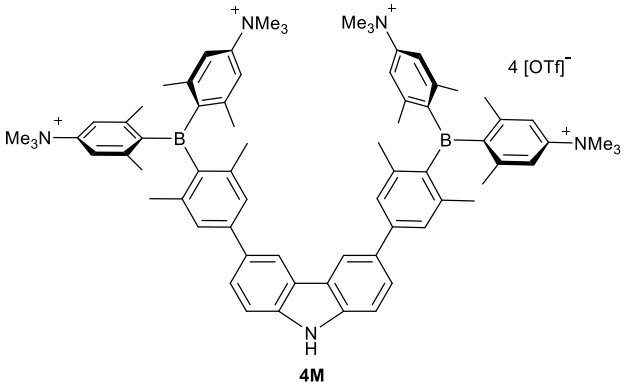
^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2): δ = 151.7, 151.4, 148.7, 143.2, 142.9, 141.2, 140.8, 138.7, 136.6, 136.3, 126.7, 126.4, 126.3, 118.0, 116.9, 112.0, 111.9, 84.4, 40.2, 28.6, 24.1, 23.9, 23.3 ppm.

^{11}B{^{1}H} NMR (160 MHz, CD_2Cl_2): δ = 73 ppm.

HRMS (ESI$^+$): *m/z* found: $[M+H]^+$ 1088.7112; calc. for $[C_{73}H_{88}B_2N_5O_2]^+$ 1088.7119 ($|\Delta|$ = 0.64 ppm).

Elem. Anal. Calc. (%) for $C_{73}H_{87}B_2N_5O_2$: C 80.58, H 8.06, N 6.44; found: C 80.65, H 8.24, N 6.53.

3,6-Bis[4-[bis[4-(*N*,*N*,*N*-trimethylammonio)-2,6-xylyl]-boryl]-3,5-xylyl]-9*H*-carbazole tetratriflate 4M



4M

In a soda-lime glass vial, compound **4** (44.0 mg, 40.1 μmol, 1.0 eq.) was dissolved in degassed DCM (6.0 mL). After the addition of MeOTf (20.6 μL, 183 μmol, 4.5 eq.), the reaction mixture was stirred at r.t. for 18 h. The pale yellow precipitate was collected by filtration and washed with Et_2O (18 mL) to obtain the methylated compound as a pale yellow solid (50.0 mg, 71%). The crude product (50.0 mg, 28.7 μmol, 1.0 eq.) was directly deprotected and therefore dissolved in MeOH (1.0 mL) in a soda-lime glass vial. After the addition of a solution of TfOH (3.0 mL) in MeOH (5.0 mL), the reaction mixture was stirred at r.t. for 1 h. The reaction mixture was quenched with water (8.0 mL) and the precipitate was collected by centrifugation and washed with water until the washing solution was pH neutral. The compound **4M** was isolated as a yellow solid (32.0 mg, 68%).

^{1}H NMR (500 MHz, CD_2Cl_2): δ = 8.49 (d, *J* = 1.3 Hz, 2H), 7.77 – 7.75 (m, 2H), 7.56 (s, 8H), 7.56 – 7.54 (m, 2H), 7.47 (s, 4H), 3.65 (s, 36H), 2.27 (s, 12H), 2.16 (s, 12H), 2.13 (s, 12H) ppm.

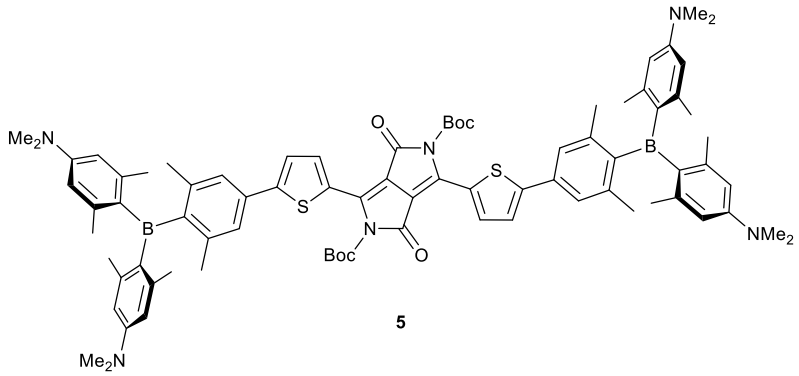
^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2): δ = 149.7, 149.5, 146.2, 144.9, 144.4, 144.1, 142.9, 141.9, 132.5, 127.9, 126.1, 125.1, 121.8 (q, *J* = 319 Hz), 120.0, 120.0, 119.6, 112.3, 57.5, 23.7, 23.6, 23.4 ppm.

Solid-State ^{11}B{^{1}H} NMR (128 MHz): Isotropic chemical shift δ_{iso} = 77.0 ppm, quadrupole coupling constant C_Q = 4.77 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.1.

HRMS (ESI$^+$): *m/z* found: $[M\text{-}2OTf]^{2+}$ 672.8241; calc. for $[C_{74}H_{91}B_2F_6N_5O_6S_2]^{2+}$ 672.8245 (|Δ| = 0.59 ppm).

Elem. Anal. Calc. (%) for $C_{76}H_{91}B_2F_{12}N_5O_{12}S_4$: C 55.51, H 5.58, N 4.26, S 7.80; found: C 53.52, H 5.71, N 4.30, S 7.51.

2,5-Di-*N*-*Boc*-3,6-bis[5-[4-[bis[4-(*N*,*N*-dimethylamino)-2,6-xylyl]boryl]-3,5-xylyl]-2-thienyl]-1,4-diketopyrrolo[3,4-c]pyrrole 5



5

Compound **6** (4.59 g, 8.83 mmol, 2.2 eq.), 2,5-di-*N*-*Boc*-3,6-di(5-bromo-thien-2-yl)-1,4-diketopyrrolo[3,4-c]pyrrole (2.55 g, 3.87 mol, 1.0 eq.) and KOH (1.30 g, 23.2 mmol, 6.0 eq.) were dissolved in a degassed mixture of H_2O (46 mL) and toluene (93 mL). The reaction mixture was degassed for 15 min and SPhos (479 mg, 1.17 mmol, 30 mol%) and $Pd_2(dba)_3$ (277.0 mg, 0.27 mmol, 7 mol%) were added. After heating to 85 °C for 3 d, the aqueous layer was extracted with DCM (7 x 100 mL) and dried over Na_2SO_4. The solvent was evaporated and the crude product was purified by automated flash column chromatography (KP-Sil 100g, hexane:ethylacetate 9:1 → 5:1) to obtain compound **5** as a violet solid (1.48 g, 29%).

^{1}H NMR (500 MHz, CD_2Cl_2): δ = 8.23 (d, *J* = 4.2 Hz, 2H), 7.47 (d, *J* = 4.2 Hz, 2H), 7.26 (s, 4H), 6.33 (s, 4H), 6.32 (s, 4H), 2.96 (s, 24H), 2.09 (s, 12H), 2.03 (s, 12H), 1.97 (s, 12H), 1.63 (s, 18H) ppm.

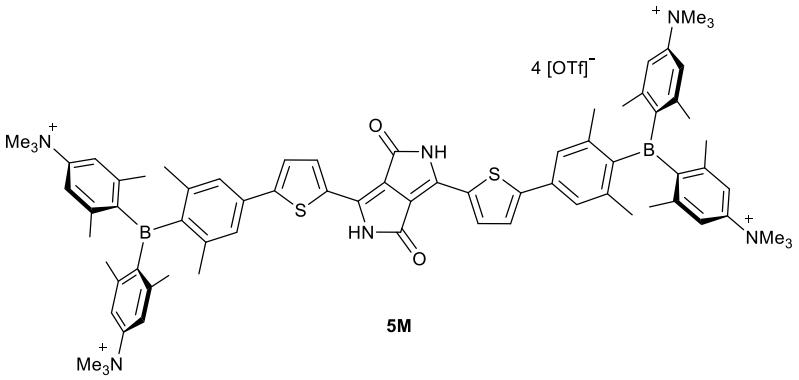
^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2): δ = 159.4, 152.2, 151.8, 151.6, 149.4, 143.4, 142.9, 141.5, 137.2, 135.8, 135.4, 132.8, 128.6, 125.2, 124.1, 111.9, 110.5, 86.1, 40.2, 27.9, 24.1, 23.9, 23.0 ppm.

Solid-State ^{11}B{^{1}H} NMR (128 MHz): Isotrope chemical shift δ_{iso} = 72.5 ppm, quadrupole coupling constant C_Q = 4.49 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.1.

HRMS (LIFDI): *m/z* found: $[M]^+$ 1320.6856; calc. for $[C_{80}H_{94}B_2N_6O_6S_2]^+$ 1320.6857 ($|\Delta|$ = 0.08 ppm).

Elem. Anal. Calc. (%) for $C_{80}H_{94}B_2N_6O_6S_2$: C 72.72, H 7.17, N 6.36, S 4.85; found: C 72.97, H 7.40, N 6.49, S 4.52.

3,6-Bis[5-[4-[bis[4-(*N*,*N*,*N*-trimethylammonio)-2,6-xylyl]boryl]-3,5-xylyl]-2-thienyl]-1,4-diketopyrrolo[3,4-c]pyrrole tetratriflate 5M



In a soda-lime glass vial, compound **5** (15.0 mg, 11.4 μmol, 1.0 eq.) was dissolved in degassed DCM (2.0 mL). After the addition of MeOTf (5.78 μL, 51.1 μmol, 4.5 eq.), the reaction mixture was stirred at r.t. for 7 h. The violet precipitate was collected by filtration and washed with Et_2O (6 mL) to obtain the methylated compound as a violet solid (22.0 mg, 97%). The crude product (22.0 mg, 11.1 μmol, 1.0 eq.) was directly deprotected and therefore dissolved in MeOH (0.2 mL) in a borosilicate glass vial. After the addition of a solution of TfOH (0.8 mL) in MeOH (2.0 mL), the reaction mixture was stirred at r.t. for 1.5 h. The reaction mixture was quenched with water (9.0 mL) and the precipitate was collected by centrifugation and washed with water until the washing solution was pH neutral. The compound **5M** was isolated as a violet solid (17.0 mg, 86%).

^{1}H NMR (500 MHz, CD_3OD): δ = 8.23 (d, *J* = 4.1 Hz, 2H), 7.69 (d, *J* = 4.1 Hz, 2H), 7.59 (s, 4H), 7.58 (s, 4H), 7.48 (s, 4H), 3.67 (s, 36H), 2.25 (s, 12H), 2.17 (s, 12H), 2.11 (s, 12H) ppm.

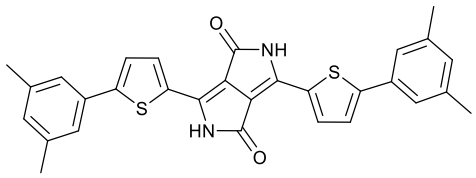
^{13}C{^{1}H} NMR (125 MHz, CD_3OD): δ = 163.7, 150.8, 149.8, 149.2, 147.0, 144.9, 144.6, 143.3, 137.9, 137.0, 134.2, 131.7, 126.8, 126.7, 112.8 (q, *J* = 319 Hz), 120.2, 120.2, 111.0, 57.5, 23.6, 23.5, 23.4 ppm.

Solid-State ^{11}B{^{1}H} NMR (128 MHz): Isotropic chemical shift δ_{iso} = 77.1 ppm, quadrupole coupling constant C_Q = 4.79 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

HRMS (ESI$^+$): *m/z* found: $[M\text{-}4OTf]^{4+}$ 295.1685; calc. for $[C_{74}H_{90}B_2N_6O_2S_2]^{4+}$ 295.1683 ($|\Delta|$ = 0.68 ppm).

Elem. Anal. Calc. (%) for $C_{78}H_{90}B_2F_{12}N_6O_{14}S_6$: C 52.70, H 5.10, N 4.73, S 10.82; found: C 51.49, H 5.40, N 4.48, S 10.14.

3,6-Bis[5-[4-[bis[3,5-xylyl]-2-thienyl]-1,4-diketopyrrolo[3,4-c]pyrrole 5A



5A

2-(3,5-dimethylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (140 mg, 0.60 mmol, 2.2 eq.), 2,5-di-*N*-*Boc*-3,6-di(5-bromo-thien-2-yl)-1,4-diketopyrrolo[3,4-c]pyrrole (180 mg, 0.27 mol, 1.0 eq.) and KOH (92.0 mg, 1.64 mmol, 6.0 eq.) were dissolved in a degassed mixture of H_2O (1.5 mL) and toluene (3 mL). The reaction mixture was degassed for 5 min and SPhos (33 mg, 82.0 μmol, 30 mol%) and $Pd_2(dba)_3$ (16.6 mg, 16.4 μmol, 6 mol%) were added. After heating to 85 °C for 3 d, the aqueous layer was extracted with DCM (3 x 30 mL). The solvent was evaporated and the crude product was purified by automated flash column chromatography (KP-Sil 100g, hexane:ethylacetate 99:1 → 97:3 → 95:5 → 90:10) to obtain the coupled compound as a violet solid (100 mg, 52%). The crude product (50.0 mg, 70.4 μmol, 1.0 eq.) was directly deprotected and therefore dissolved in DCM (1.0 mL) in a borosilicate glass vial. After the addition of a solution of TfOH (0.2 mL) in DCM (1.0 mL), the reaction mixture was stirred at r.t. for 1 h. The precipitate was collected by centrifugation and washed with water until the washing solution was pH neutral. The compound **5A** was isolated as a violet solid (30.0 mg, 84%).

^{1}H NMR (500 MHz, d^6-DMSO): δ = 11.23 (s, 2H), 8.17 (d, *J* = 4.0 Hz, 2H), 7.68 (d, *J* = 4.0 Hz, 2H), 7.36 (s, 4H), 7.05 (s, 2H), 2.34 (s, 12H) ppm.

^{13}C{^{1}H} NMR (125 MHz, d^6-DMSO): δ = 161.6, 149.4, 138.6, 135.5, 132.7, 132.5, 130.5, 129.5, 125.2, 123.6, 109.1, 20.9 ppm.

HRMS (ASAP$^-$): *m/z* found: [M]$^-$ 508.1281; calc. for [$C_{30}H_{24}N_2O_2S_2$]$^-$ 508.1285 (|Δ| = 0.79 ppm).

Elem. Anal. Calc. (%) for $C_{30}H_{24}N_2O_2S_2$: C 70.84, H 4.76, N 5.51, S 12.61; found: C 66.23, H 4.95, N 5.37, S 11.73.

Linear Optical Properties

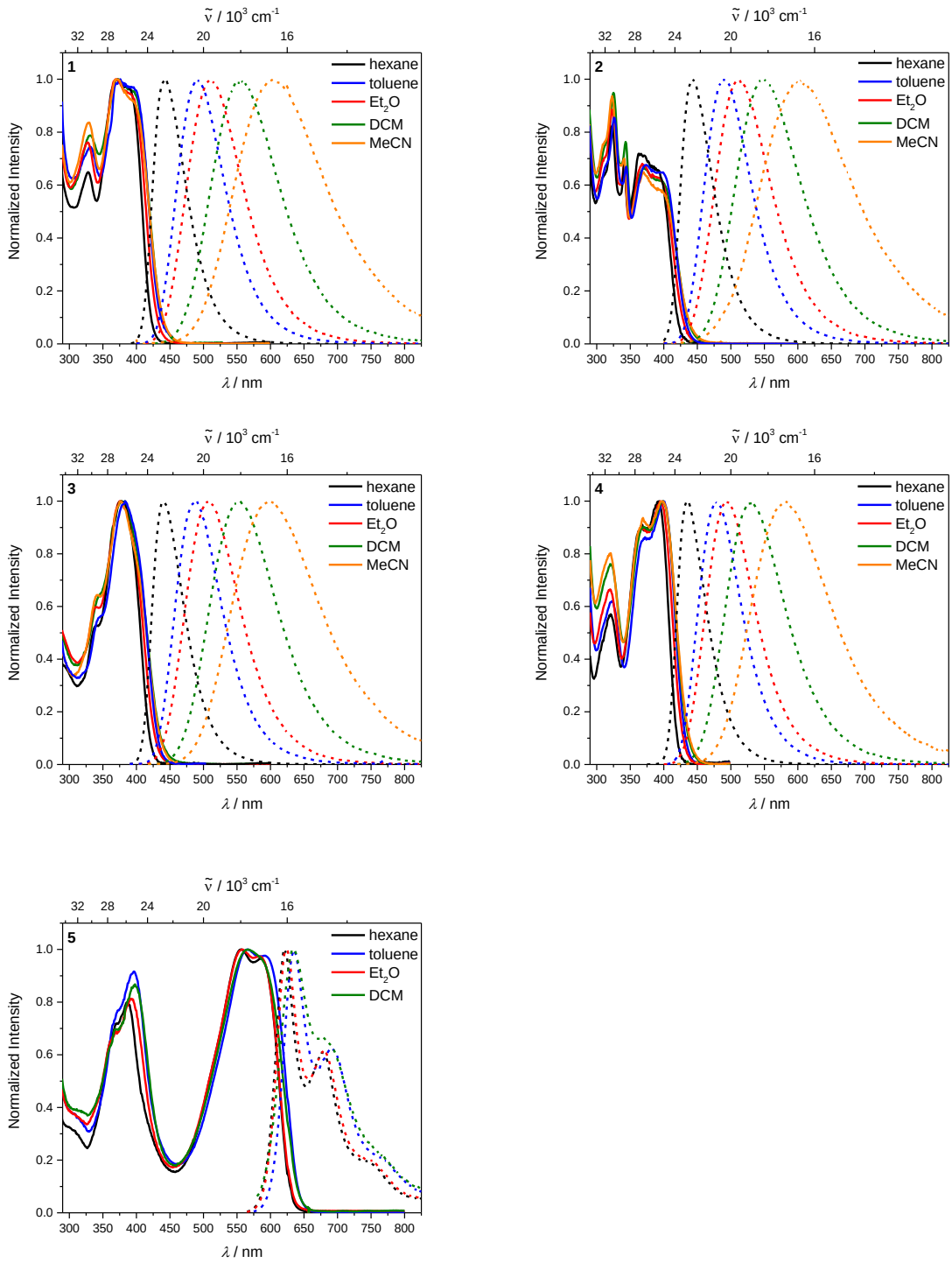


Figure S1. Absorption and emission spectra of **1** (first row, left), **2** (first row, right), **3** (second row, left), **4** (second row, right) and **5** (third row, left) in various solvents (hexane: black, toluene: blue, diethylether: red, dichloromethane: green, MeCN: orange).

Table S1. Photophysical data for compounds **1**-**5** in various solvents.

	solvent	λ_{abs} / nm	ε / M^{-1} cm^{-1}	λ_{em} / nm	Stokes shift / cm^{-1}	Φ_f	τ / ns	k_r / 10^8 s^{-1}	k_{nr} / 10^8 s^{-1}
1	hexane	372	69 000	442	4 300	0.14	1.5	0.9	5.8
	toluene	376		493	6 300	0.20	3.4	0.6	2.3
	Et_2O	369		511	7 500	0.24	5.9	0.4	1.3
	DCM	373		556	8 800	0.30	8.8	0.3	0.8
	MeCN	371		603	10 400	0.08	2.5	0.3	3.7
2	hexane	366	70 000	445	4 900	0.14	1.5	0.9	5.8
	toluene	372		490	6 500	0.23	3.6	0.6	2.2
	Et_2O	368		511	7 600	0.27	6.4	0.4	1.2
	DCM	371		545	8 600	0.34	9.6	0.4	0.6
	MeCN	370		603	10 400	0.08	2.9	0.3	3.1
3	hexane	378	82 000	441	3 800	0.16	1.5	1.1	5.6
	toluene	383		491	5 700	0.21	3.3	0.6	2.4
	Et_2O	375		509	7 000	0.23	6.5	0.4	1.1
	DCM	383		555	8 100	0.29	8.1	0.4	0.8
	MeCN	377		596	9 700	0.09	3.3	0.3	2.7
4	hexane	393	56 000	436	2 500	0.12	1.4	0.9	6.2
	toluene	399		479	4 200	0.23	3.3	0.7	2.3
	Et_2O	395		495	5 100	0.25	5.0	0.5	2.0
	DCM	399		530	6 200	0.41	10.3	0.4	0.6
	MeCN	398		581	7 900	0.15	6.3	0.2	1.4
5	hexane	557	59 000	622	1 900	0.57	2.4	2.4	1.8
	toluene	566		635	1 900	0.55	2.3	2.4	1.9
	Et_2O	558		624	1 900	0.40	2.0	2.0	3.0
	DCM	568		635	1 900	0.004	2.3	0.02	4.3

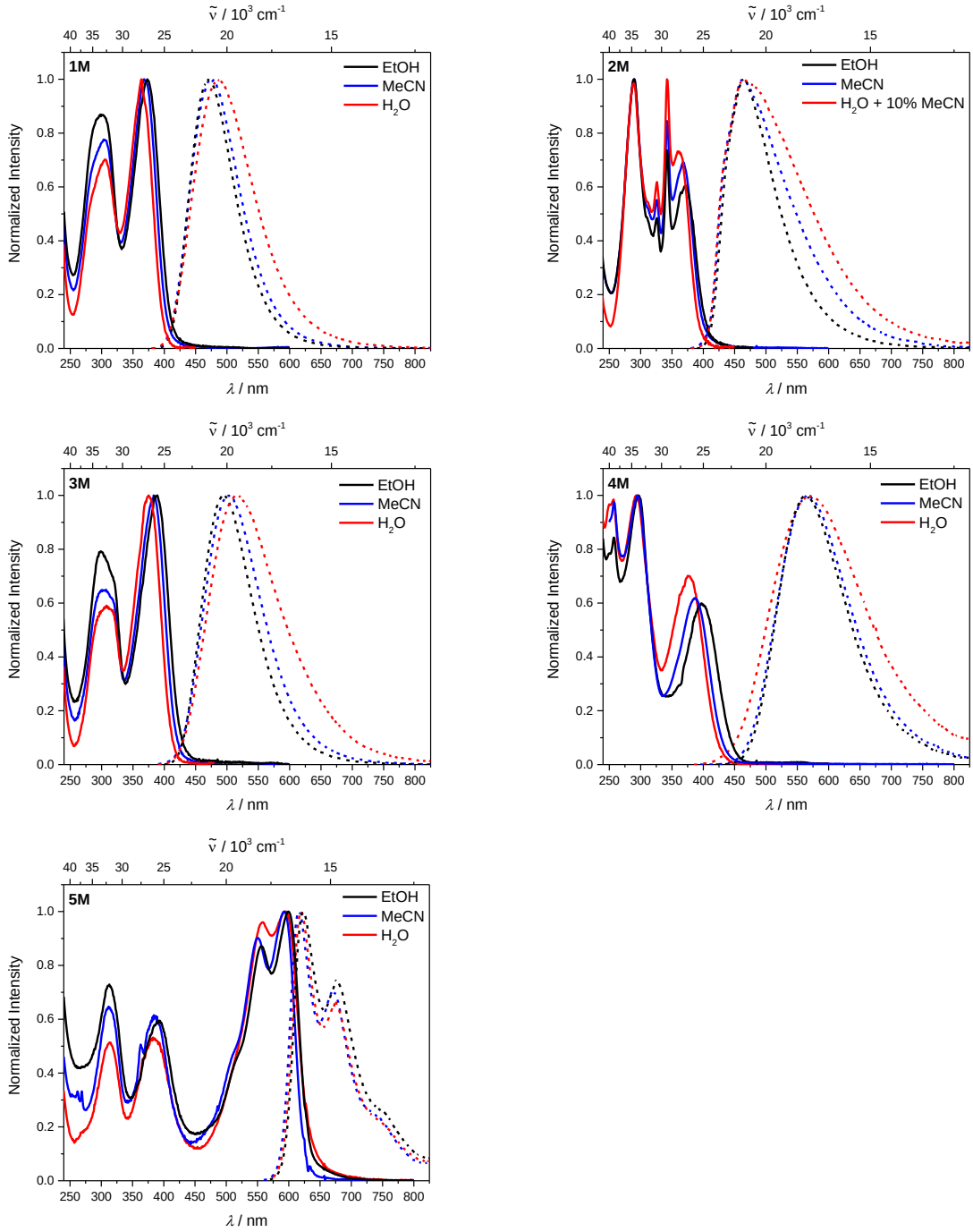


Figure S2. Absorption and emission spectra of **1M** (first row, left), **2M** (first row, right), **3M** (second row, left), **4M** (second row, right) and **5M** (third row, left) in various solvents (ethanol: black, acetonitrile: blue, water: red).

TD-DFT Calculations

Table S2. Lowest energy singlet electronic transitions of **1** in hexane solution. H = HOMO; L = LUMO

State	Symmetry	*E* (eV)	λ (nm)	*f*	Major (> 10%) contributions
S_1	B	3.50	354	0.054	H-1 → L+1 (44%), H → L (38%)
S_2	A	3.50	354	0.736	H-1 → L (38%), H → L+1 (44%),
S_3	B	3.70	335	1.496	H-4 → L (11%), H-3 → L+1 (29%), H-2 → L (37%)
S_4	A	3.77	329	0.000	H-3 → L (33%), H-2 → L+1 (42%)
S_5	B	4.19	296	0.778	H-4 → L (55%), H-3 → L+1 (15%)
S_6	A	4.37	284	0.000	H-5 → L (31%), H-4 → L+1 (42%)
S_7	A	4.59	270	0.001	H-7 → L+1 (29%), H-6 → L (25%)
S_8	B	4.59	270	0.008	H-7 → L (25%), H-6 → L+1 (29%)
S_9	B	4.62	269	0.381	H-9 → L+1 (12%), H-8 → L (14%), H-5 → L+1 (14%), H-4 → L+2 (22%)
S_{10}	A	4.62	268	0.055	H-11 → L+1 (30%), H-10 → L (39%)

Table S3. Lowest energy singlet electronic transitions of **2** in hexane solution. H = HOMO; L = LUMO

State	Symmetry	*E* (eV)	λ (nm)	*f*	Major (> 10%) contributions
S_1	A	3.50	355	0.352	H-1 → L+1 (11%), H → L+1 (29%), H → L+2 (41%)
S_2	A	3.50	355	0.427	H-1 → L+1 (25%), H-1 → L+2 (46%), H → L+1 (11%)
S_3	A	3.71	334	0.000	H-5 → L (41%), H-4 → L+1 (25%), H-4 → L+3 (20%)
S_4	A	3.72	333	1.533	H-3 → L+2 (30%), H-2 → L+1 (36%)
S_5	A	3.78	328	0.004	H-3 → L+1 (33%), H-2 → L+2 (39%)
S_6	A	3.92	317	0.345	H-4 → L (85%)
S_7	A	4.27	290	1.072	H-6 → L+2 (16%), H-5 → L+1 (51%), H-3 → L+2 (12%)
S_8	A	4.39	282	0.000	H-6 → L+1 (31%), H-5 → L+2 (41%)
S_9	A	4.55	273	0.263	H-5 → L (41%), H-4 → L+1 (39%), H-4 → L+3 (12%)
S_{10}	A	4.59	270	0.003	H-7 → L+1 (23%), H-7 → L+2 (32%)

Table S4. Lowest energy singlet electronic transitions of **3** in hexane solution. H = HOMO; L = LUMO

State	Symmetry	*E* (eV)	λ (nm)	*f*	Major (> 10%) contributions
S_1	A	3.49	354	0.384	H-1 → L (38%), H-1 → L+1 (43%), H-1 → L+2 (10%)
S_2	A	3.50	354	0.410	H → L (36%), H → L+1 (44%), H → L+2 (11%)
S_3	A	3.67	338	1.788	H-3 → L+1 (23%), H-2 → L (46%)
S_4	A	3.77	329	0.025	H-3 → L (31%), H-2 → L+1 (43%)
S_5	A	4.09	303	0.590	H-4 → L (54%), H-3 → L+1 (19%), H-2 → L+2 (13%)
S_6	A	4.34	286	0.007	H-5 → L (28%), H-4 → L+1 (45%)
S_7	A	4.54	273	0.268	H-13 → L (12%), H-5 → L+1 (26%), H-4 → L+2 (28%), H-2 → L+2 (10%)
S_8	A	4.59	270	0.008	H-7 → L (23%), H-7 → L+1 (26%)
S_9	A	4.59	270	0.004	H-6 → L (24%), H-6 → L+1 (29%)
S_{10}	A	4.61	269	0.030	H-10 → L (14%), H-10 → L+1 (10%), H-9 → L (20%). H-9 → L+1 (15%)

Table S5. Lowest energy singlet electronic transitions of **4** in hexane solution. H = HOMO; L = LUMO

State	Symmetry	*E* (eV)	λ (nm)	*f*	Major (> 10%) contributions
S_1	A	3.51	353	0.207	H-1 → L (76%)
S_2	A	3.52	352	0.581	H → L+1 (76%)
S_3	A	3.75	331	0.571	H-3 → L (34%), H-2 → L+1 (27%)
S_4	A	3.78	328	0.438	H-3 → L (35%), H-2 → L+1 (42%)
S_5	A	4.33	287	0.233	H-5 → L+1 (17%), H-4 → L (29%), H-4 →L+1 (11%)
S_6	A	4.36	284	0.157	H-5 → L (21%), H-4 →L (32%)
S_7	A	4.45	279	0.061	H-4 → L+2 (63%)
S_8	A	4.60	270	0.002	H-8 → L (55%)
S_9	A	4.60	269	0.003	H-7 → L+1 (56%)
S_{10}	A	4.64	267	0.022	H-9 → L+1 (58%)

Table S6. Lowest energy singlet electronic transitions of **5** in hexane solution. H = HOMO; L = LUMO

State	Symmetry	*E* (eV)	λ (nm)	*f*	Major (> 10%) contributions
S_1	A	2.31	537	1.739	H → L (94%)
S_2	A	3.35	370	0.294	H-2 → L (33%), H-2 → L+1 (20%), H-2 → L+2 (27%), H-2 → L+3 (10%)
S_3	A	3.35	370	0.116	H-5 → L (34%), H → L+1 (33%)
S_4	A	3.38	367	0.260	H-1 → L (28%), H-2 → L+1 (24%), H-2 → L+2 (26%), H-2 → L+3 (13%)
S_5	A	3.58	346	0.606	H-6 → L (12%), H-4 → L (28%), H-4 → L+2 (12%), H-3 → L+1 (12%)
S_6	A	3.68	337	0.012	H-3 → L (26%), H → L+1 (24%), H → L+3 (15%)
S_7	A	3.75	331	0.015	H-5 → L (43%), H → L+1 (15%)
S_8	A	3.80	326	0.122	H-1 → L (68%), H-1 → L+2 (12%), H-1→L+3 (10%)
S_9	A	3.81	325	0.161	H-2 → L (62%), H-2 → L+2 (17%), H-2 → L+3 (10%)
S_{10}	A	3.90	318	0.451	H-6 →L (41%), H-4 → L (17%)

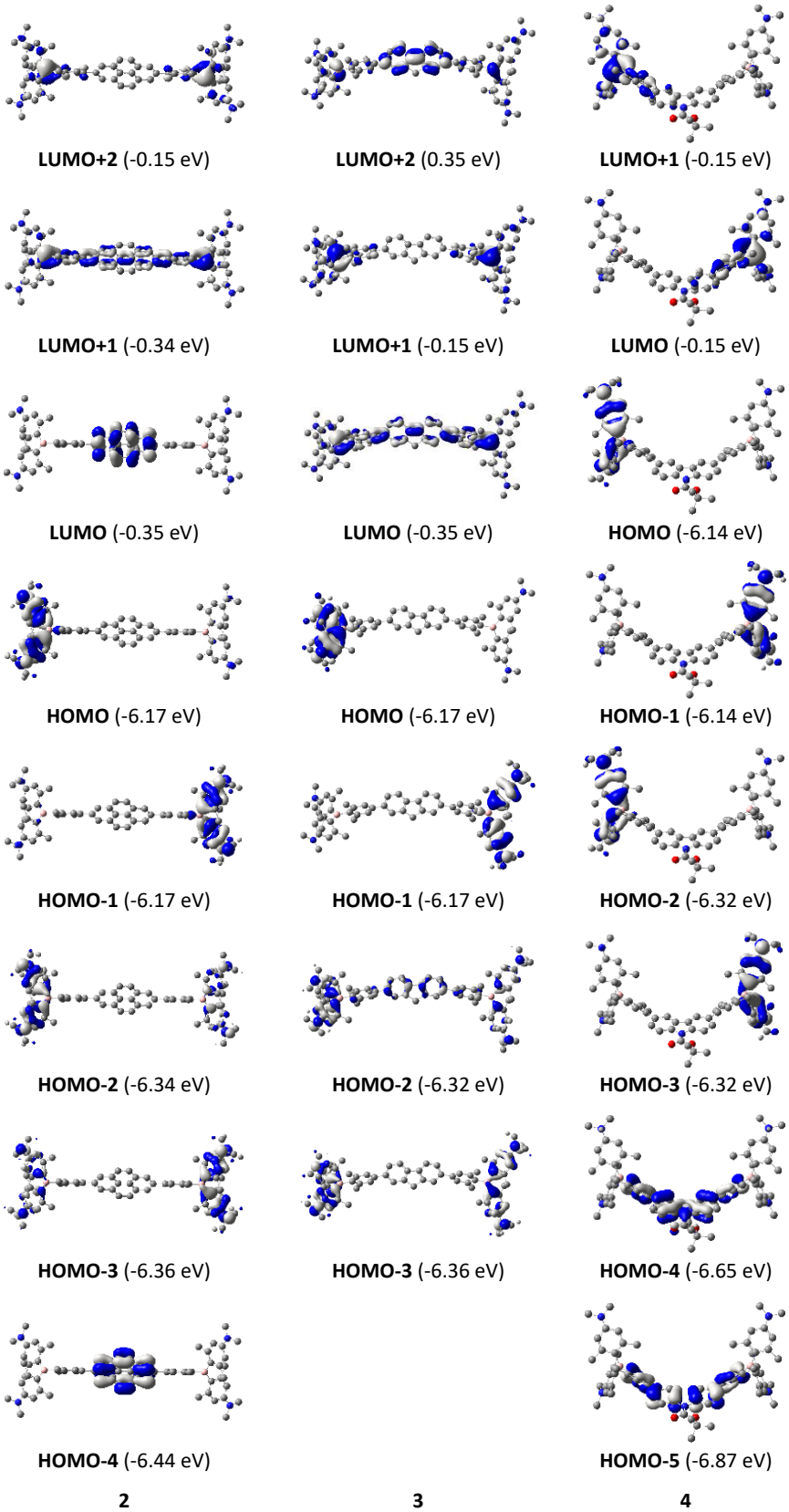


Figure S3. DFT (CAM-B3LYP/6-31 G(d))-calculated frontier orbitals for **2**-**4**. Hydrogen atoms are omitted for clarity. Surface isovalue: ± 0.03 [e a_0^{-3}]$^{1/2}$.

Table S7. Lowest energy singlet electronic transitions of **1M** in water. H = HOMO; L = LUMO[a]

State	Symmetry	*E* (eV)	λ (nm)	*f*	Major (> 10%) contributions
S_1	A	3.66	338	1.709	H-1 → L+1 (28%), H → L (53%)
S_1	*A_u*	*3.63*	*341*	*1.857*	*H-1 → L+1 (26%), H → L (56%)*
S_2	A	3.80	326	0.000	H-1 → L (38%), H → L+1 (40%)
S_2	*A_g*	*3.80*	*326*	*0.000*	*H-1 → L (37%), H → L+1 (40%)*
S_3	A	4.18	296	0.013	H-3 → L+1 (31%), H-2 → L (36%)
S_3	*A_g*	*4.18*	*297*	*0.000*	*H-3 → L (36%), H-2 → L+1 (31%)*
S_4	A	4.18	296	0.023	H-3 → L (36%), H-2 → L+1 (31%)
S_4	*A_u*	*4.18*	*297*	*0.036*	*H-3 → L+1 (31%), H-2 → L (36%)*
S_5	A	4.30	288	0.001	H-6 → L (17%), H-5 → L+1 (26%), H-4 → L (13%), H-3 → L (10%), H-2 → L+1 (12%)
S_5	*A_g*	*4.30*	*288*	*0.000*	*H-6 → L+1 (23%), H-5 → L (22%), H-3 → L (12%), H-2 → L+1 (10%)*
S_6	A	4.30	288	0.289	H-6 → L+1 (17%), H-5 → L (26%), H-4 → L+1 (13%), H-3 → L+1 (10%), H-2 → L (12%)
S_6	*A_u*	*4.30*	*288*	*0.292*	*H-6 → L (23%), H-5 → L+1 (23%), H-2 → L (12%)*
S_7	A	4.47	277	0.737	H-4 → L (10%), H → L+2 (34%)
S_7	*A_u*	*4.39*	*282*	*0.649*	*H-4 → L (12%), H-1 → L+1 (12%), H → L+2 (39%),*
S_8	A	4.64	267	0.000	H-7 → L (28%), H-6 → L+1 (11%), H-4 → L+1 (20%)
S_8	*A_g*	*4.64*	*267*	*0.000*	*H-8 → L (24%), H-4 → L+1 (24%)*

[a] black: without symmetry constraints, red: in C_i symmetry

Table S8. Lowest energy singlet electronic transitions of **2M** in water. H = HOMO; L = LUMO[a]

State	Symmetry	*E* (eV)	λ (nm)	*f*	Major (> 10%) contributions
S_1	A	3.65	339	0.004	H-1 → L+2 (29%), H → L (33%), H → L+3 (28%)
S_1	*A_u*	*3.51*	*354*	*0.005*	*H-1 → L+2 (27%), H → L (39%), H → L+3 (25%)*
S_2	A	3.69	335	1.733	H-2 → L+1 (30%), H-1 → L (52%)
S_2	*A_u*	*3.58*	*347*	*1.801*	*H-2 → L+1 (24%), H-1 → L (61%)*
S_3	A	3.81	325	0.012	H-2 → L (38%), H-1 → L+1 (39%)
S_3	*A_g*	*3.75*	*330*	*0.000*	*H-2 → L (37%), H-1 → L+1 (43%)*
S_4	A	3.92	316	0.562	H → L+2 (87%)
S_4	*A_u*	*3.86*	*321*	*0.753*	*H → L+2 (86%)*
S_5	A	4.16	298	0.021	H-3 → L (38%), H-3 → L+1 (27%)
S_5	*A_g*	*4.13*	*300*	*0.000*	*H-4 → L+1 (30%), H-3 → L (38%)*
S_6	A	4.18	297	0.016	H-4 → L (32%), H-4 → L+1 (32%)
S_6	*A_u*	*4.15*	*299*	*0.034*	*H-4 → L (38%), H-3 → L+1 (31%)*
S_7	A	4.30	288	0.119	H-7 → L (12%), H-6 → L (14%), H-6 → L+1 (14%), H-3 → L (12%)
S_7	*A_g*	*4.28*	*290*	*0.000*	*H-7 → L+1 (12%), H-6 → L (25%), H-5 → L+1 (17%), H → L+1 (18%)*
S_8	A	4.31	288	0.136	H-7 → L+1 (11%), H-6 → L (11%), H-5 → L+1 (10%), H-4 → L (11%), H-4 → L+1 (10%)
S_8	*A_u*	*4.29*	*289*	*0.086*	*H-6 → L+1 (19%), H-5 → L (13%), H-1 → L+2 (21%), H → L (16%)*

[a] black: without symmetry constraints, red: in C_i symmetry

Table S9. Lowest energy singlet electronic transitions of **3M** in water. H = HOMO; L = LUMO

State	Symmetry	*E* (eV)	λ (nm)	*f*	Major (> 10%) contributions
S_1	A	3.53	351	1.905	H-1 → L+1 (21%), H → L (60%)
S_2	A	3.74	332	0.023	H-5 → L+1 (11%), H-1 → L (34%), H-1 → L+1 (44%)
S_3	A	4.16	298	0.018	H-2 → L (32%), H-2 → L+1 (24%)
S_4	A	4.17	297	0.017	H-3 → L (28%), H-3 → L+1 (24%)
S_5	A	4.30	289	0.459	H-5 → L (18%), H-1 → L+1 (16%), H → L+2 (40%)
S_6	A	4.30	288	0.124	H-7 → L (10%), H-6 → L (16%), H-6 → L+1 (27%)
S_7	A	4.31	288	0.179	H-7 → L (18%), H-7 → L+1 (23%), H-6 → L (10%)
S_8	A	4.62	269	0.005	H-8 → L (22%), H-5 → L+1 (22%), H → L+1 (15%)

Table S10. Lowest energy singlet electronic transitions of **4M** in water. H = HOMO; L = LUMO

State	Symmetry	*E* (eV)	λ (nm)	*f*	Major (> 10%) contributions
S_1	A	3.58	346	1.113	H-5 → L (11%), H-2 → L+1 (12%), H-1 → L+1 (16%), H → L (48%)
S_2	A	3.70	335	0.298	H-5 → L+1 (15%), H-2 → L (14%), H-1 → L (20%), H → L+1 (40%)
S_3	A	4.19	296	0.013	H-3 → L (41%), H-3 → L+1 (23%)
S_4	A	4.20	296	0.019	H-4 → L (27%), H-4 →L+1 (34%)
S_5	A	4.23	293	0.021	H → L+2 (69%)
S_6	A	4.32	287	0.109	H-6 → L (27%), H-6 → L+1 (21%)
S_7	A	4.32	287	0.178	H-7 → L (17%), H-7 → L+1 (31%)
S_8	A	4.40	282	0.030	H-5 → L (19%), H → L (21%), H → L+5 (10%)

Table S11. Lowest energy singlet electronic transitions of **5M** in water. H = HOMO; L = LUMO[a]

State	Symmetry	*E* (eV)	λ (nm)	*f*	Major (> 10%) contributions
S_1	A	2.28	544	1.802	H → L (93%)
S_1	*A_u*	*2.33*	*532*	*1.596*	*H → L (94%)*
S_2	A	3.29	376	0.138	H-1 → L (22%), H → L+1 (53%), H → L+3 (10%)
S_2	*A_g*	*3.36*	*369*	*0.000*	*H-1 → L (25%), H → L+1 (45%), H → L+3 (11%)*
S_3	A	3.57	347	0.777	H-2 → L (28%), H-1 → L+1 (23%), H → L+2 (34%)
S_3	*A_u*	*3.59*	*345*	*0.917*	*H-2 → L (26%), H-1 → L+1 (24%), H → L+2 (32%)*
S_4	A	3.72	333	0.009	H-1 → L (54%), H →L+1 (19%)
S_4	*A_g*	*3.77*	*329*	*0.000*	*H-1 → L (51%), H →L+1 (20%)*
S_5	A	3.92	317	0.030	H-15 → L (23%), H-13 → L (28%)
S_5	*A_g*	*3.90*	*318*	*0.000*	*H-16 → L (27%), H-13 → L (29%), H → L+3 (10%)*
S_6	A	3.96	313	0.243	H-2 → L (43%), H → L+2 (25%)
S_6	*A_u*	*3.96*	*313*	*0.355*	*H-2 → L (53%), H → L+2 (24%)*
S_7	A	4.03	308	0.001	H-1 → L+2 (14%), H → L+3 (25%)
S_7	*A_g*	*4.00*	*310*	*0.000*	*H-1 → L+2 (18%), H → L+3 (33%)*
S_8	A	4.05	306	0.011	H-3 → L (36%), H-3 → L+1 (35%), H-3 → L+2 (13%)
S_8	*A_u*	*4.04*	*307*	*0.007*	*H-15 → L (78%)*

[a] black: without symmetry constraints, red: in C_i symmetry

Table S12. Selected angles (°) for **1M**-**5M** in the S_0 states. Calculations were performed by using the B3LYP density functional and the 6-31G(d) basis set.

angles	1M	2M	3M	4M	5M
∠ $B1C_3$-xylyl (terminal)	54.005	53.653	53.693	54.050	53.626
	54.358	53.264	53.700	54.602	53.754
∠ $B1C_3$-xylyl (central)	44.328	44.441	44.399	43.330	44.023
∠ xylyl (central)-aryl1	36.558	36.084	35.580	38.267	14.634
∠ aryl1-aryl2	37.464	0.286	0.863	2.240	3.545
∠ aryl2-aryl3					1.993
∠ aryl2/3-xylyl (central)	36.557	37.100	33.891	40.320	16.020
∠ xylyl (central)-$B2C_3$	44.338	43.858	44.598	44.783	44.020
∠ xylyl (terminal)- $B2C_3$-	54.357	54.053	53.347	54.203	54.191
	53.993	54.054	53.822	54.159	53.139

Two-Photon Absorption

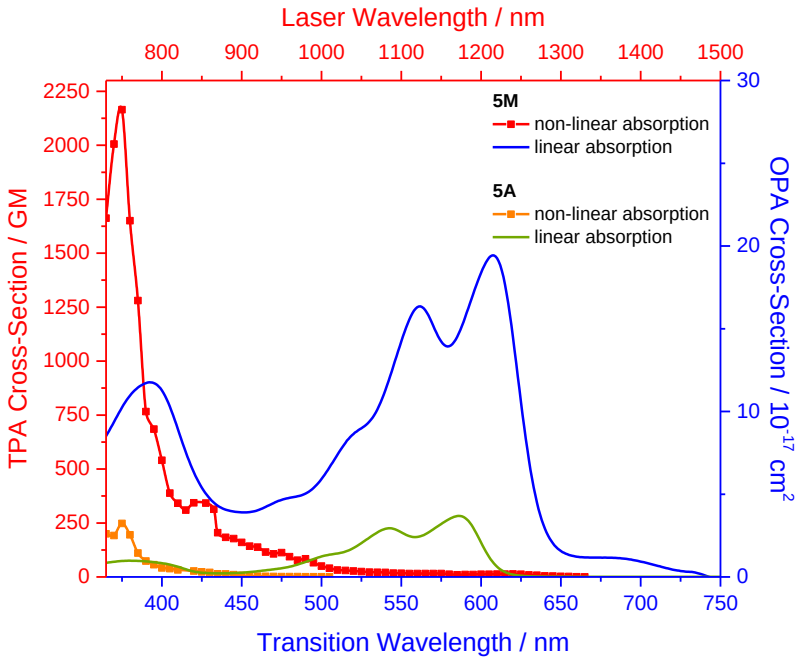


Figure S4. Two-photon absorption spectra of **5M** (red) and **5A** (orange) and one-photon absorption spectra of **5M** (blue) and **5A** (green) in DMSO.

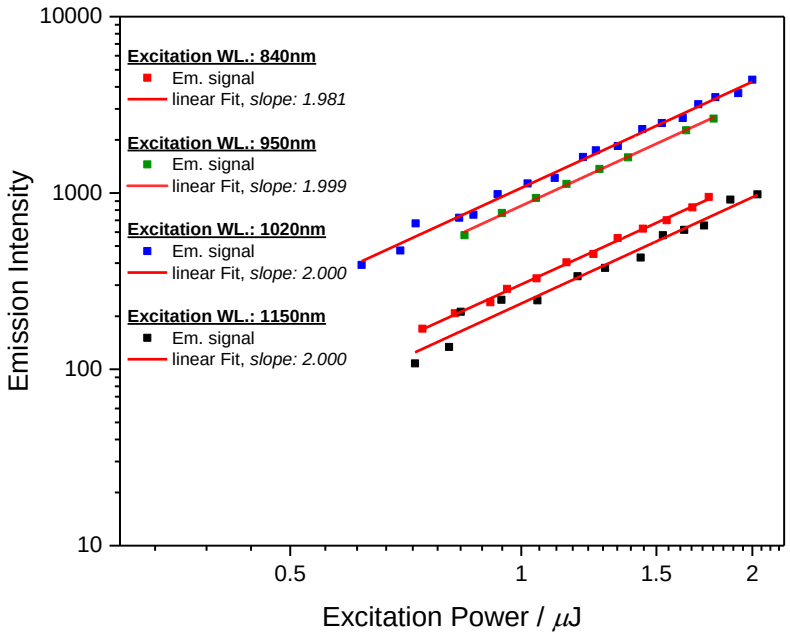


Figure S5. Power dependence of the emission intensity of **5M** in MeCN at selected excitation wavelengths.

Imaging

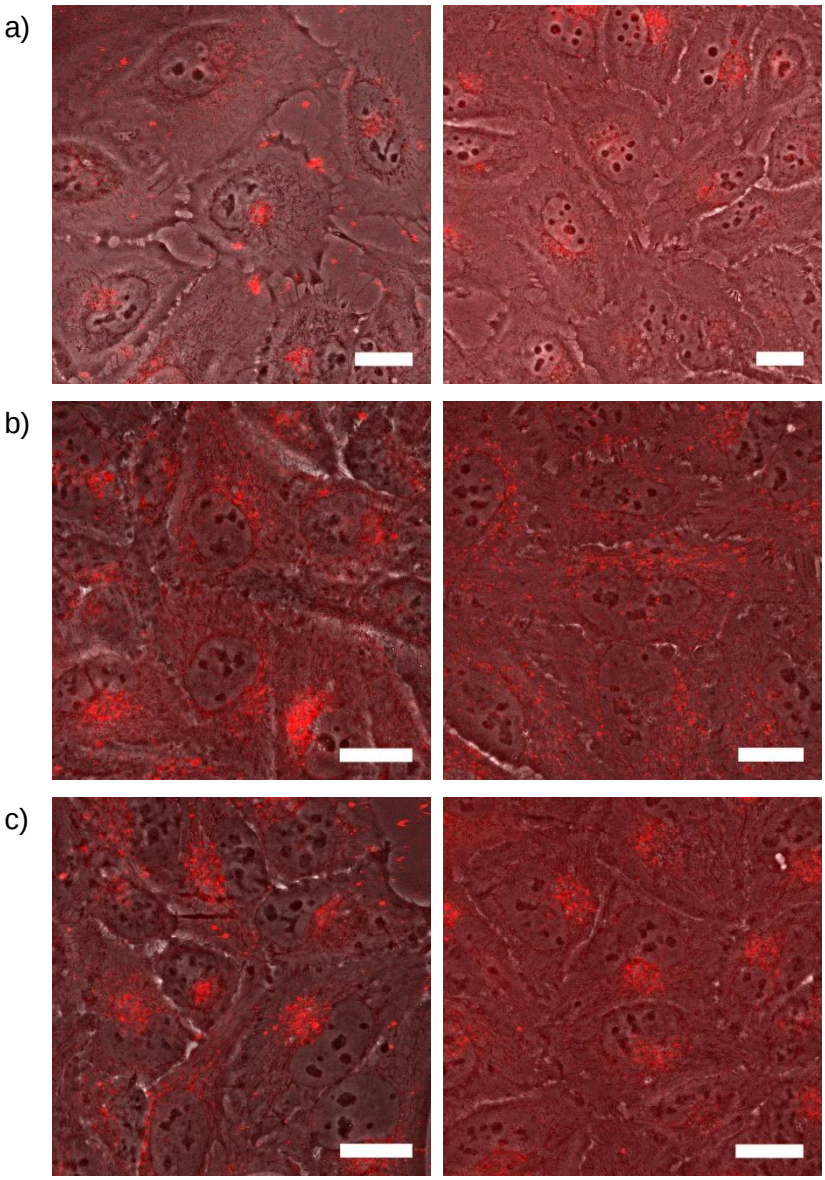


Figure S6. Confocal microscope image of HeLa cells after 1 h of incubation at 37 °C with a) **1** (5 μM), b) **2** (5 μM) and c) **3** (5 μM). Merged bright field image with fluorescence image (λ_{ex} = 405 nm; λ_{em} = 570-670 nm) before washing (left) shows the formation of nanoparticles, while after washing (right) a nominal uptake of the dye by the cell can be observed. Scale bars: 20 µm.

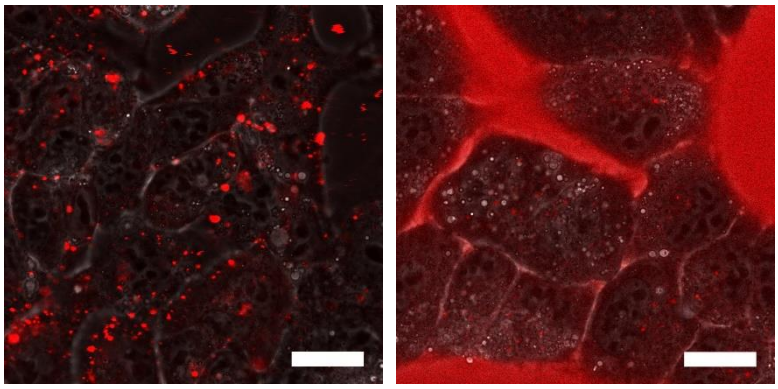


Figure S7. HepG2 cells challenged with fatty acids for 24 h and stained with **1** (5 μM) 24 h at 37 °C. Merged bright field image with fluorescence image (λ_{ex} = 405 nm; λ_{em} = 570-670 nm) without Pluronic F-127 (left) shows the formation of nanoparticles, while with the addition of 0.04% Pluronic F-127 (right) it shows the solution of the dye, but also no cellular uptake. Scale bars: 20 µm.

Table S13. Measured particle sizes of the neutral compounds in PBS containing 0.5% DMSO with DLS.

compound	particle size [nm]	error [± nm]
1	413.6	50.79
2	441.0	54.45
3	425.1	54.09

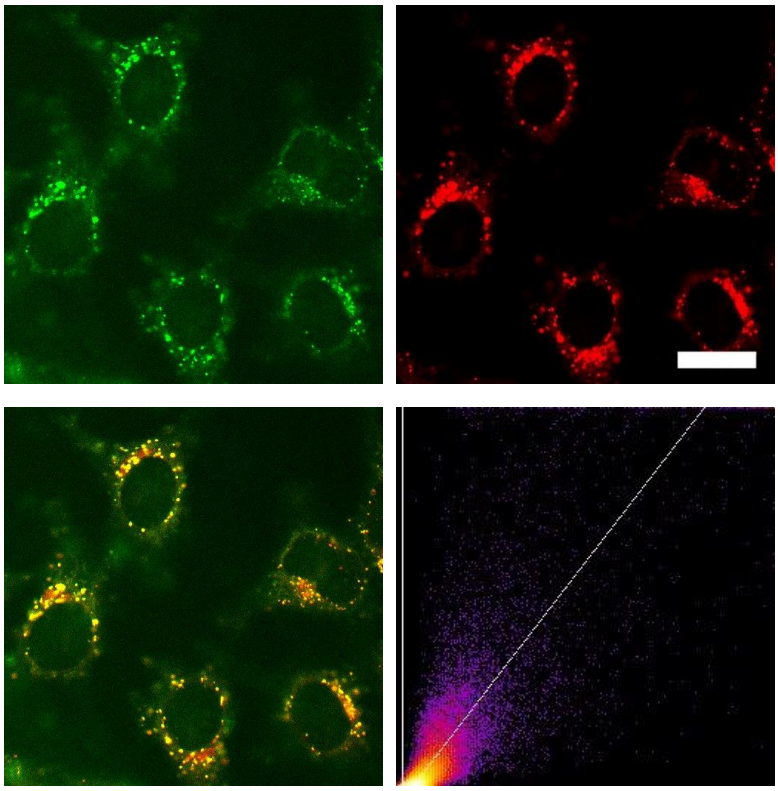


Figure S8. Co-staining experiment of HeLa cells with **1M** and LysoTracker™ Red. The cells were loaded with **1M** (0.5 μM, 2 h) and LysoTracker™ Red (0.1 μM, 20 min) at 37 °C. Fluorescence images of **1M** (top, left, λ_{ex} = 405 nm; λ_{em} = 450 – 550 nm) and LysoTracker™ Red (top, right, λ_{ex} = 561 nm; λ_{em} = 600 – 750 nm). The merged fluorescence images (bottom, left) and the correlation plot of the intensities (bottom, right, R_r = 0.80) show co-localization of the dye **1M** with lysosome. Scale bar: 20 µm.

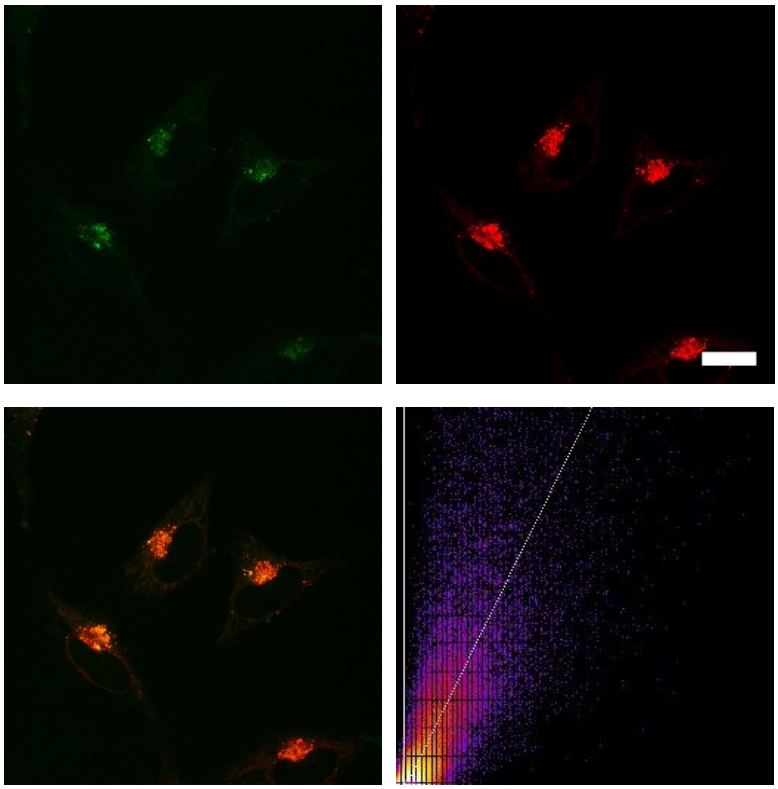


Figure S9. Co-staining experiment of HeLa cells with **2M** and LysoTracker™ Red. The cells were loaded with **2M** (0.5 μM, 2 h) and LysoTracker™ Red (0.1 μM, 20 min) at 37 °C. Fluorescence images of **2M** (top, left, λ_{ex} = 405 nm; λ_{em} = 450 – 550 nm) and LysoTracker™ Red (top, right, λ_{ex} = 561 nm; λ_{em} = 600 – 750 nm). The merged fluorescence images (bottom, left) and the correlation plot of the intensities (bottom, right, R_r = 0.73) show co-localization of the dye **2M** with lysosome. Scale bar: 20 µm.

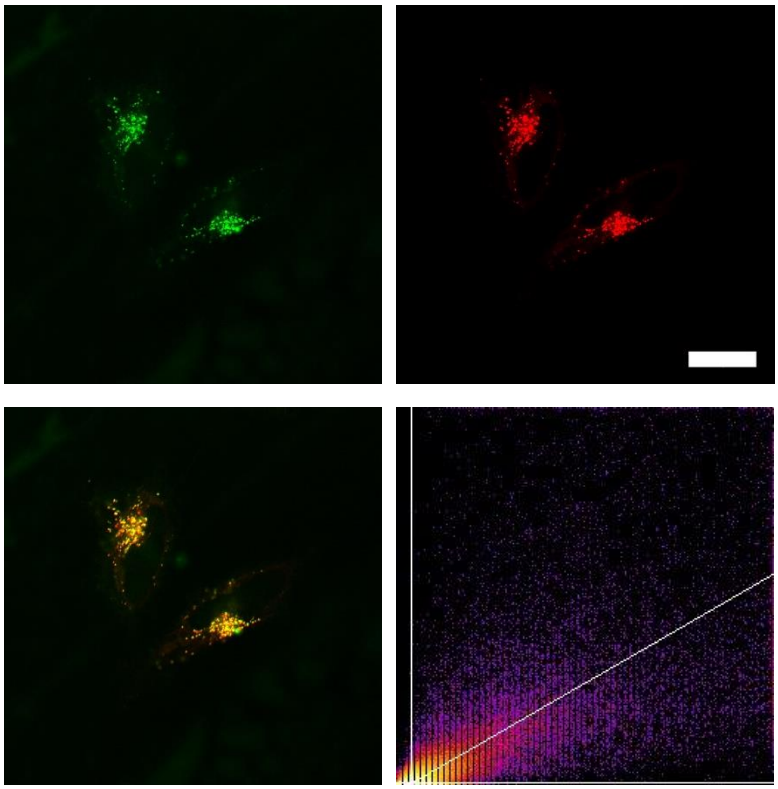


Figure S10. Co-staining experiment of HeLa cells with **3M** and LysoTracker™ Red. The cells were loaded with **3M** (0.5 μM, 2 h) and LysoTracker™ Red (0.1 μM, 20 min) at 37 °C. Fluorescence images of **3M** (top, left, λ_{ex} = 405 nm; λ_{em} = 450 – 550 nm) and LysoTracker Red (top, right, λ_{ex} = 561 nm; λ_{em} = 600 – 750 nm). The merged fluorescence images (bottom, left) and the correlation plot of the intensities (bottom, right, R_r = 0.75) show co-localization of the dye **3M** with lysosome. Scale bar: 20 µm.

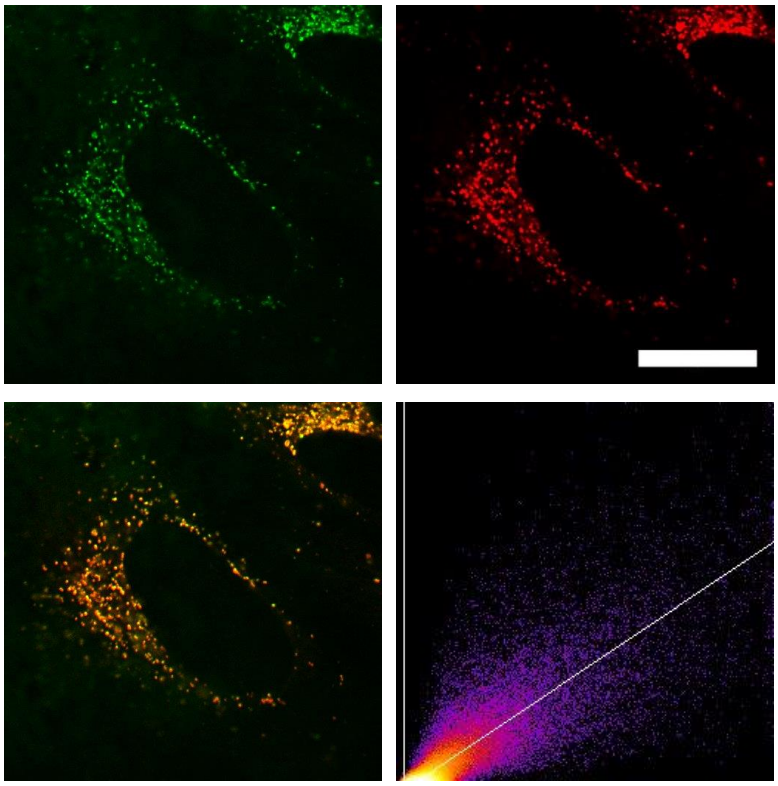


Figure S11. Co-staining experiment of HeLa cells with **4M** and LysoTracker™ Red. The cells were loaded with **4M** (0.5 μM, 2 h) and LysoTracker™ Red (0.1 μM, 20 min) at 37 °C. Fluorescence images of **4M** (top, left, λ_{ex} = 405 nm; λ_{em} = 500 – 605 nm) and LysoTracker™ Red (top, right, λ_{ex} = 561 nm; λ_{em} = 607 – 786 nm). The merged fluorescence images (bottom, left) and the correlation plot of the intensities (bottom, right, R_r = 0.83) show co-localization of the dye **4M** with lysosome. Scale bar: 20 µm.

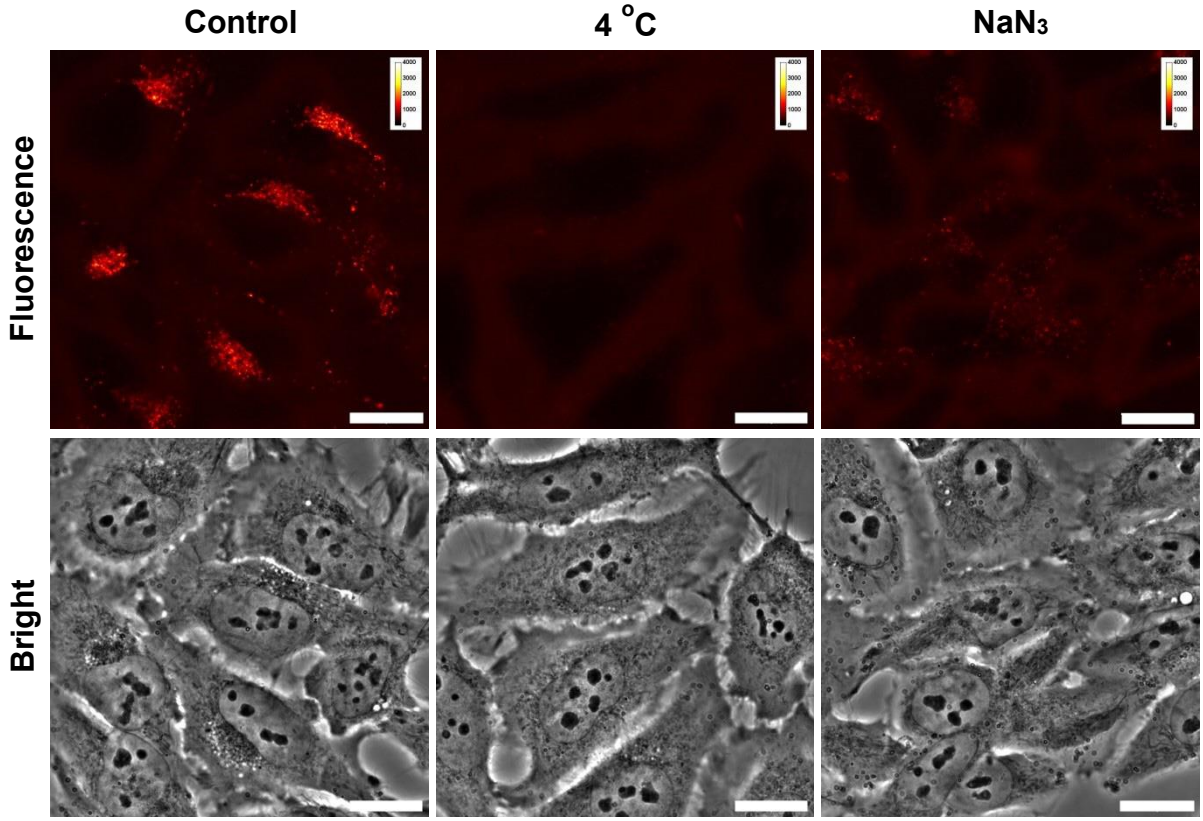


Figure S12. Cell staining with 500 nM of **5M** in DMEM for 2 h at 37 °C (left), for 2 h at 4°C (middle) and for 2 h at 37 °C with 0.1% NaN_3 (right). Fluorescence images of **5M** (top, λ_{ex} = 559 nm; λ_{em} = 570 – 670 nm) and bright field images (bottom) suggest an endocytosis pathway. Scale bars: 20 µm.

Cell Viability

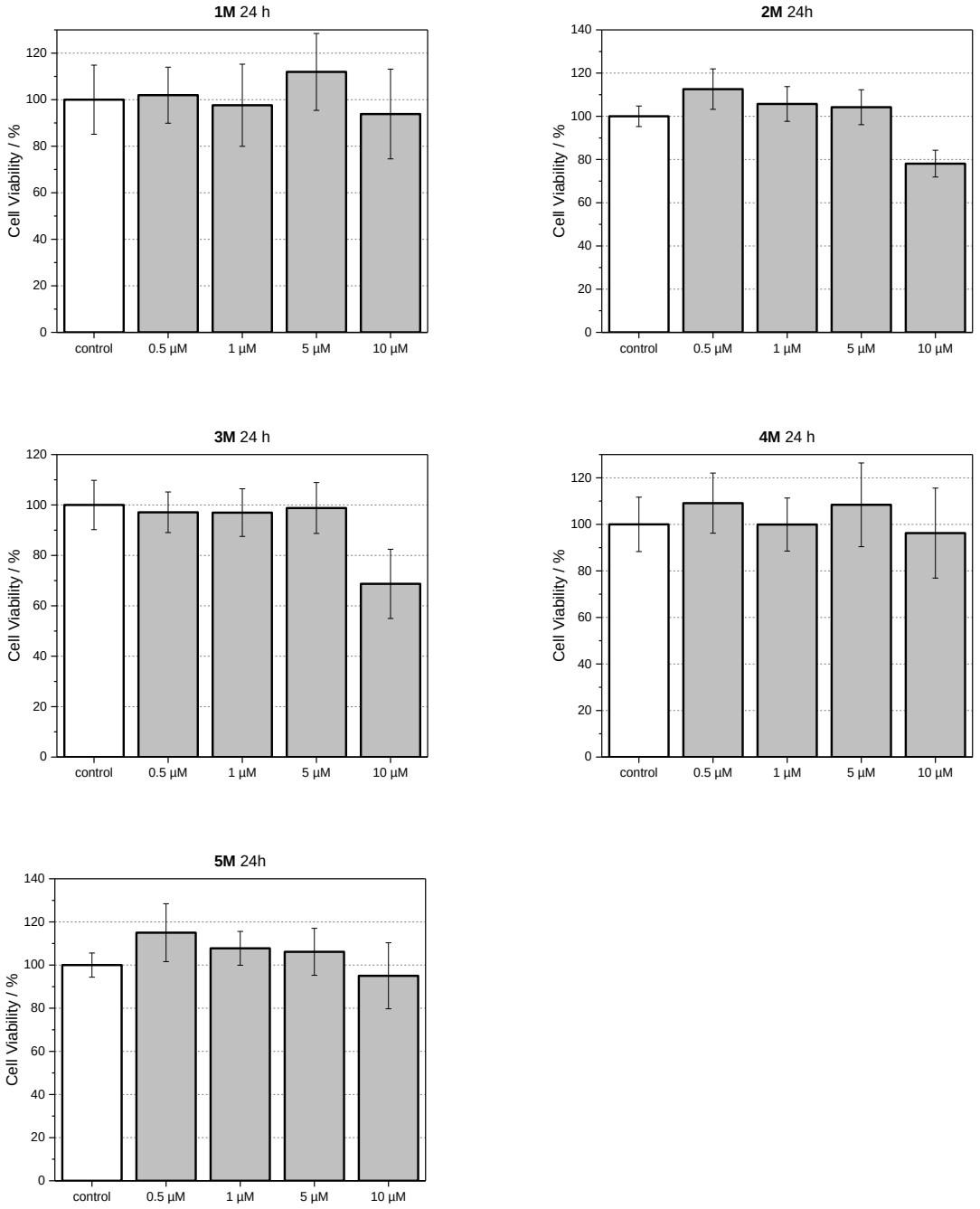


Figure S13. Cell viability of **1M**-**5M** loaded HeLa cells determined by MTT assay. The cells were incubated with **1M**-**5M** (0, 0.5, 1, 5, 10 μM) in DMEM containing 0.5% DMSO in a CO_2 incubator for 24 h. The results are expressed as percentages of the dye-free controls. All data are presented as mean standard deviation (n = 10).

NMR Spectra

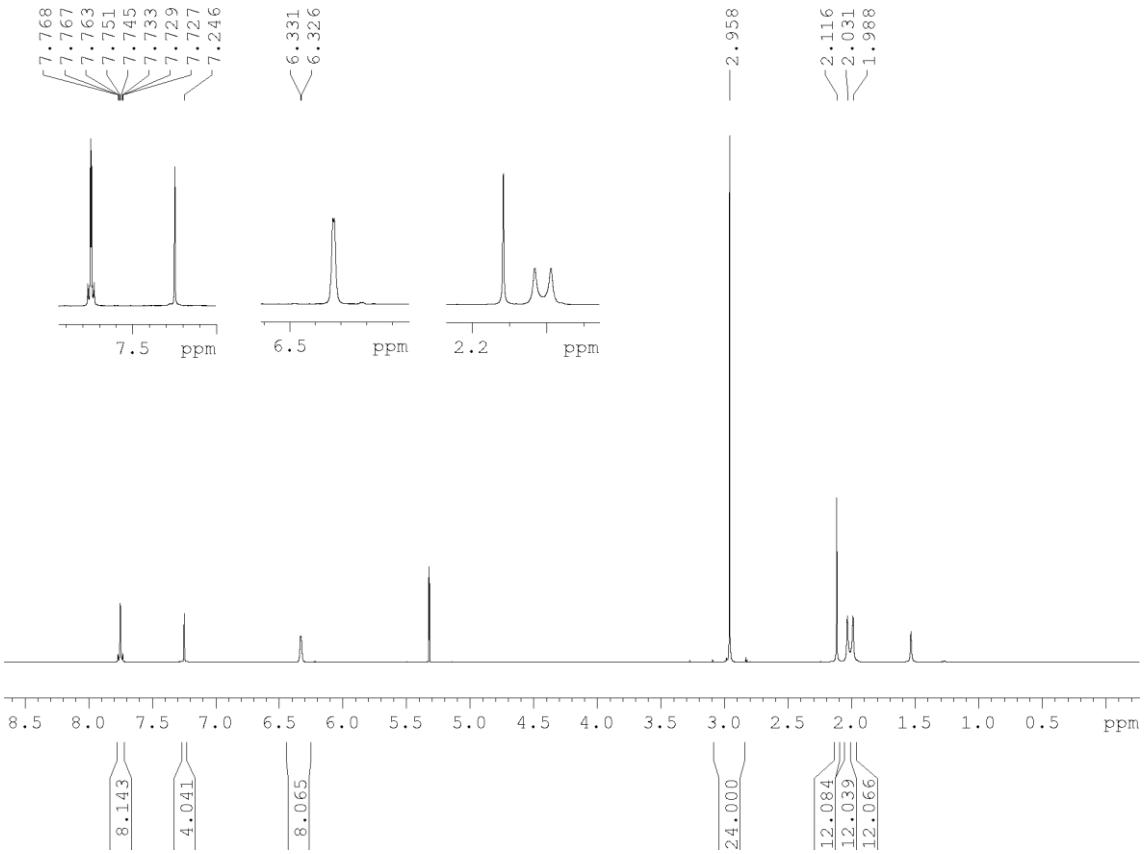


Figure S14. ^{1}H NMR spectrum of **1** in CD_2Cl_2 at 500 MHz.

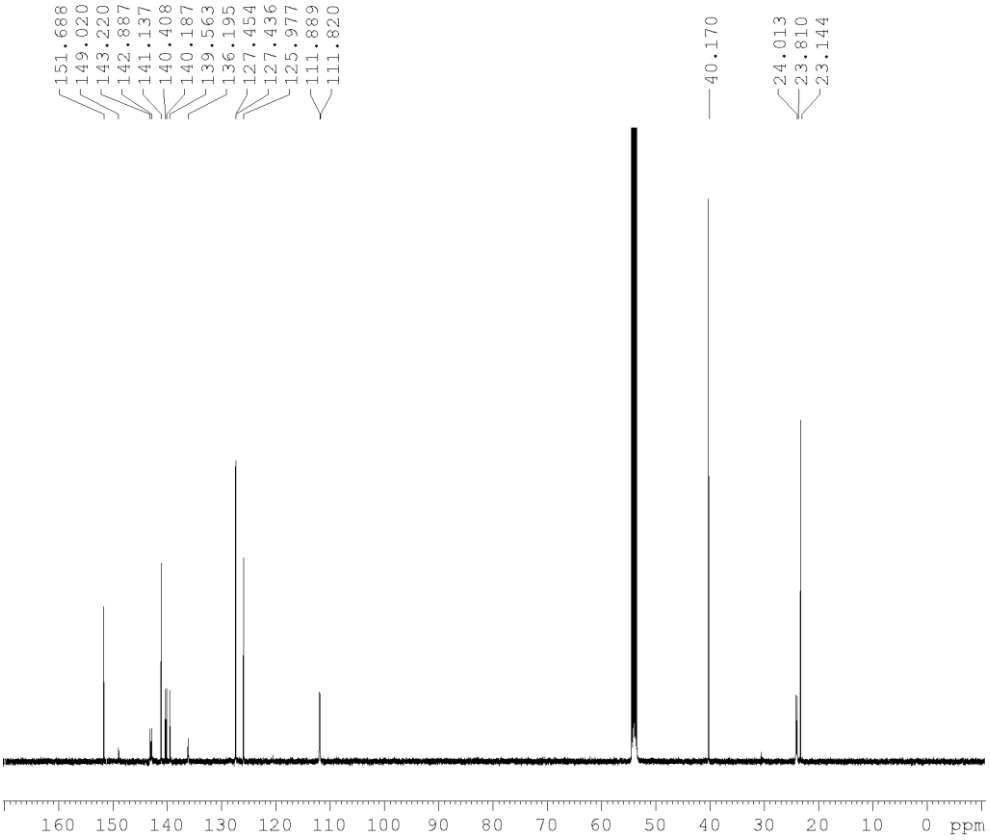


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in CD_2Cl_2 at 125 MHz.

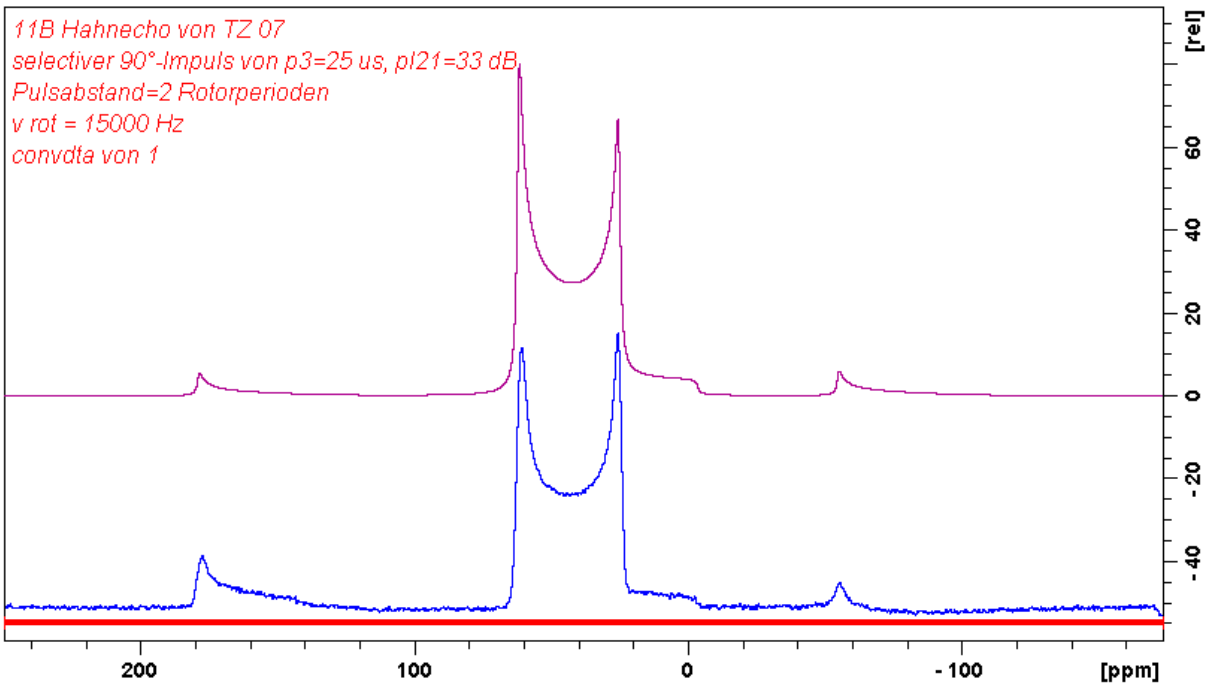


Figure S16. Solid-state $^{11}B\{^{1}H\}$ NMR spectrum of **1** at 128 MHz. (Top: Simulation) isotropic chemical shift δ_{iso} = 72.8 ppm, quadrupolar coupling constant C_Q = 4.49 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

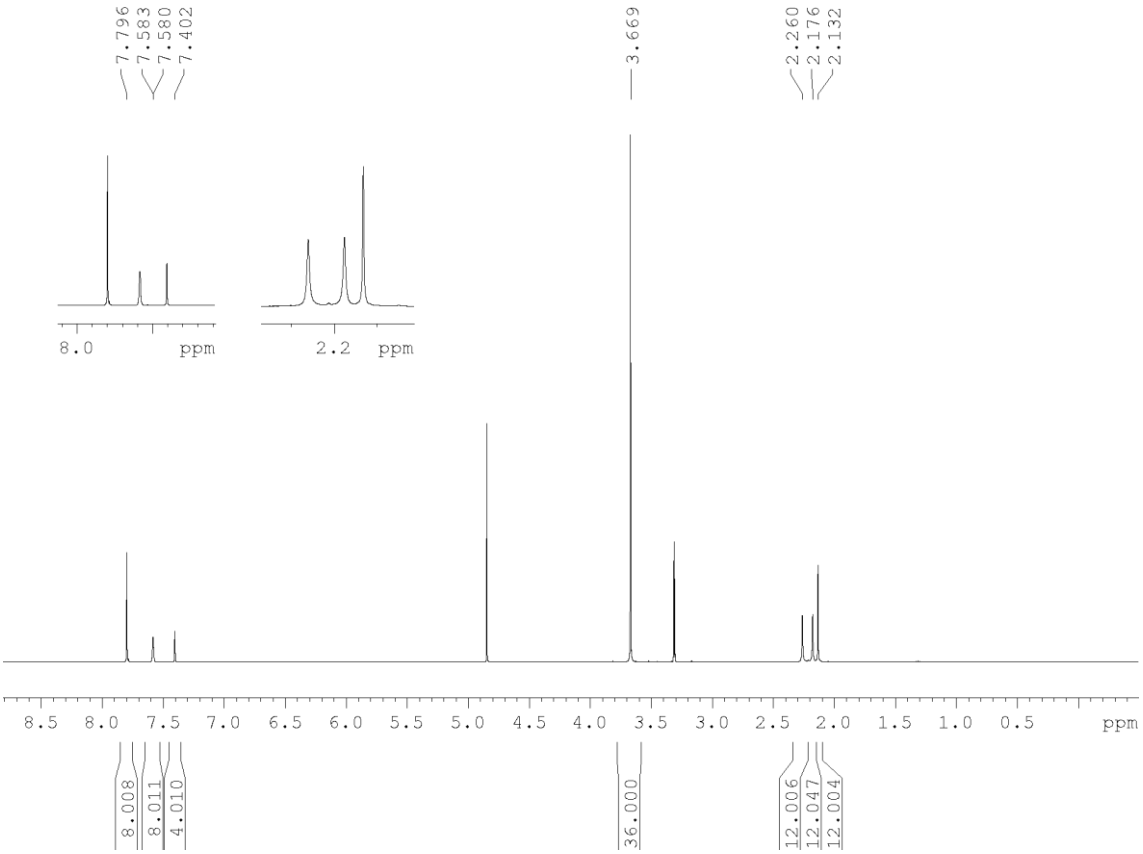


Figure S17. ^{1}H NMR spectrum of **1M** in CD_3OD at 500 MHz.

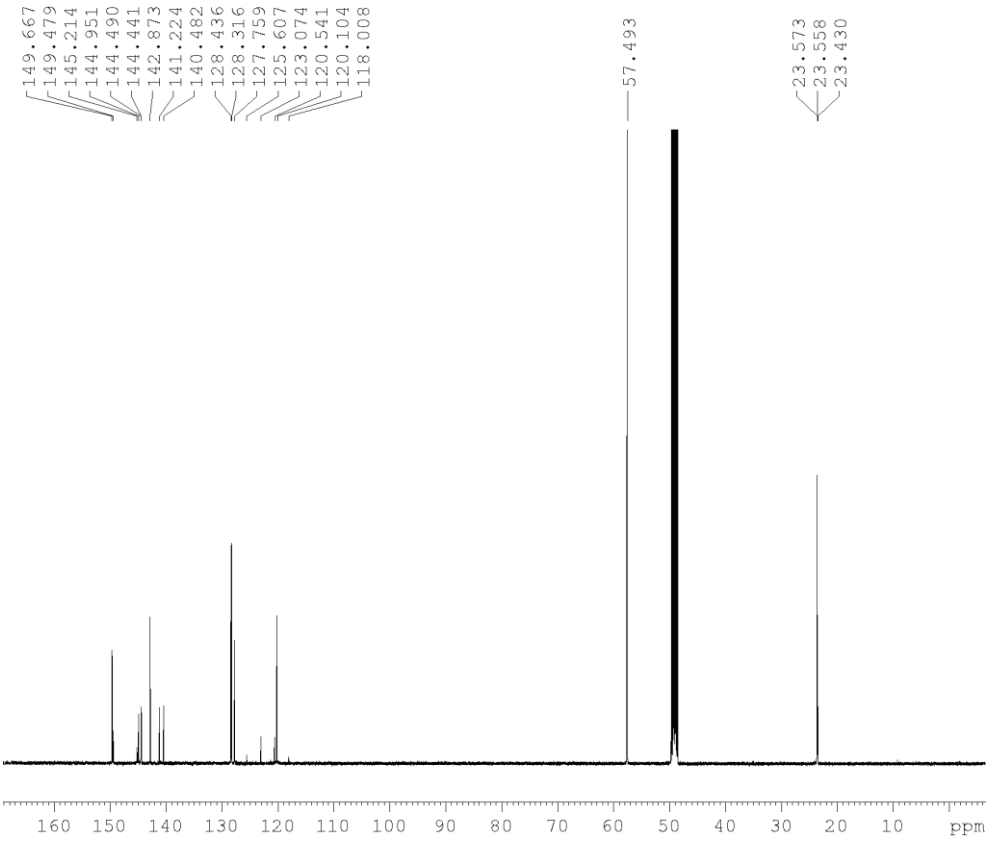


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **1M** in CD_3OD at 125 MHz.

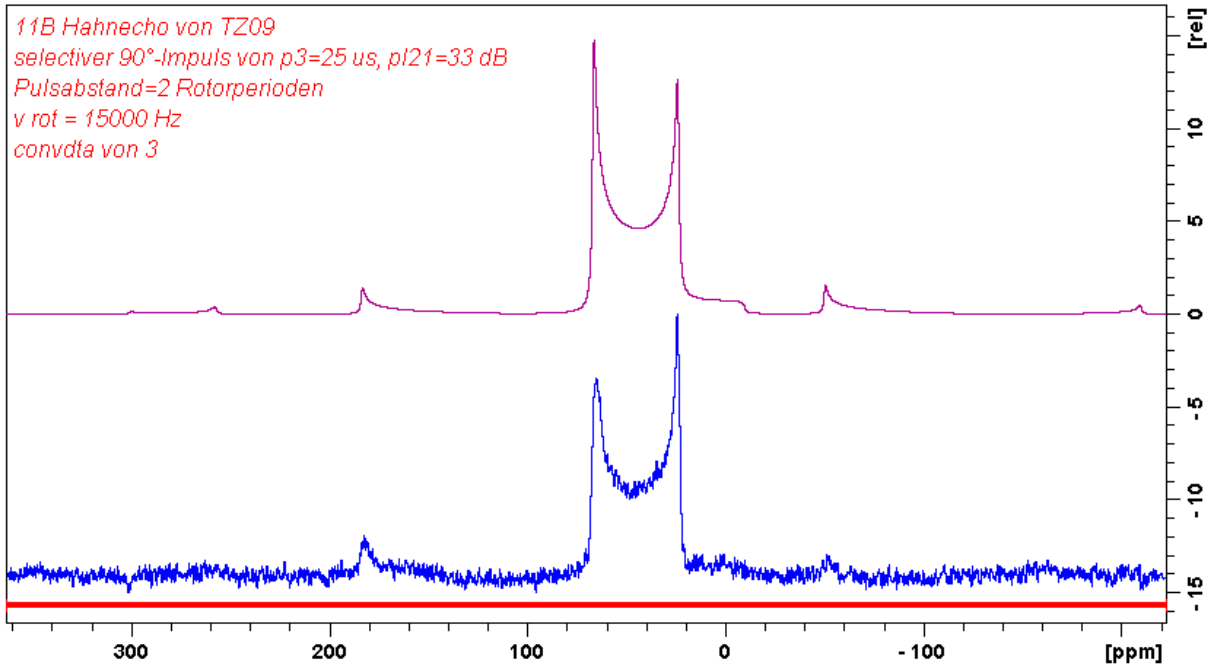


Figure S19. Solid-state $^{11}B\{^{1}H\}$ NMR spectrum of **1M** at 128 MHz. (Top: Simulation) isotropic chemical shift δ_{iso} = 79.2 ppm, quadrupolar coupling constant C_Q = 4.86 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

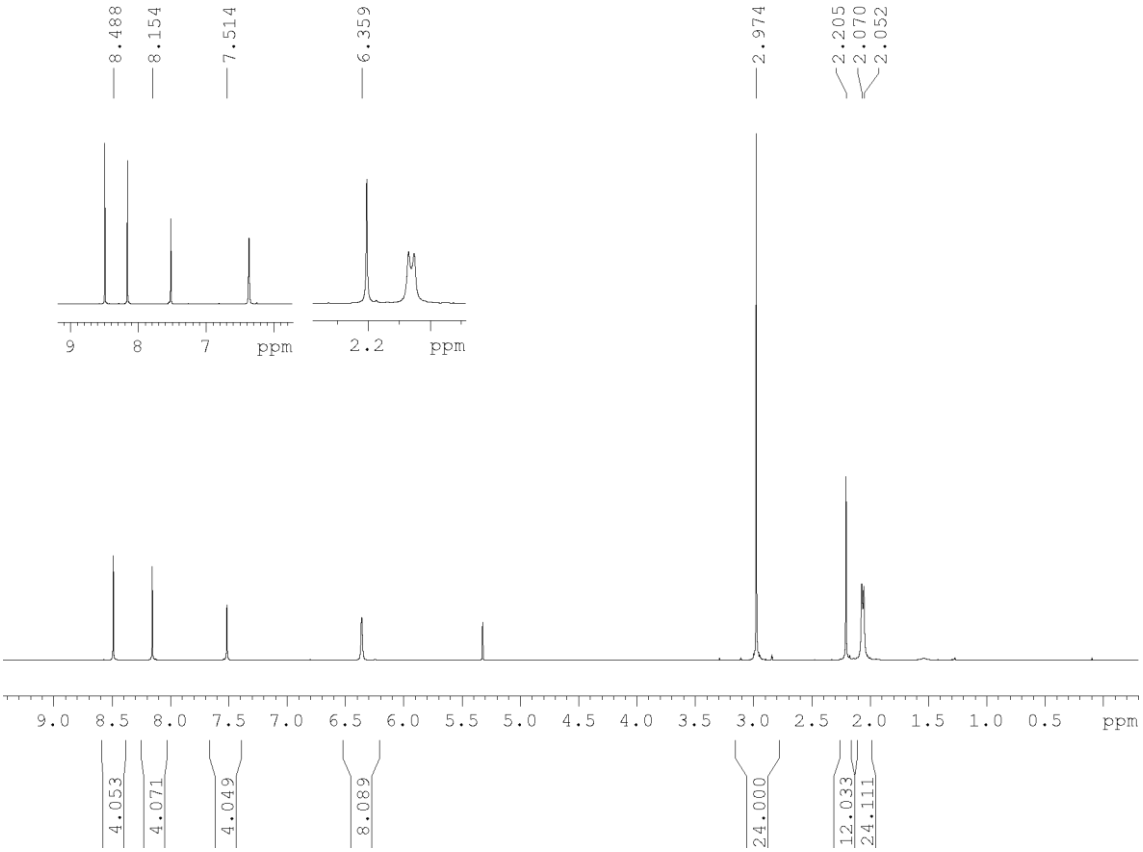


Figure S20. ^{1}H NMR spectrum of **2** in CD_2Cl_2 at 500 MHz.

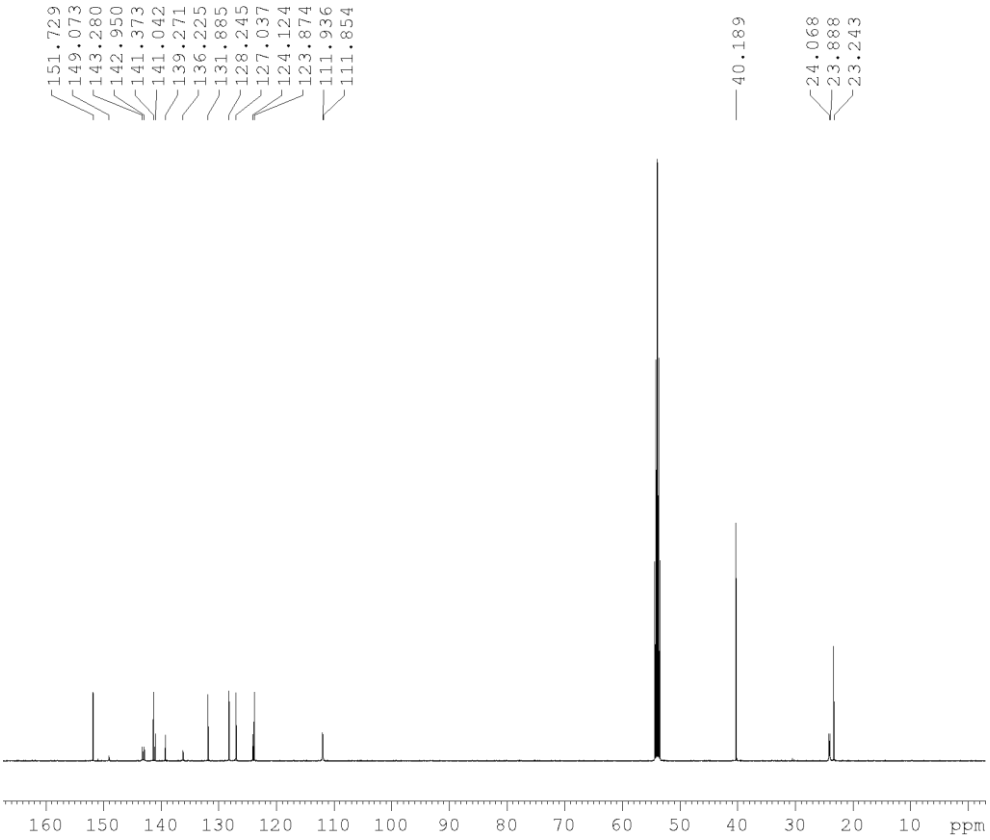


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in CD_2Cl_2 at 125 MHz.

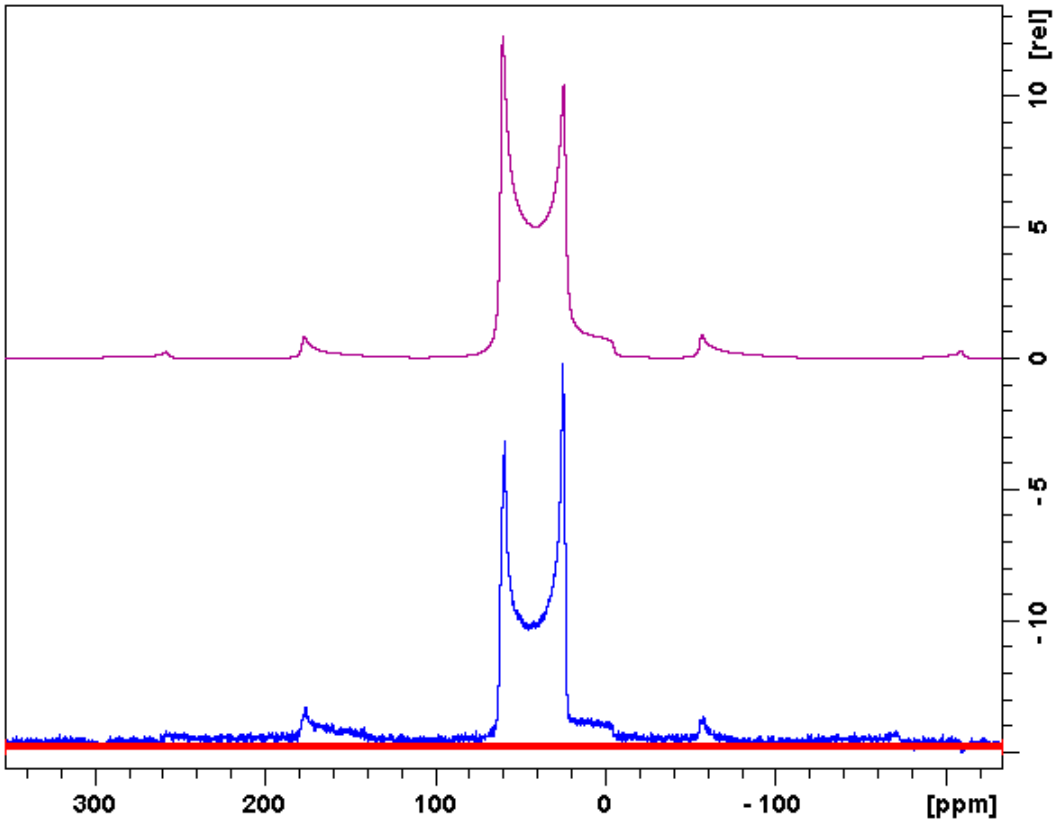


Figure S22. Solid-state $^{11}B\{^{1}H\}$ NMR spectrum of **2** at 128 MHz. (Top: Simulation) isotropic chemical shift δ_{iso} = 71.9 ppm, quadrupolar coupling constant C_Q = 4.51 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

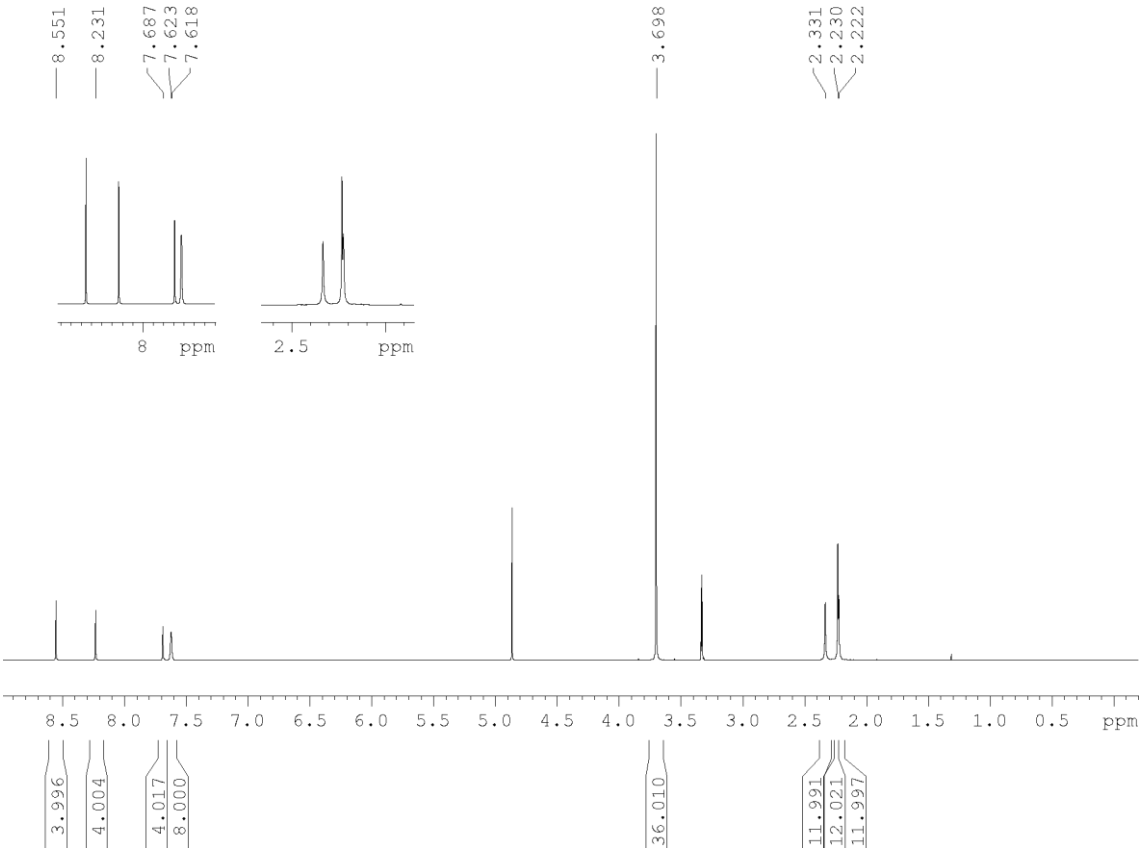


Figure S23. ^{1}H NMR spectrum of **2M** in CD_3OD at 500 MHz.

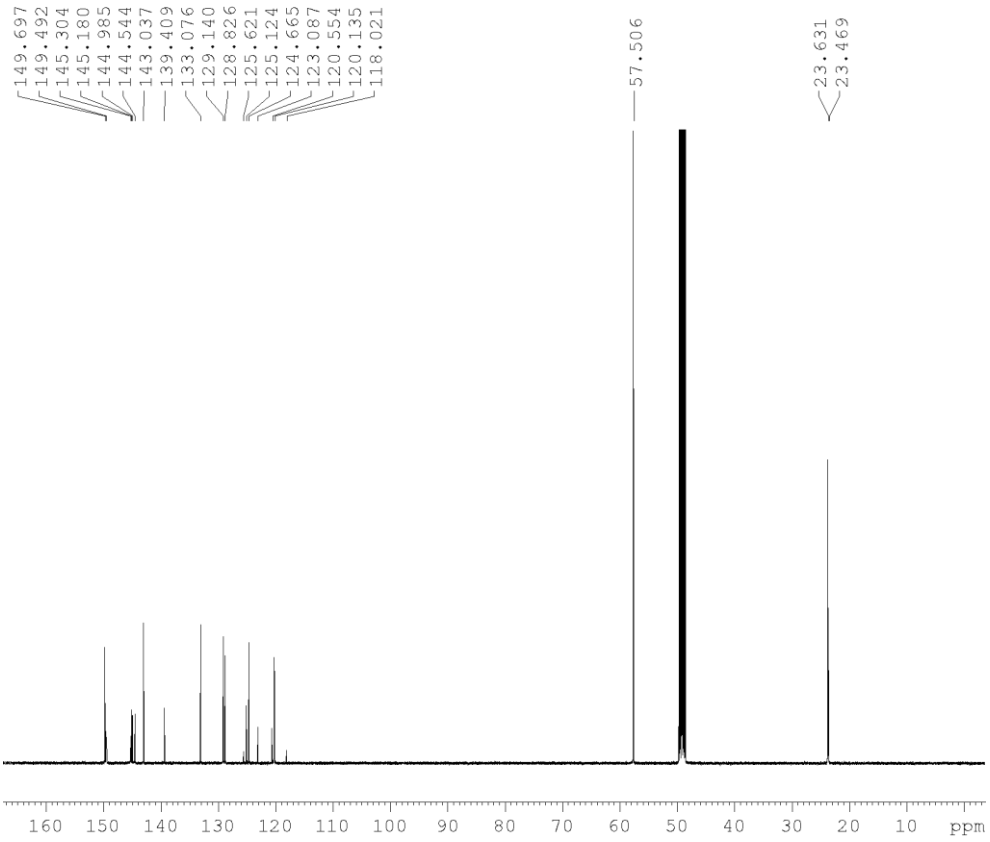


Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum of **2M** in CD_3OD at 125 MHz.

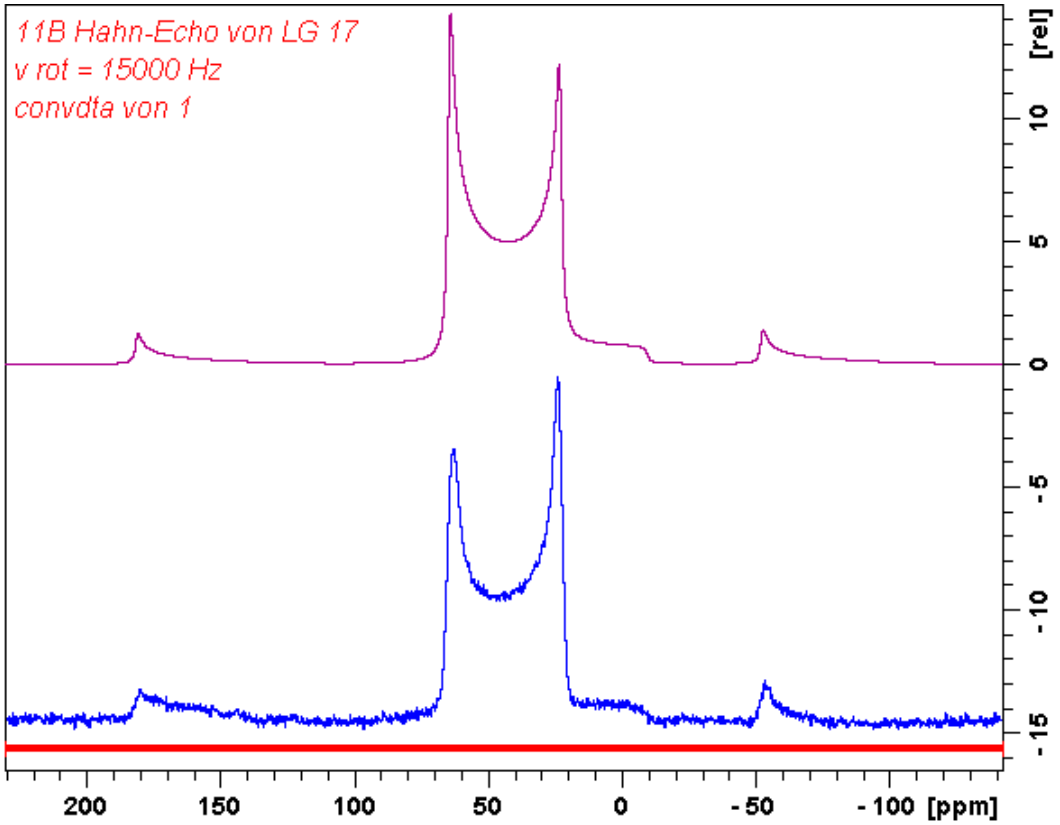


Figure S25. Solid-state $^{11}B\{^{1}H\}$ NMR spectrum of **2M** at 128 MHz. (Top: Simulation) isotropic chemical shift δ_{iso} = 77.2 ppm, quadrupolar coupling constant C_Q = 4.78 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

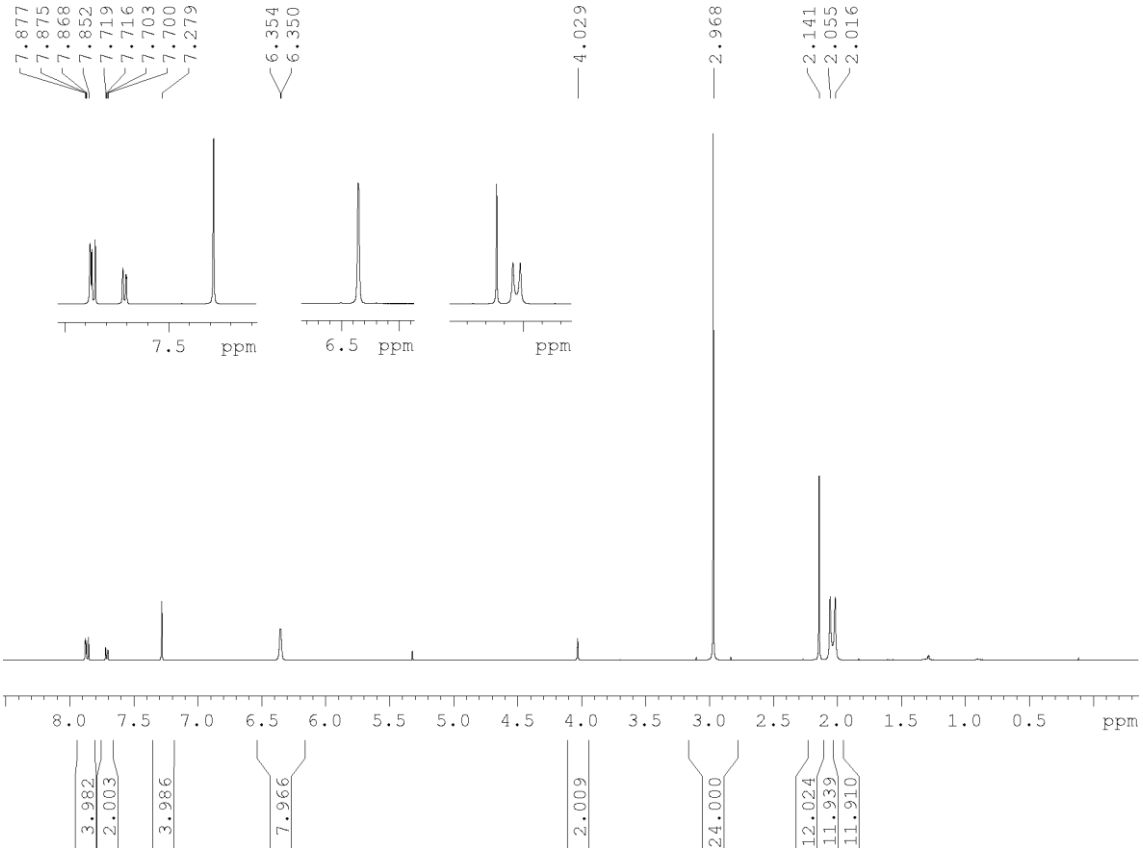


Figure S26. ^{1}H NMR spectrum of **3** in CD_2Cl_2 at 500 MHz.

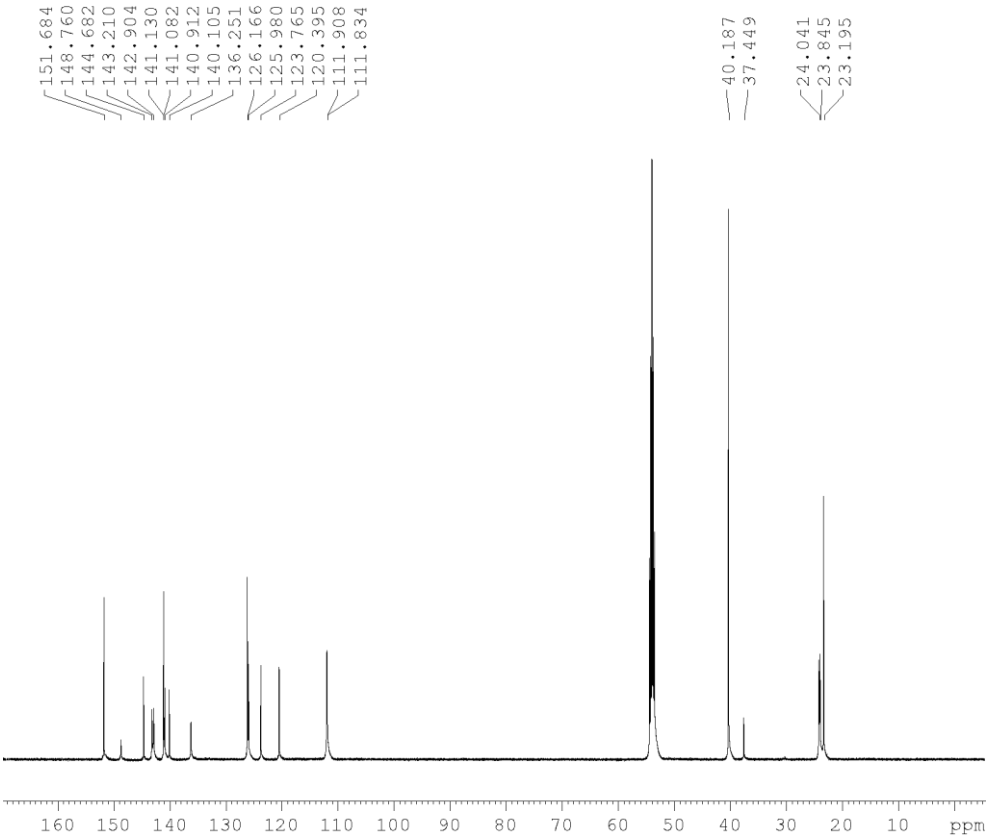


Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in CD_2Cl_2 at 125 MHz.

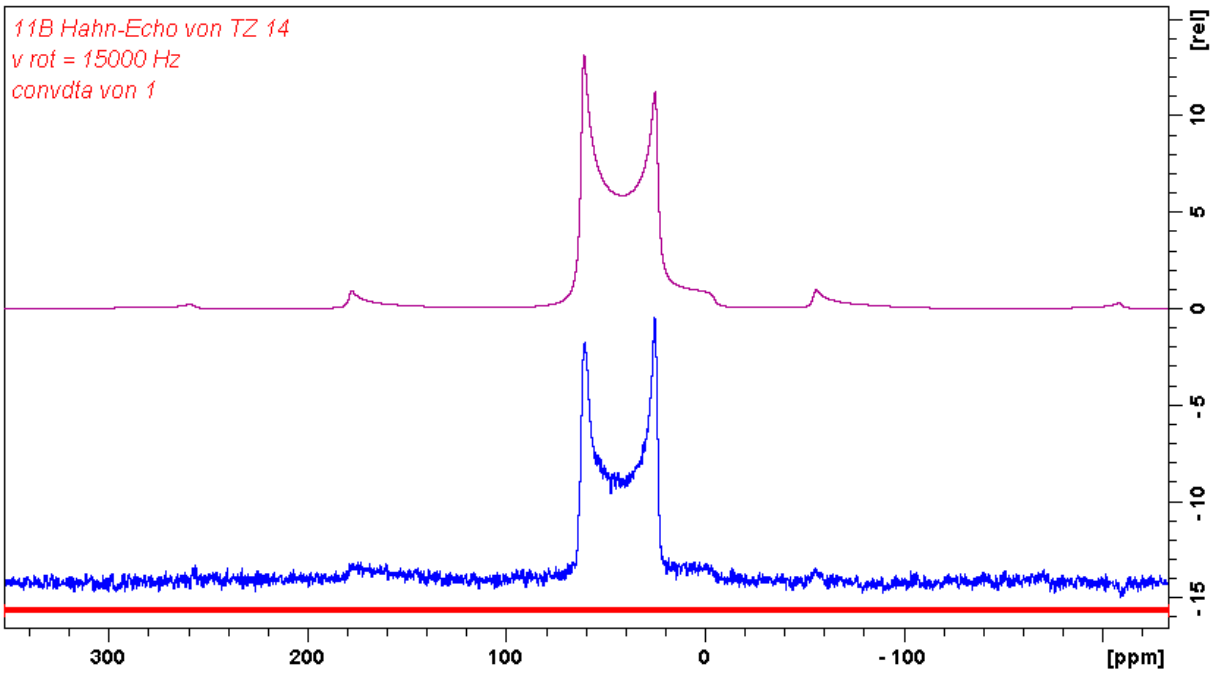


Figure S28. Solid-state $^{11}B\{^{1}H\}$ NMR spectrum of **3** at 128 MHz. (Top: Simulation) isotropic chemical shift δ_{iso} = 73.0 ppm, quadrupolar coupling constant C_Q = 4.53 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

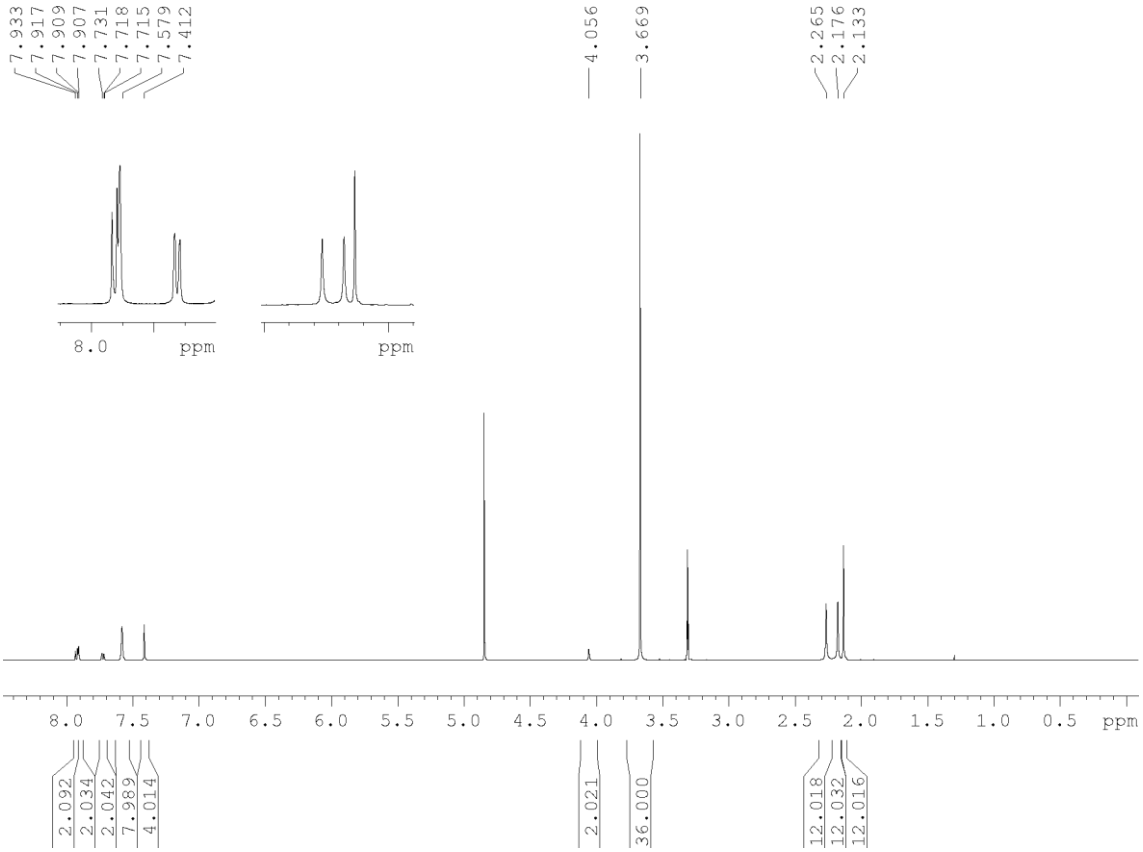


Figure S29. ^{1}H NMR spectrum of **3M** in CD_3OD at 500 MHz.

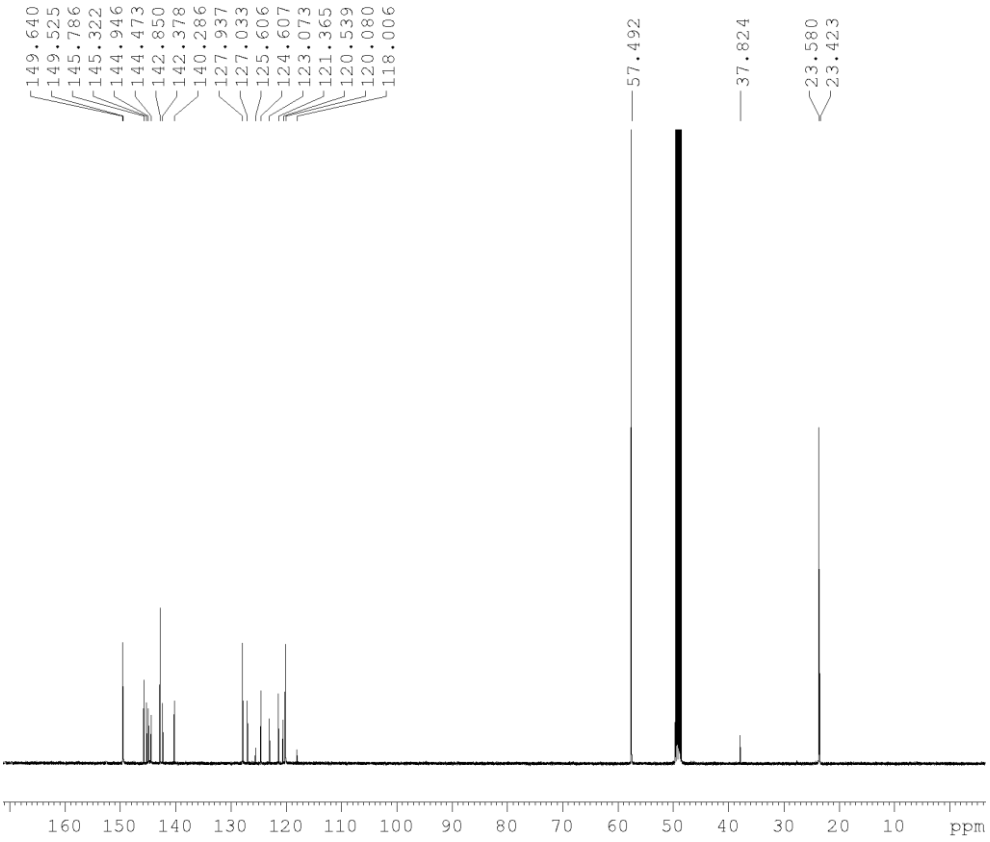


Figure S30. $^{13}C\{^{1}H\}$ NMR spectrum of **3M** in CD_3OD at 125 MHz.

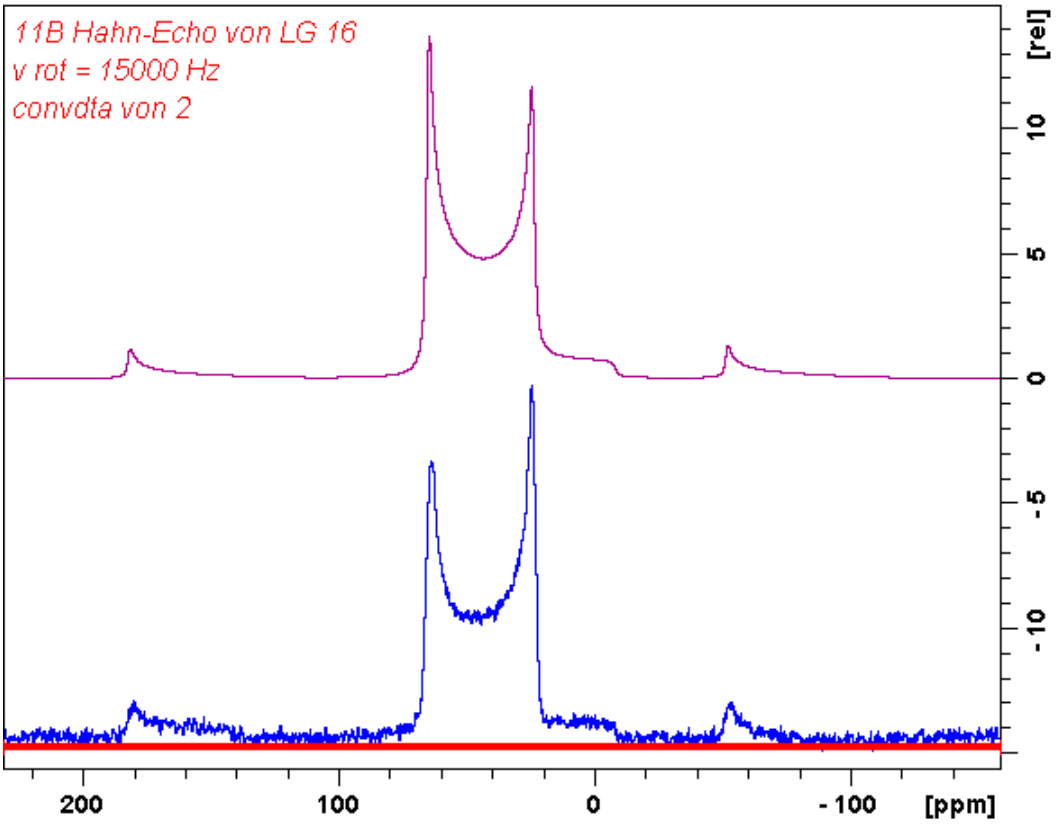


Figure S31. Solid-state $^{11}B\{^{1}H\}$ NMR spectrum of **3M** at 128 MHz. (Top: Simulation) isotropic chemical shift δ_{iso} = 77.1 ppm, quadrupolar coupling constant C_Q = 4.76 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

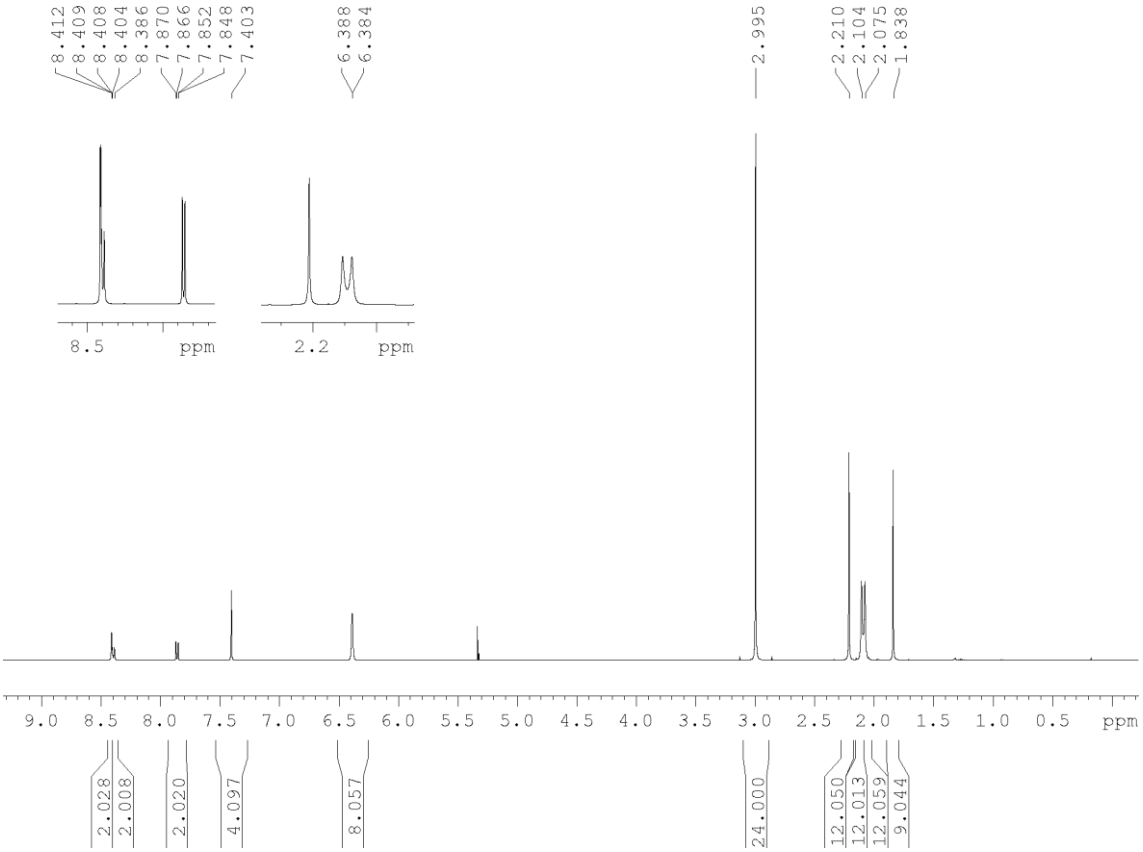


Figure S32. ^{1}H NMR spectrum of **4** in CD_2Cl_2 at 500 MHz.

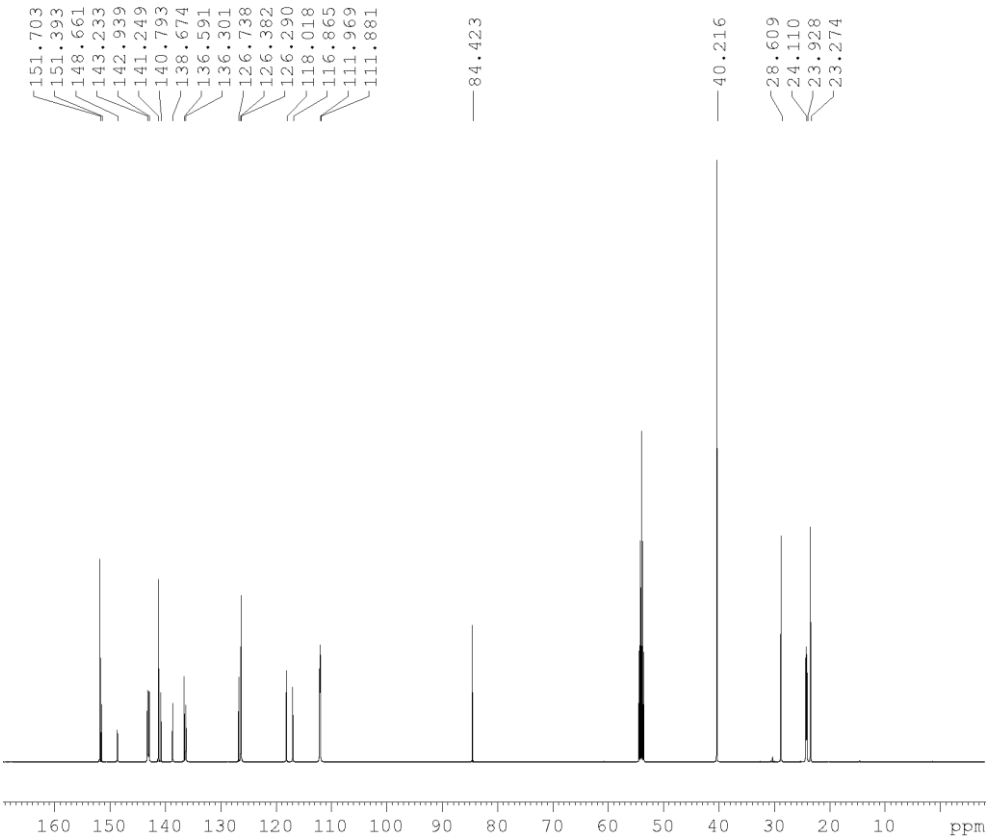


Figure S33. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2 at 125 MHz.

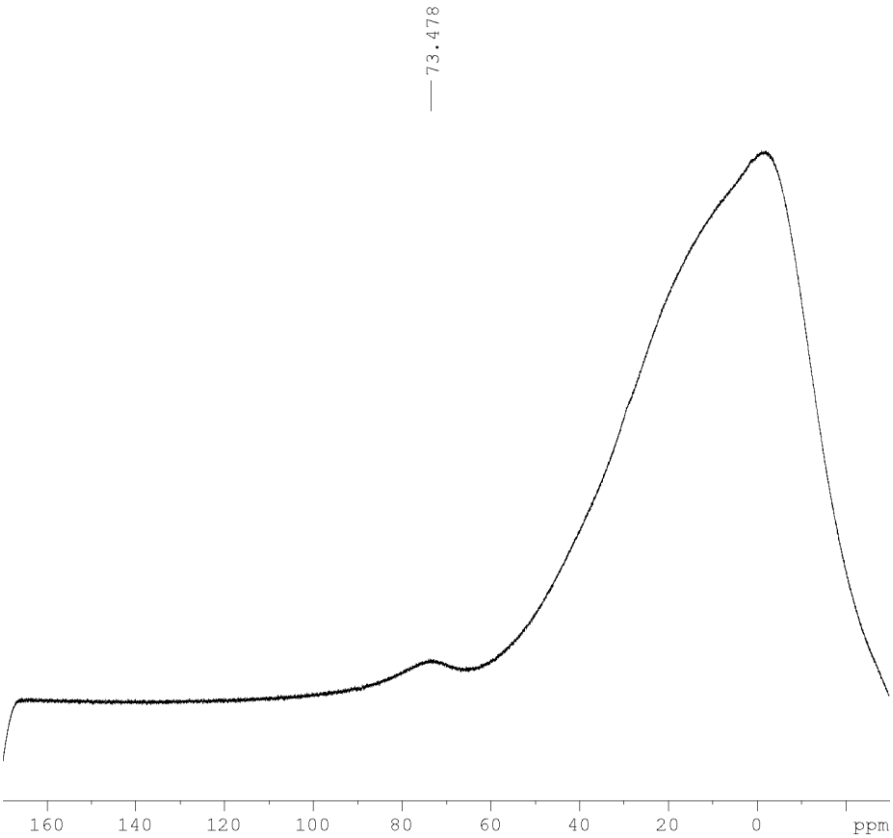


Figure S34. $^{11}B\{^{1}H\}$ NMR spectrum of **4** in CD_2Cl_2 at 160 MHz.

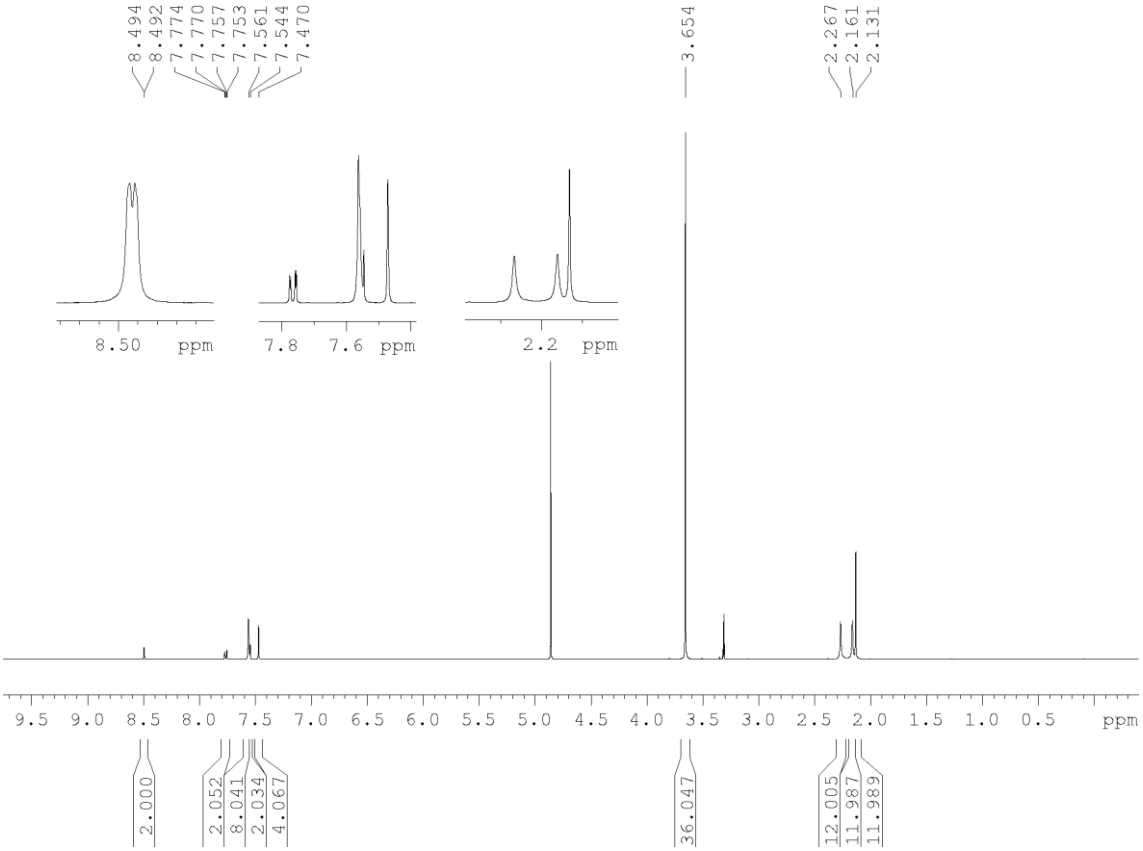


Figure S35. ^{1}H NMR spectrum of **4M** in CD_3OD at 500 MHz.

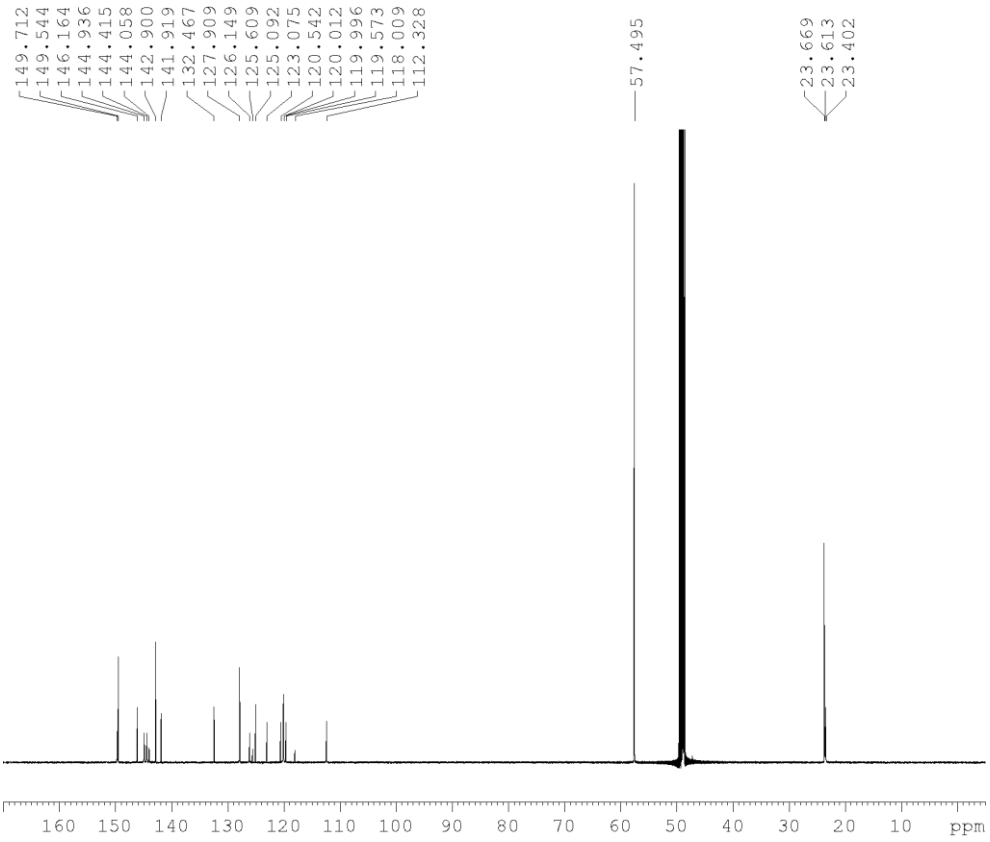


Figure S36. $^{13}C\{^{1}H\}$ NMR spectrum of **4M** in CD_3OD at 125 MHz.

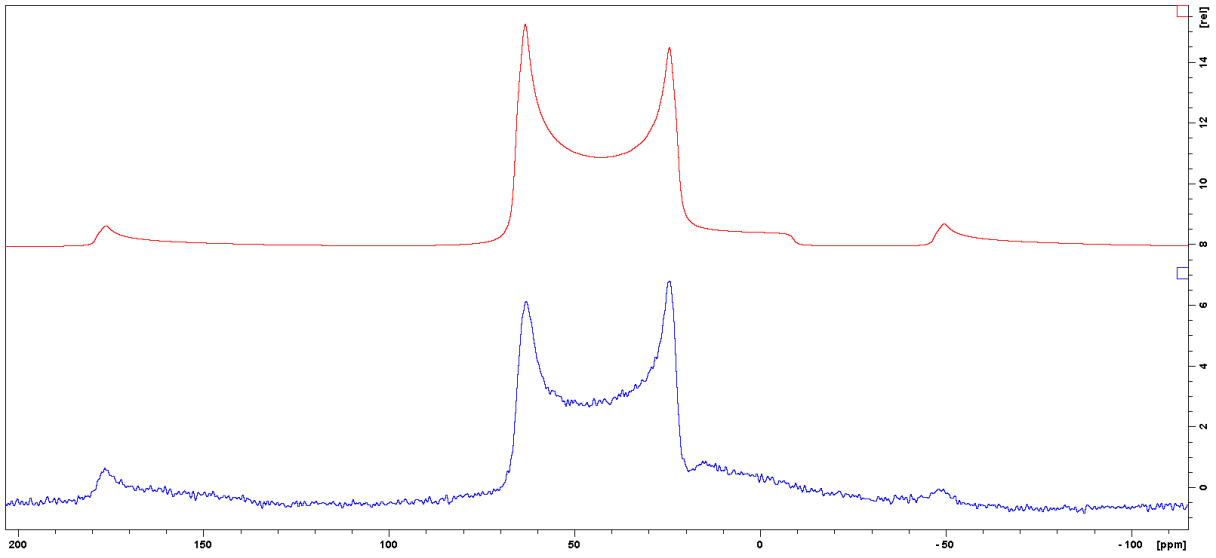


Figure S37. Solid-state $^{11}B\{^{1}H\}$ NMR spectrum of **4M** at 128 MHz. (Top: Simulation) isotropic chemical shift δ_{iso} = 77.0 ppm, quadrupolar coupling constant C_Q = 4.77 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.1.

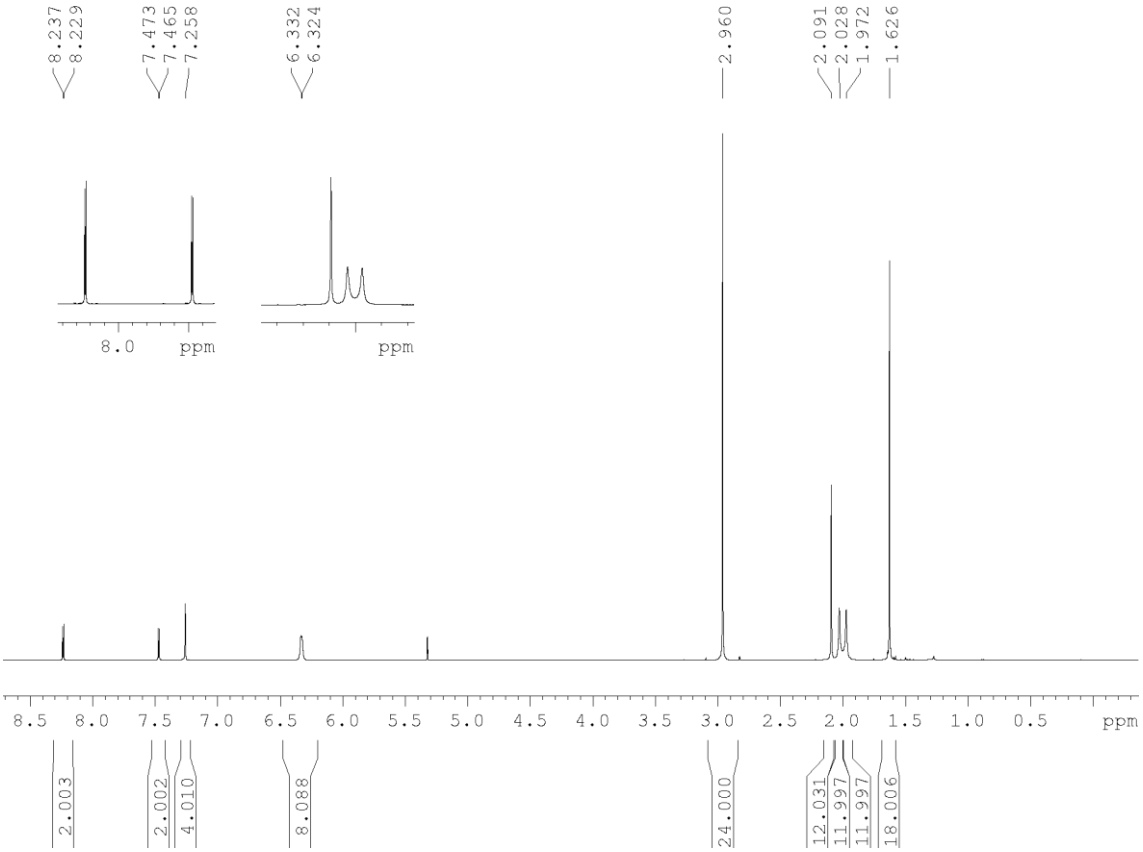


Figure S38. ^{1}H NMR spectrum of **5** in CD_2Cl_2 at 500 MHz.

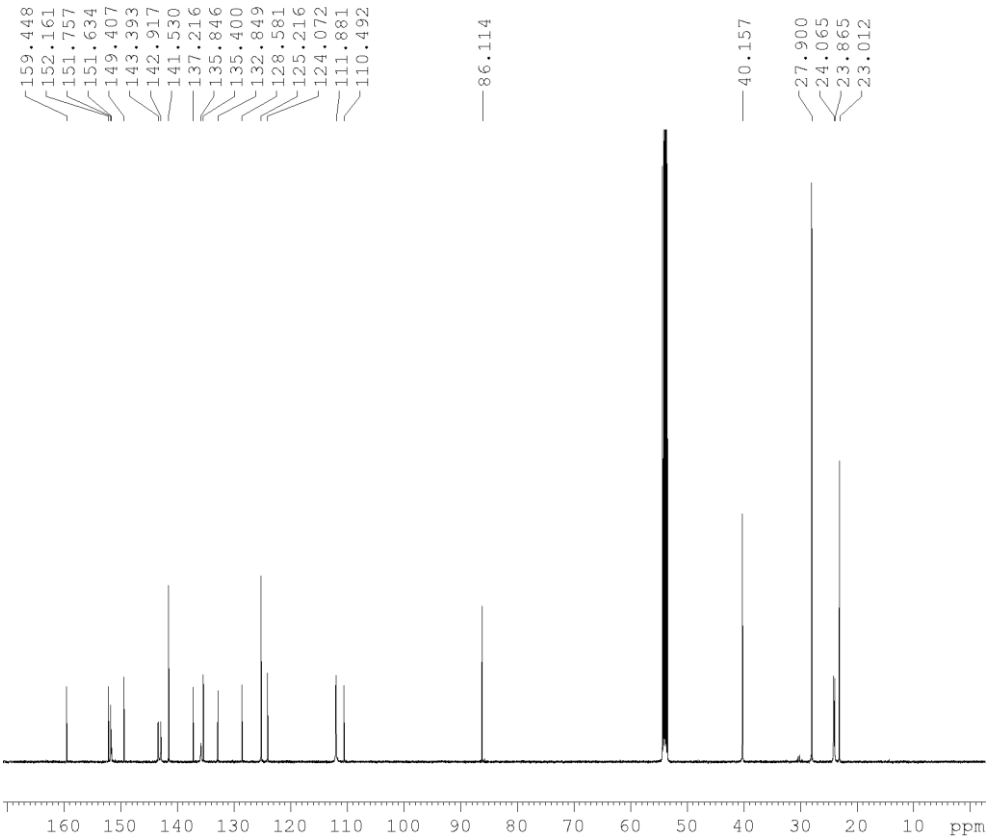


Figure S39. $^{13}C\{^{1}H\}$ NMR spectrum of **5** in CD_2Cl_2 at 125 MHz.

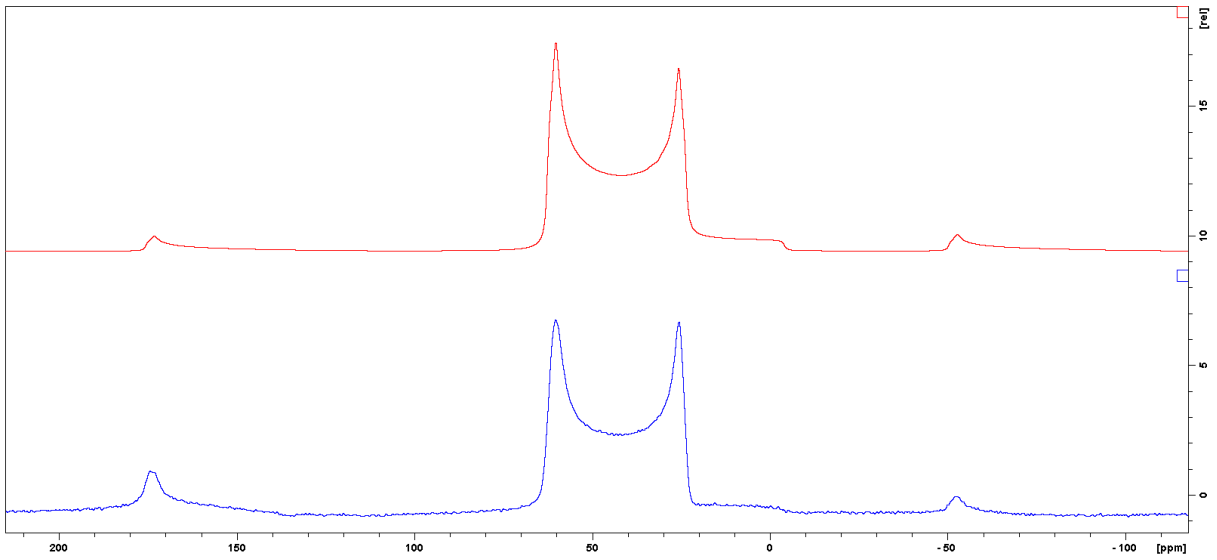


Figure S40. Solid-state $^{11}B\{^1H\}$ NMR spectrum of **5** at 128 MHz. (Top: Simulation) isotropic chemical shift δ_{iso} = 72.5 ppm, quadrupolar coupling constant C_Q = 4.49 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.1.

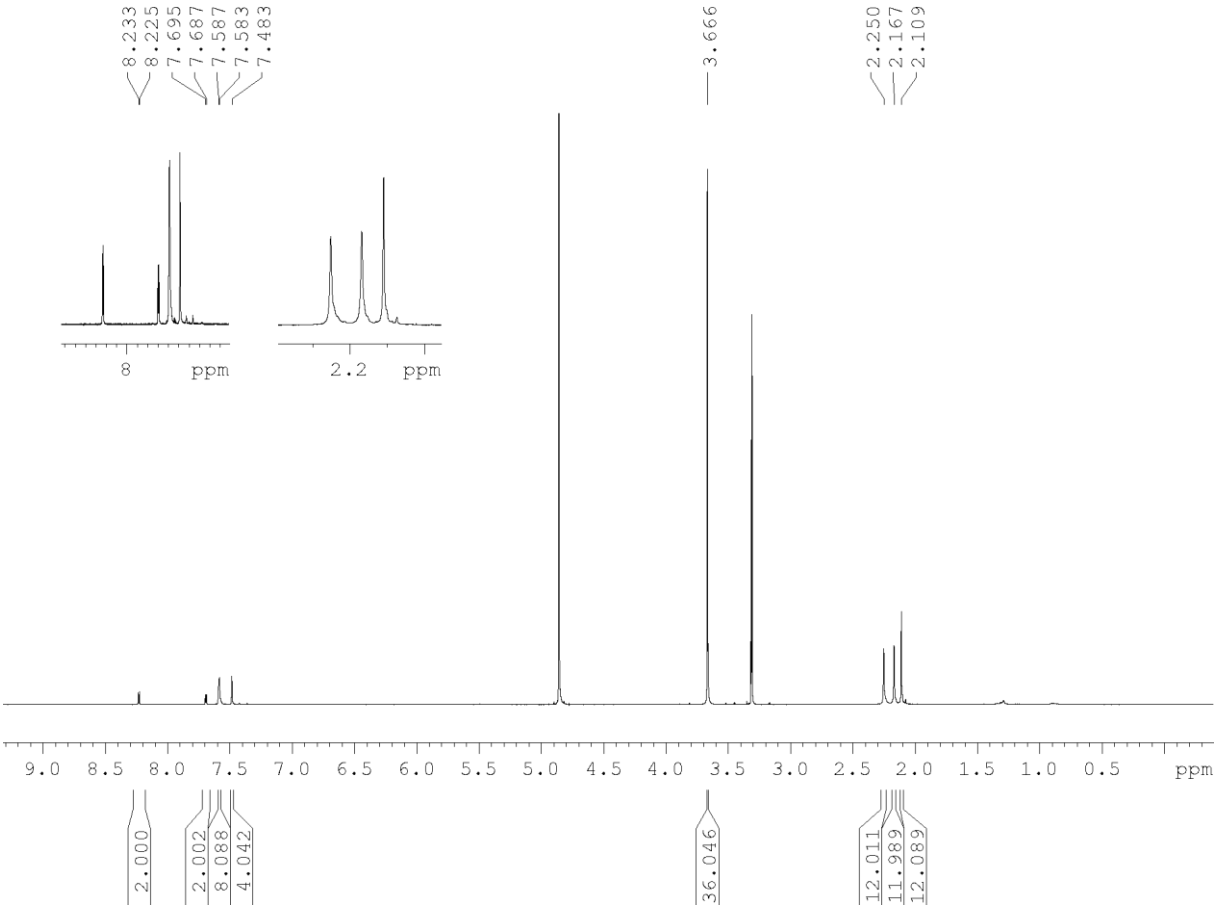


Figure S41. ^1H NMR spectrum of **5M** in CD_3OD at 500 MHz.

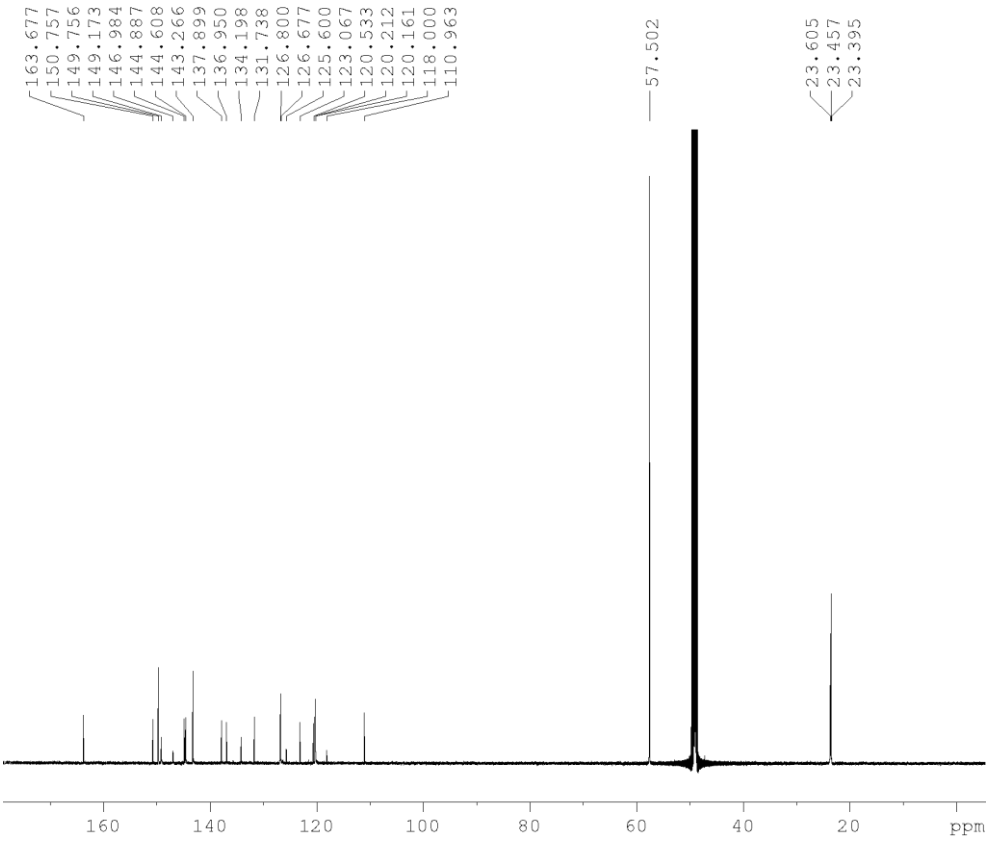


Figure S42. $^{13}C\{^{1}H\}$ NMR spectrum of **5M** in CD_3OD at 125 MHz.

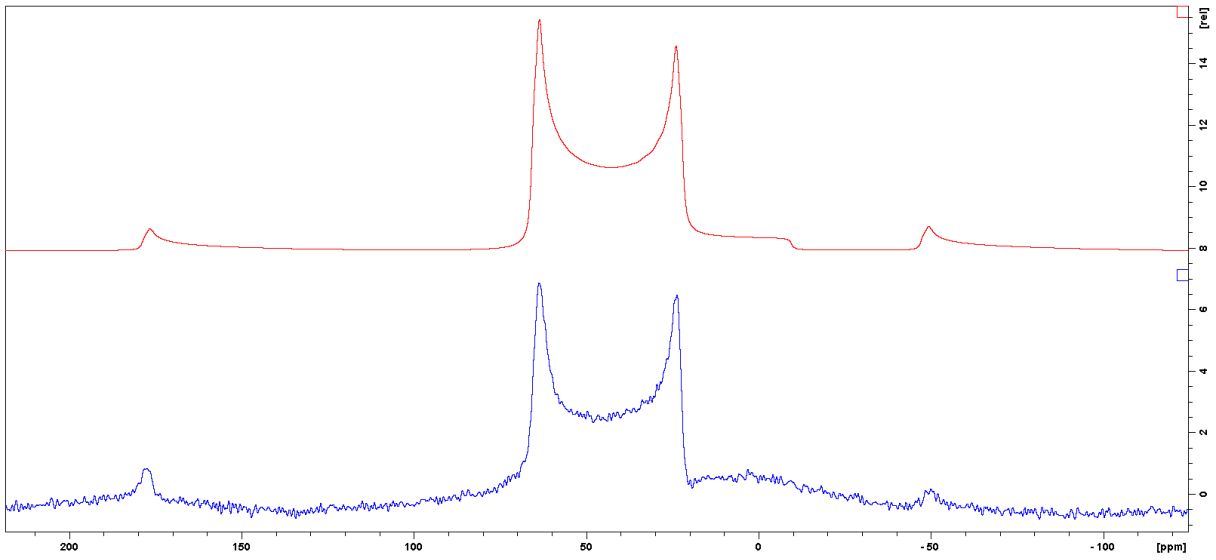


Figure S43. Solid-state $^{11}B\{^{1}H\}$ NMR spectrum of **5M** at 128 MHz. (Top: Simulation) isotropic chemical shift δ_{iso} = 77.1 ppm, quadrupolar coupling constant C_Q = 4.79 MHz, quadrupolar asymmetry parameter η_{Quad} = 0.0.

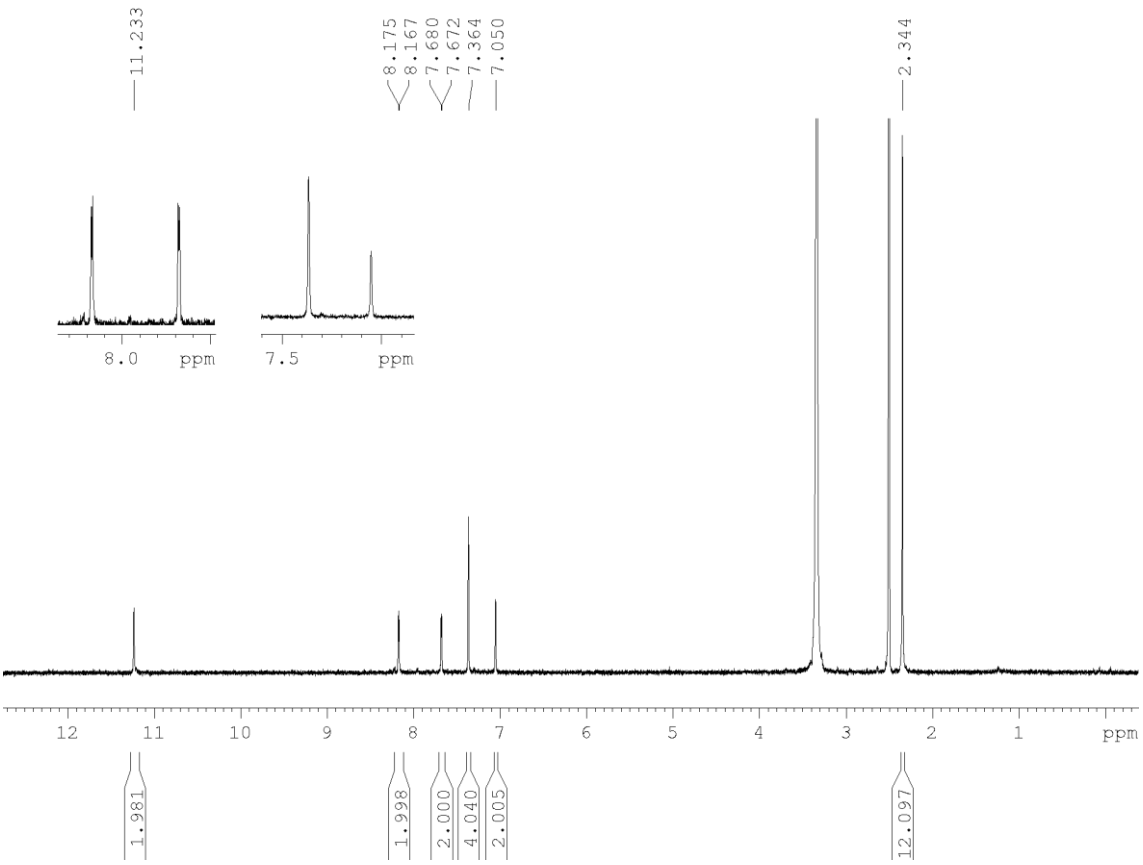


Figure S44. ^{1}H NMR spectrum of **5A** in d^{6}-DMSO at 500 MHz.

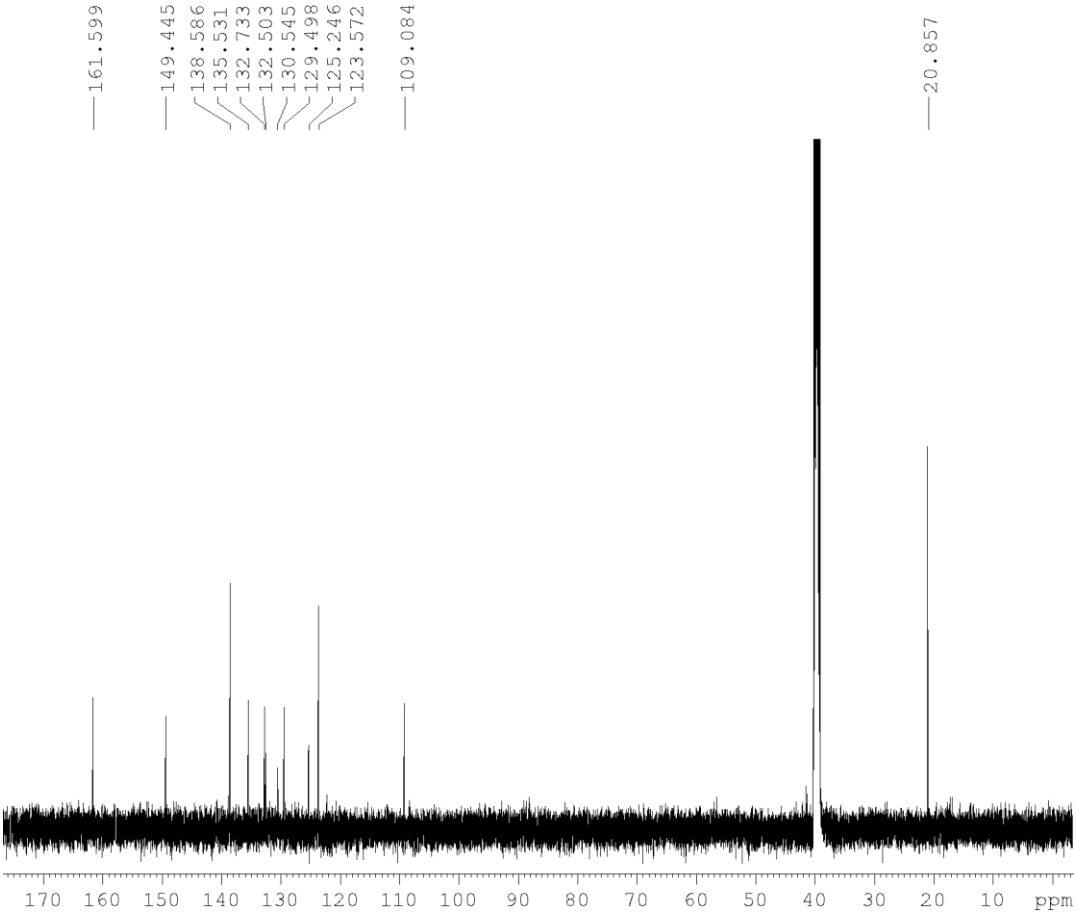
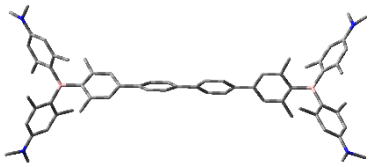


Figure S45. ^{13}C{^{1}H} NMR spectrum of **5A** in d^{6}-DMSO at 125 MHz.

Cartesian Coordinates for all DFT-Optimized Structures

Compound 1

DFT B3LYP/6-31G*, hexane, S_0



Point group: C_2

Total energy: -1823763.90 kcal mol^{-1}

Dipole moment: 0.57 D

Imaginary frequencies: 0

Symbol	X	Y	Z
C	0.000081	0.741285	-0.019291
C	0.000076	3.594646	-0.017680
C	1.144918	1.472035	0.342532
C	-1.144652	1.472447	-0.380616
C	-1.145104	2.863425	-0.377929
C	1.145355	2.863005	0.341408
H	2.043537	0.942437	0.646596
H	-2.043269	0.943193	-0.685282
H	-2.055132	3.393611	-0.644168
H	2.055393	3.392897	0.608199
C	-0.000081	-0.741285	-0.019291
C	-0.000076	-3.594646	-0.017680
C	1.144652	-1.472447	-0.380616
C	-1.144918	-1.472035	0.342532
C	-1.145355	-2.863005	0.341408
C	1.145104	-2.863425	-0.377929
H	2.043269	-0.943193	-0.685282
H	-2.043537	-0.942437	0.646596
H	-2.055393	-3.392897	0.608199
H	2.055132	-3.393611	-0.644168
C	0.000076	-5.077308	-0.016084
C	0.000577	-7.939962	-0.012238
C	0.728849	-5.807097	-0.963839
C	-0.728317	-5.804834	0.933805
C	-0.728027	-7.201991	0.959712
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C	-0.728849	5.807097	-0.963839
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H	-2.177935	-7.147361	2.560120
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H	2.186810	-7.155085	-2.579479
H	0.895387	-8.338940	-2.835091
C	-1.538974	7.881023	-2.076696
H	-0.895387	8.338940	-2.835091
H	-2.179216	8.679706	-1.687085
H	-2.186810	7.155085	-2.579479
C	1.536761	7.876059	2.052809
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H	2.177935	7.147361	2.560120
H	0.892438	8.339740	2.807011
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B	-0.000894	9.533158	-0.010505
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C	-1.005761	-11.735162	-3.757090
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C	-1.809030	-10.676420	-3.288639
C	0.116846	-12.074114	-2.975868
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H	0.771131	-12.879329	-3.290167
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C	0.427166	11.396981	1.777041
C	-1.498199	9.965546	2.108482
C	-1.811361	10.673156	3.268648
C	0.116902	12.068215	2.959726
H	-2.694944	10.377390	3.822763
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H	-2.782386	-8.923999	-0.705359
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H	2.325676	-11.055059	-0.766830
H	2.250258	-12.557724	-1.691784
H	1.414941	-12.415963	-0.137876
C	2.443208	-8.838554	1.730986
H	3.334284	-8.854232	2.367230
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H	3.340231	8.868560	-2.379041
H	1.981898	7.863958	-1.855251
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H	2.260436	12.537493	1.686312
H	1.430988	12.405246	0.128617
C	-2.443208	8.838554	1.730986
H	-1.971545	7.856994	1.839984
H	-2.782446	8.910721	0.691823
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N	-1.299280	-12.406423	-4.935631
N	-1.345483	12.449356	4.877800
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H	0.940641	14.008568	-6.218606
H	0.721497	14.417322	-4.502709
H	-0.492724	13.441585	-5.358334
C	2.555655	12.144364	-5.616083
H	2.591345	12.729334	-6.537465
H	2.639030	11.086712	-5.892402
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H	2.510857	-12.631882	6.595066
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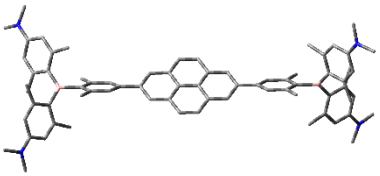
H	-2.639030	-11.086712	-5.892402
H	-3.436217	-12.405947	-5.007191
C	-0.583384	-13.628529	-5.259359
H	-0.940641	-14.008568	-6.218606
H	-0.721497	-14.417322	-4.502709
H	0.492724	-13.441585	-5.358334

Compound 2

DFT B3LYP/6-31G*, hexane, S_0



Point group: C_1

Total energy: -1919385.31 kcal mol^{-1}

Dipole moment: 0.82 D

Imaginary frequencies: 0

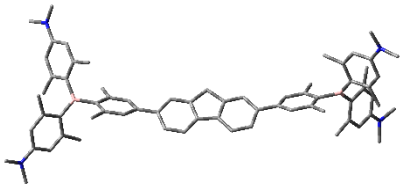
Symbol	X	Y	Z
C	-0.707661	0.018142	-0.029588
C	-3.546439	0.005920	-0.024199
C	-1.429136	0.911240	0.817689
C	-1.424647	-0.880777	-0.874514
C	-2.825665	-0.869664	-0.851681
C	-2.830089	0.888041	0.800191
H	-3.363528	-1.579247	-1.474821
H	-3.371698	1.592900	1.425449
C	0.715897	0.023479	-0.031466
C	3.552824	0.031500	-0.032530
C	1.432506	0.918448	0.818193
C	1.436896	-0.866644	-0.882496
C	2.837970	-0.841870	-0.866762
C	2.833705	0.901689	0.801340
H	3.381850	-1.539171	-1.498778
H	3.374101	1.601731	1.433336
C	5.037545	0.032622	-0.030714
C	7.898350	0.025093	-0.024817
C	5.766401	-0.135736	-1.214170
C	5.762432	0.200075	1.155295
C	7.159976	0.211729	1.175158
C	7.163951	-0.154347	-1.228288
H	5.230223	-0.232711	-2.155204
H	5.222959	0.299956	2.094123
C	-5.031100	-0.001043	-0.020753
C	-7.893594	-0.013993	-0.013807
C	-5.757672	0.239914	1.151885
C	-5.761126	-0.249213	-1.189671
C	-7.158583	-0.247953	-1.207431
C	-7.154898	0.225871	1.176440
H	-5.220374	0.412146	2.081302
H	-5.226884	-0.416959	-2.121664
C	7.832874	0.400429	2.522555
H	8.316213	1.379825	2.600906
H	8.610707	-0.347681	2.711233
H	7.098829	0.321719	3.331516

C	7.841646	-0.344787	-2.573054	C	8.825743	2.972958	-0.537145
H	8.632743	0.391620	-2.751986	H	8.862221	4.049181	-0.735869
H	7.113775	-0.248574	-3.385689	H	7.839809	2.742795	-0.121101
H	8.309099	-1.331567	-2.655472	H	8.887032	2.459716	-1.502762
C	-7.835671	-0.517143	-2.538950	C	-8.811839	2.941505	-0.520114
H	-8.324234	0.378526	-2.935854	H	-8.851692	4.023123	-0.686514
H	-8.609980	-1.289053	-2.464791	H	-7.826286	2.590678	-0.842715
H	-7.103428	-0.857080	-3.278984	H	-8.867217	2.773920	0.560772
C	-7.827937	0.487945	2.511421	C	-11.823013	-1.081168	-1.682075
H	-8.603868	1.258841	2.443196	H	-12.353703	-1.260900	-0.741575
H	-7.093825	0.826160	3.250399	H	-10.991488	-1.792807	-1.711353
H	-8.313643	-0.410288	2.905969	H	-12.501907	-1.333736	-2.503587
B	9.491958	0.011878	-0.020086	C	-11.812952	1.037135	1.675413
B	-9.486818	-0.018928	-0.010678	H	-10.981253	1.748637	1.703542
C	10.260094	-1.195601	-0.684043	H	-12.488910	1.287226	2.500157
C	11.655941	-3.387323	-1.932352	H	-12.347278	1.219485	0.737471
C	11.353978	-0.979679	-1.571066	C	-8.786322	-2.972585	0.510798
C	9.895922	-2.551227	-0.443324	H	-7.804828	-2.610364	0.833100
C	10.591992	-3.605081	-1.034526	H	-8.841630	-2.810902	-0.570968
C	12.012921	-2.047098	-2.180756	H	-8.816144	-4.053695	0.682318
H	10.294186	-4.616759	-0.783971	N	12.432130	4.408183	2.474164
H	12.823160	-1.822163	-2.864884	N	12.315106	-4.441210	-2.549058
C	10.279783	1.204023	0.648508	N	-12.393609	-3.340889	3.826129
C	11.721697	3.366873	1.894290	N	-12.380354	3.274351	-3.881649
C	11.356842	0.965721	1.549675	C	-13.599395	2.762764	-4.484147
C	9.945253	2.566694	0.404904	H	-13.986446	3.501023	-5.189410
C	10.658427	3.606112	1.001161	H	-14.385179	2.549368	-3.742003
C	12.032914	2.019416	2.164624	H	-13.406027	1.840143	-5.044695
H	10.373472	4.623919	0.760459	C	-12.126144	4.703041	-3.947866
H	12.818436	1.777822	2.871469	H	-12.717205	5.133895	-4.758696
C	-10.264064	-0.922784	1.023500	H	-11.070565	4.904033	-4.165335
C	-11.690770	-2.550449	2.927604	H	-12.386177	5.228386	-3.014693
C	-11.347031	-0.404486	1.789940	C	11.945859	5.770454	2.338530
C	-9.915268	-2.283642	1.256720	H	11.899945	6.069879	1.284484
C	-10.621035	-3.066745	2.169690	H	12.637239	6.448353	2.843250
C	-12.016377	-1.194673	2.724220	H	10.944129	5.912316	2.774551
H	-10.324935	-4.102681	2.289028	C	13.399460	4.121637	3.519220
H	-12.807107	-0.735599	3.306344	H	14.180419	3.443347	3.155787
C	-10.271061	0.881363	-1.042678	H	12.943072	3.665229	4.412395
C	-11.702728	2.501230	-2.949492	H	13.885317	5.051737	3.821337
C	-11.356538	0.359770	-1.803725	C	-13.367135	-2.725809	4.711669
C	-9.932048	2.245136	-1.272279	H	-14.152371	-2.218531	4.139046
C	-10.645487	3.026867	-2.180606	H	-12.918326	-1.989388	5.397762
C	-12.033554	1.148686	-2.733374	H	-13.846337	-3.503010	5.310690
H	-10.366668	4.069072	-2.285702	C	-11.885119	-4.657507	4.171380
H	-12.836496	0.692100	-3.300734	H	-11.824071	-5.301554	3.285938
C	11.810592	-0.433734	1.929518	H	-12.571331	-5.131733	4.876087
H	12.357851	-0.919783	1.114990	H	-10.885797	-4.621995	4.633747
H	10.972728	-1.092828	2.177900	C	12.032537	-5.803899	-2.132576
H	12.472227	-0.397475	2.801654	H	12.614443	-6.493637	-2.747346
C	8.767364	-2.935923	0.497091	H	10.972958	-6.046335	-2.276097
H	7.786216	-2.700243	0.072675	H	12.282358	-5.989078	-1.075423
H	8.827959	-2.414051	1.457961	C	13.540370	-4.185409	-3.286713
H	8.791163	-4.010616	0.706043	H	13.910139	-5.125053	-3.702139
C	11.851876	0.409251	-1.933914	H	14.333746	-3.750013	-2.658456
H	11.036002	1.093735	-2.186507	H	13.361391	-3.501489	-4.125250
H	12.522145	0.360866	-2.798798	C	-0.672640	-1.774396	-1.715269
H	12.403010	0.873531	-1.109373	H	-1.219882	-2.462155	-2.355745

C	0.689062	-1.766583	-1.720172
H	1.239554	-2.447960	-2.364660
C	-0.681603	1.811072	1.655800
H	-1.232289	2.494902	2.297537
C	0.680138	1.813473	1.657082
H	1.227187	2.499120	2.299982

Compound 3

DFT B3LYP/6-31G*, hexane, S_0



Point group: C_1

Total energy: -1847671.10 kcal mol^{-1}

Dipole moment: 1.17 D

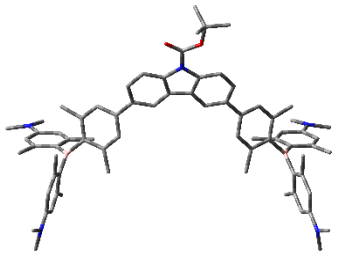
Imaginary frequencies: 0

Symbol	X	Y	Z
C	-0.719240	-1.168415	-1.182356
C	-3.477898	-0.779274	-0.777740
C	-1.637391	-1.892335	-1.946529
C	-1.180958	-0.249979	-0.216030
C	-2.539336	-0.055864	-0.014566
C	-3.000656	-1.693010	-1.738561
H	-1.301010	-2.611050	-2.689706
H	-2.888935	0.672824	0.712407
H	-3.716295	-2.275058	-2.311981
C	0.746649	-1.159959	-1.175763
C	3.496854	-0.738821	-0.746521
C	1.679961	-1.873313	-1.931475
C	1.189003	-0.236171	-0.205499
C	2.543176	-0.026274	0.008017
C	3.038908	-1.658173	-1.711275
H	1.358613	-2.595883	-2.677562
H	2.877777	0.706174	0.738277
H	3.766378	-2.231567	-2.278521
C	4.948673	-0.525587	-0.529455
C	7.750290	-0.108426	-0.108897
C	5.465792	-0.281972	0.749474
C	5.858512	-0.557924	-1.594199
C	7.230605	-0.371142	-1.405491
C	6.827897	-0.061872	0.971466
H	4.790991	-0.287513	1.602016
H	5.484837	-0.708709	-2.604035
C	-4.933867	-0.583453	-0.573745
C	-7.744244	-0.203070	-0.178484
C	-5.832636	-0.620864	-1.647581
C	-5.466082	-0.352088	0.701149
C	-6.836310	-0.179382	0.914830
C	-7.205142	-0.422245	-1.475301
H	-5.448551	-0.775416	-2.653043
H	-4.797507	-0.339663	1.558642
C	8.114670	-0.431938	-2.637847
H	8.741495	-1.329706	-2.643288
H	8.794582	0.424269	-2.708595
H	7.504162	-0.442146	-3.547023
C	7.264845	0.193953	2.402407
H	8.114255	-0.431025	2.699378
H	6.444320	-0.016094	3.096726
H	7.574588	1.233440	2.552120
C	-7.292383	0.041794	2.345603
H	-7.839895	-0.822160	2.736125
H	-7.960247	0.904941	2.442749
H	-6.431283	0.217708	2.999071
C	-8.073125	-0.463135	-2.719852
H	-8.941639	-1.120645	-2.602120
H	-7.497424	-0.829845	-3.576309
H	-8.463625	0.527120	-2.976108
B	9.308397	0.127204	0.125114
B	-9.307519	0.008563	0.041637
C	9.791194	1.414616	0.899704
C	10.651786	3.748672	2.356625
C	10.757060	1.332559	1.944013
C	9.278875	2.711226	0.609590
C	9.718586	3.837420	1.304773
C	11.155838	2.466369	2.651653
H	9.321524	4.803214	1.014066
H	11.876755	2.340479	3.451352
C	10.347338	-0.928723	-0.418903
C	12.243637	-2.842847	-1.443873
C	11.502523	-0.523302	-1.147243
C	10.173679	-2.329878	-0.232797
C	11.104406	-3.246967	-0.719992
C	12.401941	-1.459176	-1.657961
H	10.931335	-4.299709	-0.528152
H	13.242474	-1.094698	-2.237291
C	-10.072022	1.103847	-0.798891
C	-11.473823	3.083576	-2.356734
C	-11.307401	0.812082	-1.445550
C	-9.561045	2.421796	-0.971786
C	-10.254114	3.376614	-1.715210
C	-11.966081	1.770910	-2.215216
H	-9.827484	4.370067	-1.793046
H	-12.882821	1.480666	-2.715503
C	-10.071322	-0.879452	1.099325
C	-11.441541	-2.479708	3.067128
C	-10.966108	-0.300684	2.045033
C	-9.894693	-2.290492	1.173840
C	-10.579769	-3.058825	2.114669
C	-11.613155	-1.082680	3.001653
H	-10.434559	-4.132877	2.099084
H	-12.264750	-0.584924	3.710702
C	11.808883	0.934027	-1.448247
H	12.143601	1.472251	-0.555518
H	10.937023	1.475489	-1.829244
H	12.600164	1.010725	-2.201645
C	8.263232	2.956141	-0.492382
H	7.271881	2.578288	-0.222507

H	8.540694	2.467397	-1.432192
H	8.167941	4.027936	-0.695988
C	11.386916	0.018683	2.374488
H	10.645563	-0.774508	2.514933
H	11.920310	0.143198	3.322905
H	12.102602	-0.352366	1.633818
C	8.994902	-2.908946	0.529486
H	9.155794	-3.972220	0.736216
H	8.060540	-2.815424	-0.033065
H	8.834290	-2.409169	1.490557
C	-8.991124	-3.048030	0.217042
H	-9.161342	-4.126619	0.300336
H	-7.932587	-2.860359	0.423636
H	-9.161897	-2.768791	-0.827972
C	-11.248874	1.191207	2.097207
H	-11.873774	1.517537	1.259566
H	-10.334722	1.792001	2.055480
H	-11.770991	1.448904	3.024861
C	-11.963148	-0.556552	-1.375270
H	-11.256674	-1.370185	-1.568657
H	-12.766581	-0.634105	-2.115618
H	-12.397239	-0.749342	-0.388854
C	-8.259286	2.879279	-0.337611
H	-7.388910	2.425577	-0.822346
H	-8.198910	2.618942	0.724346
H	-8.155848	3.966733	-0.414802
N	13.168600	-3.763375	-1.916487
N	11.049251	4.868304	3.073853
N	-12.160308	4.044163	-3.086339
N	-12.083589	-3.246235	4.029367
C	-13.125357	-2.645929	4.844815
H	-13.504058	-3.391820	5.546601
H	-13.972698	-2.272169	4.248074
H	-12.732386	-1.808119	5.433396
C	-12.016496	-4.695280	3.953429
H	-12.541186	-5.122692	4.810426
H	-10.977463	-5.042729	3.994903
H	-12.472050	-5.098147	3.034384
C	12.854321	-5.181212	-1.870410
H	12.692343	-5.515904	-0.838757
H	13.697766	-5.747217	-2.271103
H	11.956763	-5.439188	-2.454867
C	14.226924	-3.321866	-2.808119
H	14.846785	-2.553604	-2.331082
H	13.845197	-2.908920	-3.755905
H	14.874615	-4.169593	-3.041158
C	-13.315101	3.653692	-3.876248
H	-14.089509	3.204697	-3.243268
H	-13.067155	2.932250	-4.671625
H	-13.745598	4.542114	-4.342991
C	-11.511722	5.307472	-3.393857
H	-11.248479	5.848980	-2.477314
H	-12.202985	5.935421	-3.959676
H	-10.593031	5.182462	-3.988917
C	10.641868	6.188413	2.625107
H	11.011380	6.935456	3.330671
H	9.549172	6.273048	2.596068
H	11.027862	6.439261	1.623818
C	12.169519	4.768530	3.993515
H	12.327432	5.737895	4.470681
H	13.106408	4.472630	3.495036
H	11.965181	4.039368	4.786782
C	-0.002838	0.415091	0.469858
H	-0.006642	0.241916	1.555075
H	-0.008587	1.505267	0.330964

Compound 4

DFT B3LYP/6-31G*, hexane, S_0



Point group: C_1

Total energy: -2075924.33 kcal mol^{-1}

Dipole moment: 4.27 D

Imaginary frequencies: 0

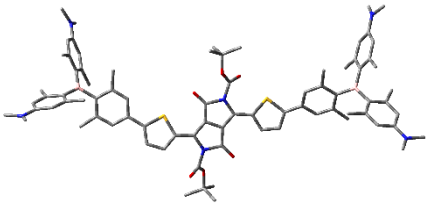
Symbol	X	Y	Z
C	-1.194946	5.048349	0.023218
C	-3.026125	2.908277	0.004686
C	-0.739984	3.710238	0.008320
C	-2.563475	5.325740	0.026829
C	-3.452573	4.253034	0.017367
C	-1.648711	2.652284	-0.000003
H	-2.932976	6.339946	0.027430
H	-4.517311	4.465537	-0.007134
H	-1.287254	1.628197	0.016694
C	0.710865	3.739387	0.011259
C	1.106209	5.093136	0.028301
N	-0.059822	5.906618	0.034333
C	2.457785	5.442910	0.038460
H	2.765537	6.478261	0.041821
C	3.395082	4.412081	0.032295
H	4.449144	4.672758	0.013017
C	1.667970	2.724509	0.005982
H	1.357155	1.683866	0.020336
C	3.031203	3.048097	0.016515
C	4.067302	1.985508	0.010299
C	6.062280	-0.067486	0.000946
C	3.894911	0.805781	-0.724195
C	5.255018	2.121118	0.739586
C	6.233123	1.122861	0.758705
C	4.864176	-0.200698	-0.752139
H	2.993272	0.681011	-1.319270
H	5.409135	3.016430	1.337181
C	-4.010270	1.797664	-0.003585

C	-5.903566	-0.349488	-0.014056	H	8.170961	-4.248862	0.212471
C	-5.208837	1.880225	0.715853	H	7.413549	-5.188518	-1.082080
C	-3.775803	0.623525	-0.729732	H	6.475319	-4.005150	-0.165921
C	-4.694913	-0.428973	-0.757830	C	8.070089	0.636749	-2.297699
C	-6.137837	0.836118	0.734058	H	8.612077	1.114801	-3.120500
H	-5.410374	2.770161	1.307411	H	8.519636	0.985748	-1.362155
H	-2.864817	0.538740	-1.317499	H	7.042187	1.013111	-2.312100
B	7.172317	-1.209448	-0.004882	C	-5.070272	-2.287179	2.300602
B	-6.955068	-1.545987	-0.017430	H	-4.775386	-1.233014	2.318653
C	7.726390	-1.748379	-1.380990	H	-4.676690	-2.707925	1.369453
C	8.693863	-2.751520	-3.904421	H	-4.560639	-2.790214	3.129146
C	8.118291	-0.874765	-2.434821	C	-9.919561	-2.063527	0.558610
C	7.843800	-3.144925	-1.637033	H	-10.914465	-2.095823	1.015424
C	8.300289	-3.619498	-2.866565	H	-9.904330	-2.786964	-0.262946
C	8.606718	-1.369712	-3.643778	H	-9.797317	-1.074919	0.104422
H	8.347283	-4.692550	-3.013020	C	-7.085411	-4.551061	-0.601276
H	8.925324	-0.656382	-4.395152	H	-7.802788	-4.627755	0.222102
C	7.702505	-1.785923	1.365369	H	-6.118737	-4.305819	-0.149562
C	8.691395	-2.794981	3.878132	H	-6.993316	-5.541606	-1.059378
C	9.096483	-1.945033	1.612771	C	-7.927285	0.233387	-2.332358
C	6.823845	-2.157631	2.422342	H	-8.484937	0.677016	-3.163938
C	7.311247	-2.666412	3.625956	H	-6.919066	0.659837	-2.341478
C	9.564545	-2.421401	2.837250	H	-8.401808	0.567651	-1.403742
H	6.593226	-2.967926	4.379917	C	-4.335217	-1.640532	-1.598542
H	10.636599	-2.500057	2.977303	H	-4.963620	-1.716911	-2.491864
C	-7.464118	-2.136173	1.354892	H	-4.456412	-2.581067	-1.049790
C	-8.417752	-3.167822	3.872155	H	-3.291561	-1.583394	-1.925478
C	-6.574827	-2.453330	2.420753	C	-7.389159	1.036501	1.569565
C	-8.850052	-2.362238	1.595592	H	-7.466063	2.077821	1.900078
C	-9.301695	-2.848773	2.822210	H	-7.389571	0.400147	2.460495
C	-7.044060	-2.973521	3.626672	H	-8.304192	0.799232	1.015611
H	-10.369381	-2.979354	2.956727	N	9.137385	-3.235307	-5.127377
H	-6.316761	-3.231939	4.387705	N	-8.782614	-3.711360	-5.133280
C	-7.472299	-2.123573	-1.391948	N	-8.879578	-3.642110	5.091894
C	-8.371772	-3.195520	-3.912291	N	9.169061	-3.258590	5.096037
C	-7.518778	-3.526485	-1.636002	C	10.578125	-3.583576	5.235130
C	-7.899683	-1.279773	-2.456256	H	10.768418	-3.918181	6.256967
C	-8.354803	-1.808777	-3.663712	H	10.903446	-4.378853	4.545469
C	-7.942753	-4.033796	-2.864055	H	11.205973	-2.702884	5.053697
H	-8.703236	-1.118789	-4.423597	C	8.238203	-3.797015	6.072514
H	-7.935428	-5.109068	-3.001197	H	8.787060	-4.071892	6.975659
C	4.569903	-1.422714	-1.603157	H	7.489602	-3.047766	6.355746
H	5.207522	-1.462504	-2.492322	H	7.703560	-4.689484	5.708929
H	3.527014	-1.414187	-1.937443	C	-10.271512	-4.035907	5.226008
H	4.732763	-2.359954	-1.059496	H	-10.552045	-4.853306	4.542623
C	7.467063	1.377979	1.605128	H	-10.451332	-4.369520	6.250048
H	7.489810	2.418979	1.944533	H	-10.941565	-3.189679	5.031892
H	8.396703	1.191186	1.056127	C	-7.929431	-4.122143	6.080258
H	7.492843	0.734961	2.490916	H	-7.221005	-3.333215	6.358975
C	5.313625	-2.064499	2.294476	H	-8.469813	-4.413578	6.983310
H	4.967555	-1.026157	2.317536	H	-7.348665	-4.990973	5.730504
H	4.824682	-2.597514	3.116741	C	-9.378141	-2.828015	-6.120673
H	4.946254	-2.497622	1.358254	H	-8.684928	-2.025075	-6.397809
C	10.155800	-1.581892	0.585994	H	-9.598528	-3.399490	-7.024697
H	11.148311	-1.568975	1.048951	H	-10.313595	-2.362257	-5.770712
H	9.986583	-0.595796	0.141552	C	-8.992709	-5.142160	-5.271880
H	10.181984	-2.296216	-0.243205	H	-9.300598	-5.360462	-6.296489
C	7.455103	-4.199058	-0.614303	H	-8.066757	-5.697591	-5.079796

H	-9.766658	-5.528280	-4.589447
C	9.697900	-2.314720	-6.101177
H	9.952591	-2.866019	-7.008736
H	8.969283	-1.543152	-6.376501
H	10.607135	-1.808202	-5.738885
C	9.420441	-4.652381	-5.276270
H	10.209448	-5.004804	-4.592752
H	8.522754	-5.255356	-5.093753
H	9.744063	-4.846312	-6.300959
C	-0.008764	7.300675	0.053261
O	1.035616	7.925072	0.063504
O	-1.242136	7.832696	0.058159
C	-1.433636	9.300378	0.077085
C	-2.958679	9.433063	0.076117
H	-3.240369	10.491023	0.089884
H	-3.388546	8.973898	-0.820087
H	-3.391680	8.949881	0.958065
C	-0.839282	9.888061	1.360598
H	-1.255234	9.382798	2.239056
H	0.246870	9.789524	1.376147
H	-1.097605	10.950934	1.426422
C	-0.834746	9.921563	-1.188416
H	0.251470	9.823536	-1.202700
H	-1.247490	9.439494	-2.081307
H	-1.093037	10.985768	-1.227261

Compound 5

DFT B3LYP/6-31G*, hexane, S_0



Point group: C_1

Total energy: -2968846.10 kcal mol^{-1}

Dipole moment: 3.34 D

Imaginary frequencies: 0

Symbol	X	Y	Z
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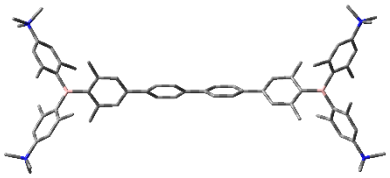
N	0.625081	-0.086907	-0.233258
C	-0.808036	-0.391054	-0.159122
O	-1.667888	0.442059	0.057226
C	-0.861280	-1.801159	-0.478008
C	0.456922	-2.258575	-0.766481
C	-1.768028	-2.853359	-0.517807
N	-1.008898	-3.991672	-0.881034
C	0.397932	-3.679061	-1.029279
O	1.240624	-4.526275	-1.294647
C	-3.189039	-2.839269	-0.294964
C	-4.065626	-3.879718	-0.002597
H	-3.735528	-4.897670	0.143024
C	-5.402416	-3.466435	0.143459
H	-6.205607	-4.144384	0.409553
C	-5.591767	-2.105670	-0.029413
S	-4.076908	-1.315713	-0.372021
C	2.805220	-1.306137	-0.707143
C	3.498710	-2.472677	-1.029792
H	2.987324	-3.390999	-1.296566
C	4.893428	-2.346833	-0.926372
H	5.577500	-3.165526	-1.118052
C	5.315437	-1.093504	-0.511640
S	3.947422	-0.032100	-0.296069
C	6.684350	-0.624027	-0.298170
C	9.372913	0.258878	0.111864
C	7.766192	-1.278074	-0.907998
C	6.971459	0.479647	0.518424
C	8.276658	0.934086	0.714661
C	9.084940	-0.870529	-0.703197
H	7.573644	-2.114328	-1.574332
H	6.158086	0.990241	1.028411
C	-6.842146	-1.349586	0.058018
C	-9.303115	0.094534	0.231708
C	-6.861011	0.020956	0.354578
C	-8.074905	-1.985518	-0.154105
C	-9.285509	-1.298443	-0.054962
C	-8.053418	0.743869	0.426200
H	-5.923767	0.535499	0.552572
H	-8.089216	-3.038618	-0.421813
C	8.462202	2.145737	1.609121
H	8.765375	3.027828	1.035938
H	9.232268	1.987992	2.372033
H	7.528574	2.385878	2.128430
C	10.172553	-1.661789	-1.405978
H	10.875024	-1.017632	-1.946011
H	9.734808	-2.353291	-2.133547
H	10.766813	-2.248693	-0.698207
C	-7.947756	2.223808	0.744540
H	-8.198461	2.842165	-0.123423
H	-6.929019	2.477149	1.055529
H	-8.624002	2.527180	1.551168
C	-10.555679	-2.093919	-0.293743
H	-10.318112	-3.083773	-0.697559
H	-11.229511	-1.602192	-1.003748
H	-11.124456	-2.234890	0.631035
B	10.872995	0.751939	0.339840
B	-10.676416	0.899575	0.332393
C	11.956096	-0.276631	0.844834
C	13.235850	-0.366779	0.223898
C	11.708424	-1.175174	1.921871
C	12.679114	-2.079888	2.350005
C	14.178917	-1.304269	0.643782
H	12.447813	-2.712227	3.199415
H	15.126646	-1.343942	0.119154
C	11.243384	2.257808	0.055728
C	12.010261	3.018414	0.985848
C	10.817058	2.937412	-1.121311
C	11.152085	4.271258	-1.350546

C	12.302688	4.362036	0.754279	H	16.730399	-2.108084	1.808701
H	10.832528	4.724628	-2.281756	H	16.814485	-3.872776	2.000609
H	12.868854	4.897663	1.507663	H	16.218682	-3.182562	0.488662
C	-10.871273	2.210010	-0.522203	C	14.646647	-3.897542	3.323510
C	-10.518112	2.278674	-1.900360	H	13.720370	-4.479189	3.246487
C	-11.395779	3.400946	0.059221	H	15.469226	-4.603438	3.454917
C	-11.531227	4.571133	-0.686996	H	14.580560	-3.273194	4.228949
C	-10.696270	3.448570	-2.637641	C	11.866330	6.971932	-1.914758
H	-11.912940	5.453600	-0.186415	H	10.794962	6.898418	-2.136098
H	-10.445490	3.430279	-3.691974	H	12.124249	8.032389	-1.881683
C	-11.815217	0.368803	1.285643	H	12.417367	6.509303	-2.749200
C	-13.165764	0.271507	0.841045	C	13.104363	7.051281	0.252387
C	-11.553777	-0.056828	2.619369	H	12.738415	7.053717	1.286416
C	-12.574950	-0.526659	3.444443	H	14.107727	6.596819	0.249553
C	-14.165501	-0.235900	1.670428	H	13.199558	8.091380	-0.065679
H	-12.322942	-0.800031	4.462593	C	-16.290528	-1.072023	3.377274
H	-15.170615	-0.308993	1.271140	H	-16.928133	-1.532375	4.134680
C	10.015060	2.249865	-2.211966	H	-16.625590	-0.033068	3.229666
H	9.986259	2.867638	-3.115566	H	-16.449686	-1.614204	2.437244
H	8.981091	2.066725	-1.902223	C	-14.628786	-1.418854	5.207260
H	10.437348	1.279295	-2.492259	H	-15.515772	-1.854538	5.671693
C	12.526881	2.436770	2.290961	H	-13.808926	-2.138021	5.320296
H	13.353441	1.737810	2.127287	H	-14.359822	-0.507756	5.765542
H	11.755997	1.883754	2.837102	C	-11.104944	5.784496	-4.218523
H	12.888299	3.234913	2.948029	H	-11.208822	6.798689	-4.609455
C	10.401308	-1.176880	2.694534	H	-10.093012	5.438445	-4.460341
H	9.580175	-1.595941	2.104000	H	-11.820708	5.136006	-4.748792
H	10.092401	-0.170056	2.994497	C	-12.018951	6.936982	-2.200672
H	10.494309	-1.775971	3.606369	H	-13.066020	6.706453	-1.948003
C	13.644089	0.516478	-0.942998	H	-11.520410	7.283797	-1.287256
H	14.562024	0.138226	-1.405294	H	-12.013661	7.764276	-2.913137
H	13.828362	1.548751	-0.628441	C	-1.450642	-5.321658	-1.170562
H	12.876788	0.561623	-1.722485	C	1.058697	1.267353	-0.299424
C	-9.970506	1.083271	-2.659842	O	-2.040065	-6.023229	-0.378343
H	-10.556475	0.174504	-2.487050	O	1.792662	1.682074	-1.171388
H	-8.940065	0.854378	-2.369324	O	0.534659	1.943267	0.714014
H	-9.976578	1.276916	-3.737577	O	-1.086482	-5.632537	-2.406858
C	-11.806929	3.487373	1.519357	C	0.516906	3.425044	0.729190
H	-12.736606	2.943083	1.714528	C	-0.319686	3.719525	1.975341
H	-11.962736	4.531489	1.810863	H	-1.312598	3.270339	1.880713
H	-11.053130	3.066240	2.192202	H	0.161305	3.309212	2.869114
C	-13.598626	0.677265	-0.557698	H	-0.429580	4.801320	2.105407
H	-14.612723	0.318183	-0.762908	C	1.944738	3.956484	0.876171
H	-12.941737	0.271211	-1.333619	H	2.425589	3.520571	1.758582
H	-13.595813	1.764453	-0.686202	H	2.545470	3.724243	-0.004850
C	-10.168819	0.013122	3.237931	H	1.916176	5.044232	1.007103
H	-9.499264	-0.747330	2.823175	C	-0.180291	3.937952	-0.533804
H	-10.222432	-0.145688	4.320039	H	-0.330781	5.020035	-0.451130
H	-9.686028	0.981982	3.072777	H	0.414381	3.739704	-1.428023
C	-11.187511	4.632630	-2.052406	H	-1.157902	3.457837	-0.642542
N	-11.319072	5.804313	-2.781877	C	-1.096696	-7.035843	-2.892375
C	-13.903801	-0.649542	2.991982	C	-0.242774	-7.901741	-1.962459
C	11.885260	5.028599	-0.415266	H	-0.717251	-8.033843	-0.988033
C	13.932465	-2.186708	1.714716	H	-0.102082	-8.888940	-2.416347
N	-14.904755	-1.160609	3.804584	H	0.738278	-7.439109	-1.817941
N	14.875120	-3.120138	2.117761	C	-2.541335	-7.527566	-3.006322
N	12.175482	6.367031	-0.630643	H	-2.551783	-8.520168	-3.470550
C	16.222752	-3.058134	1.578415	H	-3.013808	-7.596061	-2.024865

H	-3.128046	-6.851136	-3.637203
C	-0.443877	-6.899660	-4.268719
H	-1.026923	-6.229865	-4.908938
H	0.567421	-6.493406	-4.172713
H	-0.385836	-7.879975	-4.753146

Compound 1M

DFT B3LYP/6-31G*, water, S_0



Point group: C_1

Total energy: -1923472.14 kcal mol^{-1}

Imaginary frequencies: 0

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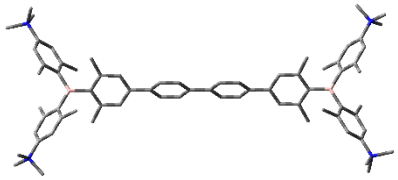
C	5.071793	0.026002	0.020497
C	5.798649	-0.952999	0.713125
C	7.193453	-0.989458	0.711149
C	7.942237	0.016678	0.024372
H	5.272940	1.783541	-1.200498
H	5.258284	-1.730784	1.245288
C	3.589766	0.028813	0.015387
C	2.856576	-0.358803	1.150972
C	2.866716	0.418181	-1.126126
C	1.465570	-0.352988	1.146125
H	3.379524	-0.647082	2.058311
C	1.475728	0.414665	-1.133056
H	3.397747	0.705675	-2.029010
C	0.742102	0.031150	0.003379
H	0.932612	-0.671457	2.037196
H	0.950789	0.734057	-2.028550
C	-0.742221	0.031145	-0.003169
C	-1.465683	-0.353183	-1.145853
C	-1.475853	0.414860	1.133197
C	-2.856689	-0.359000	-1.150704
H	-0.932723	-0.671799	-2.036869
C	-2.866840	0.418375	1.126261
H	-0.950916	0.734410	2.028636
C	-3.589884	0.028805	-0.015187
H	-3.379631	-0.647434	-2.057997
H	-3.397875	0.706028	2.029092
C	-5.071910	0.025978	-0.020306
C	-5.807108	1.001873	0.667815
C	-5.798744	-0.953175	-0.712750
C	-7.202144	1.029714	0.661762
H	-5.273092	1.783721	1.200379
C	-7.193544	-0.989666	-0.710772
H	-5.258357	-1.731054	-1.244750
C	-7.942355	0.016609	-0.024212
B	-9.509013	0.006613	-0.018858
B	9.508900	0.006656	0.018935
C	-10.339761	1.360048	-0.245825
C	-10.094118	2.153167	-1.395948
C	-11.339120	1.799845	0.663938
C	-10.827459	3.330310	-1.623259
C	-12.039218	2.988842	0.430388
C	-11.785717	3.747665	-0.709557
H	-10.610812	3.892642	-2.522251
H	-12.781190	3.296592	1.159944
C	10.339803	1.360026	0.245773
C	10.094351	2.153203	1.395910
C	11.339152	1.799679	-0.664057
C	10.827919	3.330207	1.623186
C	12.039483	2.988553	-0.430541
C	11.786211	3.747391	0.709436
H	10.611433	3.892581	2.522190
H	12.781432	3.296197	-1.160163
C	-10.319016	-1.358499	0.215057
C	-10.045498	-2.153942	1.362446
C	-11.319706	-1.810247	-0.681407
C	-10.756107	-3.339321	1.586291
C	-12.003518	-3.014970	-0.448565
C	-11.721810	-3.771445	0.681137
H	-10.524388	-3.910979	2.479181
H	-12.746677	-3.322627	-1.172582
C	10.318831	-1.358501	-0.215053
C	10.045019	-2.154072	-1.362274
C	11.319763	-1.810150	0.681198
C	10.755590	-3.339471	-1.586186
C	12.003522	-3.014889	0.448311
C	11.721531	-3.771489	-0.681244
H	10.523630	-3.911225	-2.478950
H	12.746860	-3.322468	1.172176
C	-7.840830	-2.118639	-1.492337
H	-8.659715	-1.777153	-2.133279
H	-7.104940	-2.601795	-2.141238
H	-8.248517	-2.892185	-0.831967
C	-7.858372	2.155969	1.439683
H	-7.123466	2.655524	2.077105
H	-8.284099	2.917233	0.776636
H	-8.665727	1.808043	2.091887
C	7.840766	-2.118268	1.492926
H	7.104991	-2.601053	2.142235
H	8.248103	-2.892135	0.832713
H	8.659920	-1.776704	2.133477
C	7.858232	2.155742	-1.439921
H	7.123244	2.655456	-2.077124
H	8.284352	2.916915	-0.777026
H	8.665297	1.807609	-2.092377
C	-11.682344	-1.053380	-1.942878
H	-12.108497	-0.072027	-1.714702
H	-10.809534	-0.887682	-2.583992
H	-12.416104	-1.604795	-2.537300
C	-8.996280	-1.780908	2.390925
H	-7.985855	-1.953668	2.006614
H	-9.048362	-0.727229	2.678524

H	-9.114062	-2.375325	3.301645
C	-9.048811	1.796311	-2.434733
H	-8.038859	2.007888	-2.068299
H	-9.070483	0.737361	-2.705515
H	-9.198206	2.372351	-3.352608
C	-11.672800	1.041032	1.931611
H	-12.071746	0.046540	1.711608
H	-10.791367	0.904262	2.567983
H	-12.418365	1.575070	2.527264
C	-14.057845	4.710501	-0.973131
H	-14.367799	4.252285	-0.036090
H	-14.604554	5.641738	-1.130223
H	-14.230797	4.022460	-1.800951
C	-12.213340	5.739613	-2.196408
H	-12.423655	5.089072	-3.044613
H	-12.827041	6.638272	-2.260580
H	-11.159492	6.014668	-2.172118
C	-12.304391	5.980815	0.232020
H	-12.615459	5.519863	1.167432
H	-11.235092	6.191583	0.257884
H	-12.871075	6.897664	0.061334
C	-13.178759	-4.978689	2.286286
H	-13.894023	-4.158306	2.223813
H	-13.696010	-5.922832	2.464766
H	-12.463953	-4.789601	3.084691
C	-13.462012	-5.421940	-0.098198
H	-13.926865	-6.366905	0.183687
H	-14.218500	-4.639245	-0.143886
H	-12.960298	-5.531085	-1.059066
C	-11.440835	-6.211029	1.021644
H	-10.924479	-6.263641	0.062904
H	-10.725774	-6.021460	1.819847
H	-11.980466	-7.139220	1.216826
C	11.672648	1.040822	-1.931752
H	12.071944	0.046468	-1.711745
H	10.791076	0.903744	-2.567857
H	12.417902	1.574997	-2.527672
C	9.049034	1.796530	2.434744
H	8.039050	2.007492	2.068061
H	9.071100	0.737734	2.706124
H	9.198081	2.373124	3.352324
C	12.305116	5.980483	-0.232144
H	12.871908	6.897269	-0.061475
H	12.616071	5.519516	-1.167588
H	11.235838	6.191372	-0.257935
C	12.214258	5.739229	2.196292
H	11.160474	6.014538	2.172058
H	12.424452	5.088582	3.044444
H	12.828166	6.637746	2.260478
C	14.058506	4.709906	0.972826
H	14.605355	5.641063	1.129903
H	14.231437	4.021809	1.800602
H	14.368324	4.251695	0.035737
C	8.995508	-1.781216	-2.390521
H	7.985198	-1.954070	-2.005947
H	9.047390	-0.727555	-2.678207
H	9.113135	-2.375690	-3.301224
C	11.682805	-1.053118	1.942461
H	12.109562	-0.072089	1.713995
H	10.810099	-0.886692	2.583515
H	12.416232	-1.604792	2.537055
C	11.440444	-6.211088	-1.021463
H	10.725206	-6.021590	-1.819526
H	11.980006	-7.139314	-1.216670
H	10.924291	-6.263602	-0.062607
C	13.461895	-5.421945	0.097835
H	14.218402	-4.639258	0.143275
H	12.960403	-5.531002	1.058832
H	13.926660	-6.366946	-0.184077
C	13.178094	-4.978902	-2.286624
H	13.893436	-4.158572	-2.224364
H	13.695221	-5.923100	-2.465170
H	12.463105	-4.789803	-3.084863
N	12.443223	-5.073441	-0.962463
N	12.575357	5.024316	0.915126
N	-12.443581	-5.073360	0.962313
N	-12.574658	5.024709	-0.915294

Compound 1M

DFT B3LYP/6-31G*, water, S_0



Point group: C_i

Total energy: -1923554.01 kcal mol^{-1}

Symbol	X	Y	Z
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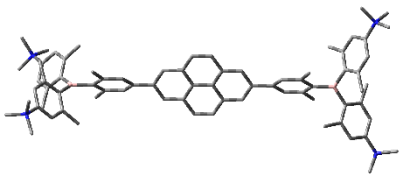
C	-0.011800	-5.099680	0.018900
C	0.827780	-5.829140	0.873010
C	0.860300	-7.224040	0.876900
C	-0.010950	-7.970140	0.023130
H	-1.527000	-5.296140	-1.492980
H	1.500960	-5.290850	1.534230
C	-0.009720	-3.617650	0.014010
C	0.173510	-2.885450	1.200470
C	-0.189750	-2.893610	-1.177970
C	0.172350	-1.494440	1.195270
H	0.295870	-3.409130	2.144200
C	-0.181360	-1.502630	-1.183570
H	-0.314930	-3.423900	-2.117630
C	-0.002320	-0.769990	0.003000
H	0.330110	-0.962300	2.128770
H	-0.336430	-0.976880	-2.121130
B	-0.004290	-9.536820	0.018870
C	-1.378660	-10.364060	0.003130
C	-2.361580	-10.116420	0.995470
C	-1.653640	-11.362270	-0.970400

C	-3.562170	-10.846800	1.011310	H	4.479570	-13.932680	-1.456610
C	-2.866920	-12.059380	-0.950500	H	6.259430	-13.739240	-1.382380
C	-3.814220	-11.804010	0.037900	H	5.256470	-12.504100	-2.191690
H	-4.273690	-10.628750	1.797140	N	5.161420	-12.484880	-0.052530
H	-3.043050	-12.800530	-1.723260	N	-5.109510	-12.589700	0.014840
C	1.378570	-10.350440	0.028950	C	0.002320	0.769990	-0.003000
C	2.364710	-10.078830	-0.959870	C	-0.172350	1.494440	-1.195270
C	1.662420	-11.352550	0.990380	C	0.181360	1.502630	1.183570
C	3.569120	-10.792610	-0.971540	C	-0.173510	2.885450	-1.200470
C	2.887520	-12.039560	0.973300	H	-0.330110	0.962300	-2.128770
C	3.832210	-11.759670	-0.005000	C	0.189750	2.893610	1.177970
H	4.289970	-10.562230	-1.749380	H	0.336430	0.976880	2.121130
H	3.060650	-12.783690	1.739740	C	0.009720	3.617650	-0.014010
C	1.831820	-7.874360	1.845210	H	-0.295870	3.409130	-2.144200
H	2.194490	-7.139850	2.569800	H	0.314930	3.423900	2.117630
H	2.708900	-8.283810	1.331640	C	0.011800	5.099680	-0.018900
H	1.380470	-8.692550	2.415140	C	0.852860	5.832250	0.831010
C	-1.858030	-7.880430	-1.795400	C	-0.827780	5.829140	-0.873010
H	-2.235580	-7.144130	-2.510430	C	0.885060	7.227200	0.830590
H	-2.725300	-8.304470	-1.277310	H	1.527000	5.296140	1.492980
H	-1.402440	-8.688470	-2.376580	C	-0.860300	7.224040	-0.876900
C	-0.684000	-11.697870	-2.084540	H	-1.500960	5.290850	-1.534230
H	0.254900	-12.099830	-1.692800	C	0.010950	7.970140	-0.023130
H	-0.434550	-10.816700	-2.686130	C	1.858030	7.880430	1.795400
H	-1.106700	-12.441710	-2.765640	C	-1.831820	7.874360	-1.845210
C	-2.190910	-9.072020	2.081380	B	0.004290	9.536820	-0.018870
H	-2.331210	-8.061480	1.683670	H	2.235580	7.144130	2.510430
H	-1.196630	-9.096920	2.535210	H	2.725300	8.304470	1.277310
H	-2.920680	-9.219460	2.882830	H	1.402440	8.688470	2.376580
C	-5.847640	-12.316930	-1.282950	H	-2.194490	7.139850	-2.569800
H	-6.781660	-12.881240	-1.276880	H	-2.708900	8.283810	-1.331640
H	-5.229760	-12.629170	-2.122580	H	-1.380470	8.692550	-2.415140
H	-6.047830	-11.247090	-1.345070	C	1.378660	10.364060	-0.003130
C	-6.038180	-12.226610	1.150010	C	-1.378570	10.350440	-0.028950
H	-6.302100	-11.172090	1.078050	C	2.361580	10.116420	-0.995470
H	-5.547870	-12.438520	2.099520	C	1.653640	11.362270	0.970400
H	-6.935570	-12.838090	1.054470	C	-2.364710	10.078830	0.959870
C	-4.814150	-14.073680	0.126450	C	-1.662420	11.352550	-0.990380
H	-5.759870	-14.618010	0.116620	C	3.562170	10.846800	-1.011310
H	-4.283280	-14.248430	1.062520	C	2.190910	9.072020	-2.081380
H	-4.198690	-14.384780	-0.715280	C	2.866920	12.059380	0.950500
C	2.181830	-9.028370	-2.037310	C	0.684000	11.697870	2.084540
H	2.286840	-8.018510	-1.627850	C	-3.569120	10.792610	0.971540
H	1.195280	-9.077420	-2.506320	C	-2.181830	9.028370	2.037310
H	2.927270	-9.147640	-2.828950	C	-2.887520	12.039560	-0.973300
C	0.693860	-11.713490	2.098210	C	-0.693860	11.713490	-2.098210
H	-0.232630	-12.137610	1.700140	C	3.814220	11.804010	-0.037900
H	0.419320	-10.840300	2.700250	H	4.273690	10.628750	-1.797140
H	1.130080	-12.448370	2.780460	H	2.331210	8.061480	-1.683670
C	6.294310	-11.485180	0.090450	H	1.196630	9.096920	-2.535210
H	6.250430	-10.769470	-0.728210	H	2.920680	9.219460	-2.882830
H	7.240980	-12.027250	0.061770	H	3.043050	12.800530	1.723260
H	6.178280	-10.969120	1.043760	H	-0.254900	12.099830	1.692800
C	5.314770	-13.504440	1.052180	H	0.434550	10.816700	2.686130
H	4.534320	-14.258830	0.958550	H	1.106700	12.441710	2.765640
H	5.253980	-13.003200	2.017560	C	-3.832210	11.759670	0.005000
H	6.293430	-13.971760	0.941130	H	-4.289970	10.562230	1.749380
C	5.299930	-13.219560	-1.372920	H	-2.286840	8.018510	1.627850

H	-1.195280	9.077420	2.506320
H	-2.927270	9.147640	2.828950
H	-3.060650	12.783690	-1.739740
H	0.232630	12.137610	-1.700140
H	-0.419320	10.840300	-2.700250
H	-1.130080	12.448370	-2.780460
N	5.109510	12.589700	-0.014840
N	-5.161420	12.484880	0.052530
C	5.847640	12.316930	1.282950
C	6.038180	12.226610	-1.150010
C	4.814150	14.073680	-0.126450
C	-6.294310	11.485180	-0.090450
C	-5.314770	13.504440	-1.052180
C	-5.299930	13.219560	1.372920
H	6.781660	12.881240	1.276880
H	5.229760	12.629170	2.122580
H	6.047830	11.247090	1.345070
H	6.302100	11.172090	-1.078050
H	5.547870	12.438520	-2.099520
H	6.935570	12.838090	-1.054470
H	5.759870	14.618010	-0.116620
H	4.283280	14.248430	-1.062520
H	4.198690	14.384780	0.715280
H	-6.250430	10.769470	0.728210
H	-7.240980	12.027250	-0.061770
H	-6.178280	10.969120	-1.043760
H	-4.534320	14.258830	-0.958550
H	-5.253980	13.003200	-2.017560
H	-6.293430	13.971760	-0.941130
H	-4.479570	13.932680	1.456610
H	-6.259430	13.739240	1.382380
H	-5.256470	12.504100	2.191690

Compound 2M

DFT B3LYP/6-31G*, water, S_0



Point group: C_1

Total energy: -2019094.10 kcal mol^{-1}

Imaginary frequencies: 0

Symbol	X	Y	Z
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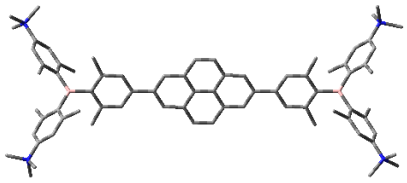
C	3.545794	0.024793	0.059944
C	1.429377	-1.203978	0.160054
C	1.430765	1.257366	-0.020720
C	2.832034	1.230939	-0.029167
C	2.830707	-1.179938	0.156861
H	3.370759	2.173550	-0.074053
H	3.368217	-2.123456	0.196854
C	-0.711158	0.028223	0.074262
C	-3.544068	0.029632	0.072091
C	-1.428988	-1.201933	0.165920
C	-1.427669	1.259263	-0.016285
C	-2.829003	1.234486	-0.020568
C	-2.830293	-1.175708	0.168129
H	-3.366914	2.177545	-0.066484
H	-3.369238	-2.118237	0.212778
C	-5.028577	0.028921	0.064443
C	-7.898460	0.018338	0.036469
C	-5.755122	0.932804	-0.723525
C	-5.763647	-0.876834	0.842817
C	-7.158633	-0.911654	0.830991
C	-7.150508	0.958408	-0.738329
H	-5.214599	1.620787	-1.367300
H	-5.230619	-1.559636	1.498342
C	5.029944	0.022452	0.048764
C	7.900609	0.011830	0.018178
C	5.765518	-0.883092	0.825916
C	5.755616	0.924987	-0.741180
C	7.150351	0.925140	-0.787089
C	7.161022	-0.893216	0.842511
H	5.231987	-1.584525	1.461077
H	5.213962	1.631217	-1.364013
C	-7.818377	-1.936498	1.736242
H	-8.235880	-2.775692	1.168797
H	-8.632316	-1.513925	2.334232
H	-7.087834	-2.350290	2.437059
C	-7.798260	1.985123	-1.650075
H	-8.598239	1.563316	-2.266648
H	-7.056099	2.408231	-2.332863
H	-8.231357	2.818024	-1.084740
C	7.793911	1.955883	-1.697361
H	8.225199	1.498469	-2.594432
H	8.593933	2.518526	-1.204870
H	7.049081	2.684029	-2.030284
C	7.816397	-1.925343	1.742577
H	8.596373	-2.501218	1.233533
H	7.072180	-2.641718	2.101359
H	8.277356	-1.466548	2.624099
B	-9.465222	-0.000254	0.005681
B	9.466872	-0.002371	-0.007761
C	-10.307806	1.362744	0.081664
C	-11.780965	3.771292	0.261295
C	-11.295323	1.691546	-0.879896
C	-10.079765	2.281999	1.143100
C	-10.825517	3.463770	1.226482
C	-12.014267	2.895027	-0.790242
H	-10.627772	4.132989	2.057392
H	-12.744396	3.106765	-1.560293
C	-10.265966	-1.385527	-0.110064
C	-11.662803	-3.832553	-0.368367
C	-11.295782	-1.741546	0.802379
C	-9.962694	-2.294830	-1.156160
C	-10.672015	-3.501492	-1.282539
C	-11.972311	-2.959489	0.671346
H	-10.410846	-4.155900	-2.103800
H	-12.740402	-3.199700	1.399073

C	10.314223	-0.124951	1.349287
C	11.791241	-0.298177	3.756880
C	11.307711	-1.118715	1.530382
C	10.085383	0.788852	2.415407
C	10.833316	0.699660	3.595506
C	12.027072	-1.206634	2.733609
H	10.633727	1.422617	4.379797
H	12.760232	-1.997347	2.826506
C	10.265106	0.102978	-1.395598
C	11.650421	0.240784	-3.858991
C	11.273298	1.079764	-1.615573
C	9.979876	-0.804602	-2.447660
C	10.683421	-0.735826	-3.662179
C	11.942812	1.146984	-2.842570
H	10.434948	-1.458203	-4.428926
H	12.691620	1.921414	-2.974121
C	-11.693218	-0.855657	1.965163
H	-12.155982	0.074594	1.621484
H	-10.831481	-0.580509	2.582495
H	-12.409097	-1.361097	2.619365
C	-9.042550	2.047852	2.223330
H	-8.027638	2.139338	1.824461
H	-9.118286	1.049798	2.665394
H	-9.152508	2.773499	3.034356
C	-11.613305	0.794338	-2.059150
H	-10.711537	0.494318	-2.602458
H	-12.266746	1.300912	-2.774968
H	-12.119013	-0.122624	-1.739778
C	-8.877511	-2.039870	-2.184322
H	-8.971570	-2.728484	-3.029043
H	-7.881933	-2.176425	-1.749756
H	-8.908074	-1.023225	-2.585599
C	8.915855	-1.879276	-2.341068
H	9.028347	-2.621227	-3.137050
H	7.912256	-1.449407	-2.423706
H	8.950957	-2.413097	-1.387621
C	11.653260	2.102824	-0.565367
H	12.148237	1.632670	0.290091
H	10.779029	2.637686	-0.180283
H	12.336248	2.853329	-0.973177
C	11.632008	-2.147526	0.466310
H	10.734613	-2.654041	0.097057
H	12.300644	-2.920401	0.855614
H	12.123343	-1.687951	-0.397217
C	9.040253	1.884224	2.346032
H	8.029737	1.471136	2.425977
H	9.078655	2.440793	1.405300
H	9.173278	2.604497	3.158530
N	-12.428265	-5.136598	-0.467012
N	-12.540926	5.076086	0.389474
N	12.407394	0.353265	-5.166315
N	12.553687	-0.362708	5.064188
C	-13.908882	-4.852064	-0.637631
H	-14.439078	-5.802975	-0.711569
H	-14.043294	-4.268508	-1.548645
H	-14.270791	-4.291313	0.221918
C	-12.212602	-5.952267	0.794579
H	-12.759162	-6.891924	0.698274
H	-12.580958	-5.394715	1.653524
H	-11.144286	-6.140741	0.902581
C	-11.992661	-5.987473	-1.636872
H	-12.592933	-6.897469	-1.628982
H	-10.938838	-6.240769	-1.526520
H	-12.163980	-5.442134	-2.564349
C	-11.567887	6.239790	0.339599
H	-11.033263	6.198794	-0.609633
H	-10.865108	6.159238	1.166578
H	-12.133776	7.169404	0.420270
C	-13.549601	5.280731	-0.716185
H	-14.281559	4.474260	-0.690297
H	-13.034266	5.305150	-1.675693
H	-14.046994	6.234971	-0.541651
C	-13.296016	5.104364	1.705398
H	-13.987000	4.261297	1.722451
H	-13.842082	6.046763	1.772221
H	-12.590633	5.025091	2.530208
C	13.323924	0.927997	5.272828
H	14.014473	1.054143	4.438676
H	13.871188	0.857890	6.214312
H	12.626849	1.762855	5.309058
C	11.583452	-0.564165	6.213564
H	11.038451	-1.492882	6.042973
H	10.889655	0.273309	6.252182
H	12.152922	-0.620039	7.142730
C	13.549644	-1.498151	5.108411
H	14.283149	-1.367270	4.313617
H	13.022782	-2.445128	4.996269
H	14.048258	-1.466794	6.077404
C	13.892393	0.167456	-4.917090
H	14.417302	0.244423	-5.870691
H	14.045383	-0.817754	-4.476015
H	14.243868	0.940076	-4.236041
C	11.984018	-0.682636	-6.181527
H	12.573876	-0.524675	-7.084671
H	10.925547	-0.555995	-6.406190
H	12.178426	-1.678443	-5.784770
C	12.165254	1.719292	-5.782139
H	12.711004	1.776151	-6.725274
H	12.518559	2.491001	-5.101154
H	11.094484	1.833930	-5.951989
C	0.680220	-2.429952	0.242794
H	1.227065	-3.367227	0.305160
C	-0.681139	-2.428864	0.245890
H	-1.228988	-3.365383	0.310906
C	0.682975	2.484538	-0.098273
H	1.230865	3.421129	-0.161691
C	-0.678390	2.485339	-0.096406
H	-1.225161	3.422680	-0.158487

Compound 2M

DFT B3LYP/6-31G*, water, S_0



Point group: C_i

Total energy: -2019170.38 kcal mol^{-1}

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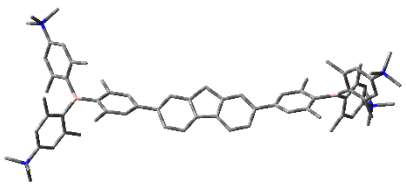
C	1.406530	-0.870400	-0.873610
C	1.406000	0.914340	0.830980
C	2.807230	0.885290	0.825720
C	2.807830	-0.857160	-0.850830
H	3.345310	1.583000	1.461660
H	3.345950	-1.561200	-1.479710
C	-0.689110	-0.025360	0.025090
C	-3.521930	-0.009360	0.007430
C	-1.406000	-0.914340	-0.830980
C	-1.406530	0.870400	0.873610
C	-2.807830	0.857160	0.850830
C	-2.807230	-0.885290	-0.825720
H	-3.345950	1.561200	1.479710
H	-3.345310	-1.583000	-1.461660
C	-5.052350	0.035500	-0.039010
C	-7.922330	0.021870	-0.026080
C	-5.783560	0.895900	0.792140
C	-5.782780	-0.828080	-0.868040
C	-7.177780	-0.864250	-0.865090
C	-7.179020	0.919910	0.801260
H	-5.246820	1.549050	1.474220
H	-5.245930	-1.474850	-1.556170
C	-7.832160	-1.839980	-1.826750
H	-8.251800	-2.708330	-1.306740
H	-8.643440	-1.386720	-2.405570
H	-7.097780	-2.215600	-2.544850
C	-7.832160	1.896450	1.762920
H	-8.634860	1.442080	2.352210
H	-7.093760	2.283140	2.470920
H	-8.263110	2.757930	1.240400
B	-9.489210	0.000810	-0.004210
C	-10.332510	1.365450	-0.012000
C	-11.806720	3.779330	-0.071000
C	-11.325090	1.642230	0.960670
C	-10.099920	2.339860	-1.022010
C	-10.846220	3.523980	-1.046330
C	-12.044560	2.848370	0.931380
H	-10.644870	4.236450	-1.839550
H	-12.778700	3.018550	1.707890
C	-10.289390	-1.389100	0.033850
C	-11.685500	-3.847150	0.154920
C	-11.314340	-1.696770	-0.901370
C	-9.990600	-2.352460	1.031740
C	-10.699560	-3.564520	1.090350
C	-11.990520	-2.920320	-0.838550
H	-10.441960	-4.261440	1.877030
H	-12.754770	-3.122000	-1.581850
C	-11.706690	-0.750650	-2.017500
H	-12.171920	0.159800	-1.627280
H	-10.842100	-0.442660	-2.615020
H	-12.418880	-1.221060	-2.701190
C	-9.057130	2.163930	-2.107910
H	-8.044300	2.234680	-1.699650
H	-9.129850	1.190700	-2.602680
H	-9.163630	2.931530	-2.879840
C	-11.648220	0.683540	2.089040
H	-10.748940	0.355610	2.620200
H	-12.305650	1.151050	2.827430
H	-12.151580	-0.215470	1.718930
C	-8.910780	-2.151820	2.077430
H	-9.008490	-2.884330	2.883940
H	-7.912930	-2.264570	1.641240
H	-8.944170	-1.157910	2.531920
N	-12.450380	-5.155010	0.180390
N	-12.567100	5.088670	-0.133590
C	-13.932060	-4.880750	0.358410
H	-14.461840	-5.834540	0.379130
H	-14.071500	-4.346430	1.298420
H	-14.290130	-4.275380	-0.471980
C	-12.227750	-5.902480	-1.121600
H	-12.774020	-6.846220	-1.078040
H	-12.592260	-5.300340	-1.951600
H	-11.158750	-6.084370	-1.234070
C	-12.019930	-6.066520	1.305630
H	-12.619410	-6.975150	1.246450
H	-10.965360	-6.313030	1.187300
H	-12.196320	-5.571260	2.259860
C	-11.595270	6.248620	-0.017150
H	-11.065360	6.157610	0.931250
H	-10.888310	6.212450	-0.843690
H	-12.161510	7.180890	-0.051230
C	-13.581450	5.233800	0.976280
H	-14.312610	4.429440	0.903950
H	-13.070940	5.207560	1.938310
H	-14.078750	6.195680	0.850120
C	-13.315630	5.186310	-1.449950
H	-14.005830	4.344960	-1.515180
H	-13.862130	6.130630	-1.469420
H	-12.606070	5.151300	-2.274240
C	0.658310	-1.762250	-1.719690
H	1.205860	-2.447270	-2.361840
C	-0.703020	-1.756250	-1.726270
H	-1.250150	-2.436440	-2.373900
C	0.703020	1.756250	1.726270
H	1.250150	2.436440	2.373900
C	-0.658310	1.762250	1.719690
H	-1.205860	2.447270	2.361840
C	5.052350	-0.035500	0.039010
C	5.783560	-0.895900	-0.792140

C	5.782780	0.828080	0.868040
C	7.179020	-0.919910	-0.801260
H	5.246820	-1.549050	-1.474220
C	7.177780	0.864250	0.865090
H	5.245930	1.474850	1.556170
C	7.922330	-0.021870	0.026080
C	7.832160	-1.896450	-1.762920
C	7.832160	1.839980	1.826750
B	9.489210	-0.000810	0.004210
H	8.634860	-1.442080	-2.352210
H	7.093760	-2.283140	-2.470920
H	8.263110	-2.757930	-1.240400
H	8.251800	2.708330	1.306740
H	8.643440	1.386720	2.405570
H	7.097780	2.215600	2.544850
C	10.332510	-1.365450	0.012000
C	10.289390	1.389100	-0.033850
C	11.325090	-1.642230	-0.960670
C	10.099920	-2.339860	1.022010
C	11.314340	1.696770	0.901370
C	9.990600	2.352460	-1.031740
C	12.044560	-2.848370	-0.931380
C	11.648220	-0.683540	-2.089040
C	10.846220	-3.523980	1.046330
C	9.057130	-2.163930	2.107910
C	11.990520	2.920320	0.838550
C	11.706690	0.750650	2.017500
C	10.699560	3.564520	-1.090350
C	8.910780	2.151820	-2.077430
C	11.806720	-3.779330	0.071000
H	12.778700	-3.018550	-1.707890
H	10.748940	-0.355610	-2.620200
H	12.305650	-1.151050	-2.827430
H	12.151580	0.215470	-1.718930
H	10.644870	-4.236450	1.839550
H	8.044300	-2.234680	1.699650
H	9.129850	-1.190700	2.602680
H	9.163630	-2.931530	2.879840
C	11.685500	3.847150	-0.154920
H	12.754770	3.122000	1.581850
H	12.171920	-0.159800	1.627280
H	10.842100	0.442660	2.615020
H	12.418880	1.221060	2.701190
H	10.441960	4.261440	-1.877030
H	9.008490	2.884330	-2.883940
H	7.912930	2.264570	-1.641240
H	8.944170	1.157910	-2.531920
N	12.567100	-5.088670	0.133590
N	12.450380	5.155010	-0.180390
C	11.595270	-6.248620	0.017150
C	13.581450	-5.233800	-0.976280
C	13.315630	-5.186310	1.449950
C	13.932060	4.880750	-0.358410
C	12.227750	5.902480	1.121600
C	12.019930	6.066520	-1.305630
H	11.065360	-6.157610	-0.931250
H	10.888310	-6.212450	0.843690
H	12.161510	-7.180890	0.051230
H	14.312610	-4.429440	-0.903950
H	13.070940	-5.207560	-1.938310
H	14.078750	-6.195680	-0.850120
H	14.005830	-4.344960	1.515180
H	13.862130	-6.130630	1.469420
H	12.606070	-5.151300	2.274240
H	14.461840	5.834540	-0.379130
H	14.071500	4.346430	-1.298420
H	14.290130	4.275380	0.471980
H	12.774020	6.846220	1.078040
H	12.592260	5.300340	1.951600
H	11.158750	6.084370	1.234070
H	12.619410	6.975150	-1.246450
H	10.965360	6.313030	-1.187300
H	12.196320	5.571260	-2.259860

Compound 3M

DFT B3LYP/6-31G*, water, S_0



Point group: C_1

Total energy: -1947382.60 kcal mol^{-1}

Imaginary frequencies: 0

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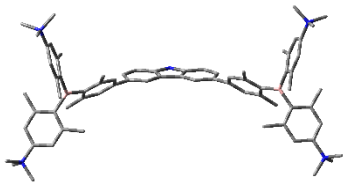
C	-3.478062	-0.881140	-0.327342
C	-1.632553	-2.392732	-0.868008
C	-1.187115	-0.143453	-0.050765
C	-2.548027	0.113164	0.042941
C	-2.995565	-2.127301	-0.778429
H	-2.900854	1.088362	0.368570
H	-3.702625	-2.910844	-1.033028
C	0.741409	-1.382584	-0.509275
C	3.487756	-0.817872	-0.339974
C	1.667591	-2.362492	-0.874593
C	1.184666	-0.121904	-0.055414
C	2.541108	0.159222	0.033428
C	3.025744	-2.072145	-0.789702
H	2.877151	1.140280	0.359253
H	3.745847	-2.842339	-1.048487
C	4.943213	-0.547138	-0.265133
C	7.773937	-0.081449	-0.104046
C	5.496418	0.261444	0.739124
C	5.832900	-1.100428	-1.199052
C	7.211597	-0.904357	-1.128702
C	6.865991	0.517144	0.824784
H	4.841140	0.679158	1.498134
H	5.433501	-1.685009	-2.022601
C	-4.937327	-0.634548	-0.248932
C	-7.773337	-0.203778	-0.088426

C	-5.818345	-1.189981	-1.188934	H	10.824713	0.357813	-2.580073
C	-5.501543	0.153481	0.765239	H	12.515438	-0.126053	-2.660567
C	-6.877538	0.358774	0.874115	C	8.631592	2.549334	-1.706410
C	-7.196255	-0.978426	-1.143051	H	7.606292	2.405060	-1.352062
H	-5.412228	-1.786359	-2.000768	H	8.864421	1.696368	-2.350850
H	-4.849157	0.593656	1.514379	H	8.648405	3.446177	-2.332530
C	8.042279	-1.560709	-2.217180	C	11.276879	0.731923	2.318306
H	8.569021	-2.449565	-1.851755	H	10.421606	0.179504	2.719718
H	8.795866	-0.889586	-2.641450	H	11.819057	1.150574	3.170891
H	7.399809	-1.882450	-3.041738	H	11.934568	0.003067	1.833451
C	7.320847	1.397519	1.974912	C	9.019219	-2.424353	1.644062
H	8.153114	0.963905	2.539061	H	9.213044	-3.260303	2.322521
H	6.501263	1.553575	2.681928	H	8.064584	-2.614439	1.142742
H	7.645469	2.385567	1.629999	H	8.879005	-1.530071	2.256964
C	-7.342633	1.225024	2.031188	C	-9.001468	-2.469983	1.778789
H	-7.834540	0.636677	2.813458	H	-9.218175	-3.372304	2.358073
H	-8.047427	2.003962	1.721325	H	-7.947128	-2.218194	1.934544
H	-6.489934	1.730454	2.493204	H	-9.109610	-2.724552	0.721318
C	-8.015669	-1.643059	-2.235139	C	-11.175260	2.162775	1.200144
H	-8.871130	-2.203968	-1.844338	H	-11.725454	1.999206	0.268302
H	-7.397453	-2.350758	-2.794371	H	-10.237720	2.664843	0.939161
H	-8.407961	-0.915808	-2.954318	H	-11.755417	2.860262	1.810822
B	9.321466	0.131439	0.009795	C	-11.796658	-1.627543	-0.852536
B	-9.322178	-0.002008	0.018015	H	-10.980315	-2.328897	-0.653270
C	9.943329	1.582676	0.292536	H	-12.572433	-2.180922	-1.389170
C	11.044205	4.152131	0.730092	H	-12.211755	-1.330098	0.115842
C	10.850341	1.820587	1.354408	C	-8.653749	2.335363	-1.816113
C	9.600121	2.678218	-0.547758	H	-7.715475	1.817269	-2.038424
C	10.162480	3.941117	-0.327231	H	-8.602264	2.643587	-0.767865
C	11.383766	3.101618	1.572203	H	-8.687091	3.244639	-2.423411
H	9.882446	4.746459	-0.998640	N	13.002822	-4.505463	-0.577393
H	12.059548	3.231889	2.407626	N	11.607628	5.543710	0.933982
C	10.325378	-1.109661	-0.152222	N	-12.136466	-0.611238	5.222859
C	12.061182	-3.331211	-0.402701	N	-12.484765	1.343709	-4.836276
C	11.412128	-1.091973	-1.068162	C	14.427668	-4.070323	-0.290069
C	10.144349	-2.273792	0.638424	H	15.085264	-4.932717	-0.411061
C	11.020180	-3.365976	0.514687	H	14.472305	-3.697069	0.733264
C	12.256293	-2.201008	-1.192558	H	14.714327	-3.285315	-0.986991
H	10.844936	-4.225940	1.147763	C	12.909865	-5.025875	-2.000050
H	13.061259	-2.152197	-1.918487	H	13.583209	-5.878486	-2.102719
C	-10.199823	0.341448	-1.279982	H	13.198740	-4.238082	-2.693061
C	-11.711690	0.979288	-3.585660	H	11.879320	-5.327927	-2.187752
C	-11.333069	-0.424776	-1.649184	C	12.685954	-5.656530	0.348382
C	-9.849427	1.448698	-2.101631	H	13.409927	-6.448382	0.155224
C	-10.613895	1.760180	-3.232371	H	11.679887	-6.019923	0.141952
C	-12.070490	-0.109561	-2.802378	H	12.772108	-5.323334	1.382085
H	-10.316212	2.617920	-3.826806	C	10.474851	6.520872	1.188592
H	-12.914838	-0.739911	-3.049358	H	9.934174	6.194982	2.077487
C	-10.073278	-0.149629	1.427619	H	9.807047	6.530909	0.329417
C	-11.405768	-0.475316	3.902463	H	10.900384	7.513925	1.342425
C	-10.933049	0.861214	1.935916	C	12.553181	5.628216	2.109230
C	-9.904597	-1.327094	2.200343	H	13.395609	4.957895	1.942585
C	-10.582286	-1.484015	3.421614	H	12.020896	5.360878	3.021329
C	-11.577264	0.694845	3.166885	H	12.908541	6.656542	2.178219
H	-10.430120	-2.406458	3.966773	C	12.377621	5.972812	-0.301034
H	-12.212142	1.498643	3.524893	H	13.185273	5.259488	-0.466371
C	11.695218	0.091340	-1.970721	H	12.780212	6.972418	-0.129385
H	11.971109	0.978997	-1.393809	H	11.708566	5.984007	-1.159031

C	-13.038649	2.750472	-4.707518
H	-13.692551	2.783755	-3.835832
H	-13.598162	2.987515	-5.613868
H	-12.216787	3.452907	-4.584093
C	-11.566622	1.270353	-6.042642
H	-11.178627	0.254210	-6.116443
H	-10.746417	1.973928	-5.914719
H	-12.142460	1.525798	-6.933717
C	-13.651298	0.419191	-5.097172
H	-14.346059	0.468745	-4.259404
H	-13.283800	-0.597148	-5.234875
H	-14.147404	0.757262	-6.007134
C	-13.633418	-0.523662	4.991934
H	-14.140083	-0.627490	5.952813
H	-13.924181	-1.329982	4.318258
H	-13.874844	0.439747	4.547218
C	-11.861148	-1.925699	5.915292
H	-12.425789	-1.935333	6.847766
H	-10.795852	-2.005221	6.129171
H	-12.189597	-2.745900	5.277860
C	-11.704435	0.498002	6.164230
H	-12.231100	0.373835	7.111894
H	-11.952147	1.462586	5.725502
H	-10.627130	0.421287	6.312634
H	-1.291165	-3.365967	-1.209314
H	1.342594	-3.341532	-1.215312
C	-0.008715	0.759996	0.264546
H	-0.009669	1.085901	1.313694
H	-0.018343	1.674269	-0.344474

Compound 4M

DFT B3LYP/6-31G*, water, S_0



Point group: C_1

Total energy: -1957452.61 kcal mol^{-1}

Imaginary frequencies: 0

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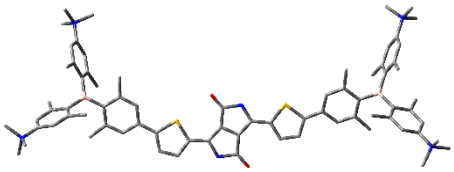
C	-1.632553	-2.392732	-0.868008
C	-1.187115	-0.143453	-0.050765
C	-2.548027	0.113164	0.042941
C	-2.995565	-2.127301	-0.778429
H	-2.900854	1.088362	0.368570
H	-3.702625	-2.910844	-1.033028
C	0.741409	-1.382584	-0.509275
C	3.487756	-0.817872	-0.339974
C	1.667591	-2.362492	-0.874593
C	1.184666	-0.121904	-0.055414
C	2.541108	0.159222	0.033428
C	3.025744	-2.072145	-0.789702
H	2.877151	1.140280	0.359253
H	3.745847	-2.842339	-1.048487
C	4.943213	-0.547138	-0.265133
C	7.773937	-0.081449	-0.104046
C	5.496418	0.261444	0.739124
C	5.832900	-1.100428	-1.199052
C	7.211597	-0.904357	-1.128702
C	6.865991	0.517144	0.824784
H	4.841140	0.679158	1.498134
H	5.433501	-1.685009	-2.022601
C	-4.937327	-0.634548	-0.248932
C	-7.773337	-0.203778	-0.088426
C	-5.818345	-1.189981	-1.188934
C	-5.501543	0.153481	0.765239
C	-6.877538	0.358774	0.874115
C	-7.196255	-0.978426	-1.143051
H	-5.412228	-1.786359	-2.000768
H	-4.849157	0.593656	1.514379
C	8.042279	-1.560709	-2.217180
H	8.569021	-2.449565	-1.851755
H	8.795866	-0.889586	-2.641450
H	7.399809	-1.882450	-3.041738
C	7.320847	1.397519	1.974912
H	8.153114	0.963905	2.539061
H	6.501263	1.553575	2.681928
H	7.645469	2.385567	1.629999
C	-7.342633	1.225024	2.031188
H	-7.834540	0.636677	2.813458
H	-8.047427	2.003962	1.721325
H	-6.489934	1.730454	2.493204
C	-8.015669	-1.643059	-2.235139
H	-8.871130	-2.203968	-1.844338
H	-7.397453	-2.350758	-2.794371
H	-8.407961	-0.915808	-2.954318
B	9.321466	0.131439	0.009795
B	-9.322178	-0.002008	0.018015
C	9.943329	1.582676	0.292536
C	11.044205	4.152131	0.730092
C	10.850341	1.820587	1.354408
C	9.600121	2.678218	-0.547758
C	10.162480	3.941117	-0.327231
C	11.383766	3.101618	1.572203
H	9.882446	4.746459	-0.998640
H	12.059548	3.231889	2.407626
C	10.325378	-1.109661	-0.152222
C	12.061182	-3.331211	-0.402701
C	11.412128	-1.091973	-1.068162
C	10.144349	-2.273792	0.638424
C	11.020180	-3.365976	0.514687
C	12.256293	-2.201008	-1.192558
H	10.844936	-4.225940	1.147763
H	13.061259	-2.152197	-1.918487
C	-10.199823	0.341448	-1.279982
C	-11.711690	0.979288	-3.585660
C	-11.333069	-0.424776	-1.649184

C	-9.849427	1.448698	-2.101631
C	-10.613895	1.760180	-3.232371
C	-12.070490	-0.109561	-2.802378
H	-10.316212	2.617920	-3.826806
H	-12.914838	-0.739911	-3.049358
C	-10.073278	-0.149629	1.427619
C	-11.405768	-0.475316	3.902463
C	-10.933049	0.861214	1.935916
C	-9.904597	-1.327094	2.200343
C	-10.582286	-1.484015	3.421614
C	-11.577264	0.694845	3.166885
H	-10.430120	-2.406458	3.966773
H	-12.212142	1.498643	3.524893
C	11.695218	0.091340	-1.970721
H	11.971109	0.978997	-1.393809
H	10.824713	0.357813	-2.580073
H	12.515438	-0.126053	-2.660567
C	8.631592	2.549334	-1.706410
H	7.606292	2.405060	-1.352062
H	8.864421	1.696368	-2.350850
H	8.648405	3.446177	-2.332530
C	11.276879	0.731923	2.318306
H	10.421606	0.179504	2.719718
H	11.819057	1.150574	3.170891
H	11.934568	0.003067	1.833451
C	9.019219	-2.424353	1.644062
H	9.213044	-3.260303	2.322521
H	8.064584	-2.614439	1.142742
H	8.879005	-1.530071	2.256964
C	-9.001468	-2.469983	1.778789
H	-9.218175	-3.372304	2.358073
H	-7.947128	-2.218194	1.934544
H	-9.109610	-2.724552	0.721318
C	-11.175260	2.162775	1.200144
H	-11.725454	1.999206	0.268302
H	-10.237720	2.664843	0.939161
H	-11.755417	2.860262	1.810822
C	-11.796658	-1.627543	-0.852536
H	-10.980315	-2.328897	-0.653270
H	-12.572433	-2.180922	-1.389170
H	-12.211755	-1.330098	0.115842
C	-8.653749	2.335363	-1.816113
H	-7.715475	1.817269	-2.038424
H	-8.602264	2.643587	-0.767865
H	-8.687091	3.244639	-2.423411
N	13.002822	-4.505463	-0.577393
N	11.607628	5.543710	0.933982
N	-12.136466	-0.611238	5.222859
N	-12.484765	1.343709	-4.836276
C	14.427668	-4.070323	-0.290069
H	15.085264	-4.932717	-0.411061
H	14.472305	-3.697069	0.733264
H	14.714327	-3.285315	-0.986991
C	12.909865	-5.025875	-2.000050
H	13.583209	-5.878486	-2.102719
H	13.198740	-4.238082	-2.693061
H	11.879320	-5.327927	-2.187752
C	12.685954	-5.656530	0.348382
H	13.409927	-6.448382	0.155224
H	11.679887	-6.019923	0.141952
H	12.772108	-5.323334	1.382085
C	10.474851	6.520872	1.188592
H	9.934174	6.194982	2.077487
H	9.807047	6.530909	0.329417
H	10.900384	7.513925	1.342425
C	12.553181	5.628216	2.109230
H	13.395609	4.957895	1.942585
H	12.020896	5.360878	3.021329
H	12.908541	6.656542	2.178219
C	12.377621	5.972812	-0.301034
H	13.185273	5.259488	-0.466371
H	12.780212	6.972418	-0.129385
H	11.708566	5.984007	-1.159031
C	-13.038649	2.750472	-4.707518
H	-13.692551	2.783755	-3.835832
H	-13.598162	2.987515	-5.613868
H	-12.216787	3.452907	-4.584093
C	-11.566622	1.270353	-6.042642
H	-11.178627	0.254210	-6.116443
H	-10.746417	1.973928	-5.914719
H	-12.142460	1.525798	-6.933717
C	-13.651298	0.419191	-5.097172
H	-14.346059	0.468745	-4.259404
H	-13.283800	-0.597148	-5.234875
H	-14.147404	0.757262	-6.007134
C	-13.633418	-0.523662	4.991934
H	-14.140083	-0.627490	5.952813
H	-13.924181	-1.329982	4.318258
H	-13.874844	0.439747	4.547218
C	-11.861148	-1.925699	5.915292
H	-12.425789	-1.935333	6.847766
H	-10.795852	-2.005221	6.129171
H	-12.189597	-2.745900	5.277860
C	-11.704435	0.498002	6.164230
H	-12.231100	0.373835	7.111894
H	-11.952147	1.462586	5.725502
H	-10.627130	0.421287	6.312634
H	-1.291165	-3.365967	-1.209314
H	1.342594	-3.341532	-1.215312
C	-0.008715	0.759996	0.264546
H	-0.009669	1.085901	1.313694
H	-0.018343	1.674269	-0.344474

Compound 5M

DFT B3LYP/6-31G*, water, S_0



Point group: C_1

Total energy: - 2633343.06 kcal mol^{-1}

Imaginary frequencies: 0

Symbol	X	Y	Z
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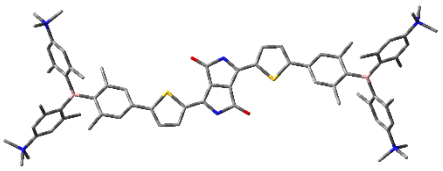
C	-3.478062	-0.881140	-0.327342
C	-1.632553	-2.392732	-0.868008
C	-1.187115	-0.143453	-0.050765
C	-2.548027	0.113164	0.042941
C	-2.995565	-2.127301	-0.778429
H	-2.900854	1.088362	0.368570
H	-3.702625	-2.910844	-1.033028
C	0.741409	-1.382584	-0.509275
C	3.487756	-0.817872	-0.339974
C	1.667591	-2.362492	-0.874593
C	1.184666	-0.121904	-0.055414
C	2.541108	0.159222	0.033428
C	3.025744	-2.072145	-0.789702
H	2.877151	1.140280	0.359253
H	3.745847	-2.842339	-1.048487
C	4.943213	-0.547138	-0.265133
C	7.773937	-0.081449	-0.104046
C	5.496418	0.261444	0.739124
C	5.832900	-1.100428	-1.199052
C	7.211597	-0.904357	-1.128702
C	6.865991	0.517144	0.824784
H	4.841140	0.679158	1.498134
H	5.433501	-1.685009	-2.022601
C	-4.937327	-0.634548	-0.248932
C	-7.773337	-0.203778	-0.088426
C	-5.818345	-1.189981	-1.188934
C	-5.501543	0.153481	0.765239
C	-6.877538	0.358774	0.874115
C	-7.196255	-0.978426	-1.143051
H	-5.412228	-1.786359	-2.000768
H	-4.849157	0.593656	1.514379
C	8.042279	-1.560709	-2.217180
H	8.569021	-2.449565	-1.851755
H	8.795866	-0.889586	-2.641450
H	7.399809	-1.882450	-3.041738
C	7.320847	1.397519	1.974912
H	8.153114	0.963905	2.539061
H	6.501263	1.553575	2.681928
H	7.645469	2.385567	1.629999
C	-7.342633	1.225024	2.031188
H	-7.834540	0.636677	2.813458
H	-8.047427	2.003962	1.721325
H	-6.489934	1.730454	2.493204
C	-8.015669	-1.643059	-2.235139
H	-8.871130	-2.203968	-1.844338
H	-7.397453	-2.350758	-2.794371
H	-8.407961	-0.915808	-2.954318
B	9.321466	0.131439	0.009795
B	-9.322178	-0.002008	0.018015
C	9.943329	1.582676	0.292536
C	11.044205	4.152131	0.730092
C	10.850341	1.820587	1.354408
C	9.600121	2.678218	-0.547758
C	10.162480	3.941117	-0.327231
C	11.383766	3.101618	1.572203
H	9.882446	4.746459	-0.998640
H	12.059548	3.231889	2.407626
C	10.325378	-1.109661	-0.152222
C	12.061182	-3.331211	-0.402701
C	11.412128	-1.091973	-1.068162
C	10.144349	-2.273792	0.638424
C	11.020180	-3.365976	0.514687
C	12.256293	-2.201008	-1.192558
H	10.844936	-4.225940	1.147763
H	13.061259	-2.152197	-1.918487
C	-10.199823	0.341448	-1.279982
C	-11.711690	0.979288	-3.585660
C	-11.333069	-0.424776	-1.649184
C	-9.849427	1.448698	-2.101631
C	-10.613895	1.760180	-3.232371
C	-12.070490	-0.109561	-2.802378
H	-10.316212	2.617920	-3.826806
H	-12.914838	-0.739911	-3.049358
C	-10.073278	-0.149629	1.427619
C	-11.405768	-0.475316	3.902463
C	-10.933049	0.861214	1.935916
C	-9.904597	-1.327094	2.200343
C	-10.582286	-1.484015	3.421614
C	-11.577264	0.694845	3.166885
H	-10.430120	-2.406458	3.966773
H	-12.212142	1.498643	3.524893
C	11.695218	0.091340	-1.970721
H	11.971109	0.978997	-1.393809
H	10.824713	0.357813	-2.580073
H	12.515438	-0.126053	-2.660567
C	8.631592	2.549334	-1.706410
H	7.606292	2.405060	-1.352062
H	8.864421	1.696368	-2.350850
H	8.648405	3.446177	-2.332530
C	11.276879	0.731923	2.318306
H	10.421606	0.179504	2.719718
H	11.819057	1.150574	3.170891
H	11.934568	0.003067	1.833451
C	9.019219	-2.424353	1.644062
H	9.213044	-3.260303	2.322521
H	8.064584	-2.614439	1.142742
H	8.879005	-1.530071	2.256964
C	-9.001468	-2.469983	1.778789

H	-9.218175	-3.372304	2.358073
H	-7.947128	-2.218194	1.934544
H	-9.109610	-2.724552	0.721318
C	-11.175260	2.162775	1.200144
H	-11.725454	1.999206	0.268302
H	-10.237720	2.664843	0.939161
H	-11.755417	2.860262	1.810822
C	-11.796658	-1.627543	-0.852536
H	-10.980315	-2.328897	-0.653270
H	-12.572433	-2.180922	-1.389170
H	-12.211755	-1.330098	0.115842
C	-8.653749	2.335363	-1.816113
H	-7.715475	1.817269	-2.038424
H	-8.602264	2.643587	-0.767865
H	-8.687091	3.244639	-2.423411
N	13.002822	-4.505463	-0.577393
N	11.607628	5.543710	0.933982
N	-12.136466	-0.611238	5.222859
N	-12.484765	1.343709	-4.836276
C	14.427668	-4.070323	-0.290069
H	15.085264	-4.932717	-0.411061
H	14.472305	-3.697069	0.733264
H	14.714327	-3.285315	-0.986991
C	12.909865	-5.025875	-2.000050
H	13.583209	-5.878486	-2.102719
H	13.198740	-4.238082	-2.693061
H	11.879320	-5.327927	-2.187752
C	12.685954	-5.656530	0.348382
H	13.409927	-6.448382	0.155224
H	11.679887	-6.019923	0.141952
H	12.772108	-5.323334	1.382085
C	10.474851	6.520872	1.188592
H	9.934174	6.194982	2.077487
H	9.807047	6.530909	0.329417
H	10.900384	7.513925	1.342425
C	12.553181	5.628216	2.109230
H	13.395609	4.957895	1.942585
H	12.020896	5.360878	3.021329
H	12.908541	6.656542	2.178219
C	12.377621	5.972812	-0.301034
H	13.185273	5.259488	-0.466371
H	12.780212	6.972418	-0.129385
H	11.708566	5.984007	-1.159031
C	-13.038649	2.750472	-4.707518
H	-13.692551	2.783755	-3.835832
H	-13.598162	2.987515	-5.613868
H	-12.216787	3.452907	-4.584093
C	-11.566622	1.270353	-6.042642
H	-11.178627	0.254210	-6.116443
H	-10.746417	1.973928	-5.914719
H	-12.142460	1.525798	-6.933717
C	-13.651298	0.419191	-5.097172
H	-14.346059	0.468745	-4.259404
H	-13.283800	-0.597148	-5.234875
H	-14.147404	0.757262	-6.007134
C	-13.633418	-0.523662	4.991934
H	-14.140083	-0.627490	5.952813
H	-13.924181	-1.329982	4.318258
H	-13.874844	0.439747	4.547218
C	-11.861148	-1.925699	5.915292
H	-12.425789	-1.935333	6.847766
H	-10.795852	-2.005221	6.129171
H	-12.189597	-2.745900	5.277860
C	-11.704435	0.498002	6.164230
H	-12.231100	0.373835	7.111894
H	-11.952147	1.462586	5.725502
H	-10.627130	0.421287	6.312634
H	-1.291165	-3.365967	-1.209314
H	1.342594	-3.341532	-1.215312
C	-0.008715	0.759996	0.264546
H	-0.009669	1.085901	1.313694
H	-0.018343	1.674269	-0.344474

Compound 5M

DFT B3LYP/6-31G*, water, S_0



Point group: C_i

Total energy: -2633397.46 kcal mol^{-1}

Symbol	X	Y	Z
C	1.332320	0.994310	-0.567460
N	0.314620	1.831600	-1.017960
H	0.450370	2.703510	-1.510550
C	-0.980160	1.338470	-0.729070
O	-2.020840	1.916790	-1.036130
C	-0.706900	0.088170	-0.039640
C	0.706900	-0.088170	0.039640
C	-1.332320	-0.994310	0.567460
N	-0.314620	-1.831600	1.017960
H	-0.450370	-2.703510	1.510550
C	0.980160	-1.338470	0.729070
O	2.020840	-1.916790	1.036130
C	-2.714330	-1.314190	0.759080
C	-3.250230	-2.442200	1.365810
H	-2.649200	-3.247080	1.774030
C	-4.658360	-2.453550	1.388310
H	-5.235790	-3.270990	1.803720
C	-5.233700	-1.339090	0.800160
S	-3.997920	-0.246510	0.213050
C	-6.656220	-1.032850	0.643320
C	-9.442210	-0.467220	0.344540
C	-7.110530	-0.084470	-0.285180
C	-7.619130	-1.690600	1.425420
C	-8.983940	-1.443070	1.277300
C	-8.464290	0.220990	-0.430460
H	-6.394540	0.423820	-0.925600
H	-7.298680	-2.404660	2.177820

C	-8.819360	1.272510	-1.465040	H	-14.450910	-5.045340	-2.524040
H	-9.148450	2.205580	-0.996040	C	-16.245490	-3.925140	-0.913160
H	-7.948510	1.504570	-2.085040	H	-16.574300	-3.231960	-0.142080
H	-9.620540	0.950420	-2.137730	H	-16.101820	-3.400100	-1.857110
C	-9.923120	-2.228970	2.173110	H	-16.971650	-4.729930	-1.027690
H	-9.360350	-2.737840	2.961160	C	-15.083560	-5.286990	0.802250
H	-10.669030	-1.595240	2.663160	H	-14.118660	-5.714320	1.073300
H	-10.469900	-2.994040	1.611900	H	-15.421640	-4.599210	1.573680
B	-10.981990	-0.162870	0.171540	H	-15.824220	-6.073020	0.653640
C	-11.505840	1.340630	0.152590	C	2.714330	1.314190	-0.759080
C	-12.417060	4.012210	0.126850	C	3.250230	2.442200	-1.365810
C	-11.149660	2.243080	1.191500	S	3.997920	0.246510	-0.213050
C	-12.336470	1.818950	-0.891190	H	2.649200	3.247080	-1.774030
C	-12.771350	3.152810	-0.903200	C	4.658360	2.453550	-1.388310
C	-11.620470	3.559000	1.174430	C	5.233700	1.339090	-0.800160
H	-13.386880	3.478920	-1.730410	H	5.235790	3.270990	-1.803720
H	-11.341230	4.213480	1.992370	C	6.656220	1.032850	-0.643320
C	-12.026590	-1.352450	0.004250	C	7.110530	0.084470	0.285180
C	-13.891830	-3.443670	-0.341570	C	7.619130	1.690600	-1.425420
C	-13.204480	-1.419170	0.796820	C	8.464290	-0.220990	0.430460
C	-11.814060	-2.368920	-0.961390	H	6.394540	-0.423820	0.925600
C	-12.754250	-3.395910	-1.134250	C	8.983940	1.443070	-1.277300
C	-14.114100	-2.466240	0.623950	H	7.298680	2.404660	-2.177820
H	-12.557940	-4.140630	-1.893320	C	9.442210	0.467220	-0.344540
H	-14.995170	-2.489420	1.255220	C	8.819360	-1.272510	1.465040
C	-10.270780	1.845530	2.360930	C	9.923120	2.228970	-2.173110
H	-10.582950	0.900830	2.816640	B	10.981990	0.162870	-0.171540
H	-9.227770	1.723840	2.051600	H	9.148450	-2.205580	0.996040
H	-10.300320	2.610650	3.141840	H	7.948510	-1.504570	2.085040
C	-12.787090	0.948630	-2.048000	H	9.620540	-0.950420	2.137730
H	-13.558000	0.237060	-1.733780	H	9.360350	2.737840	-2.961160
H	-13.208760	1.561160	-2.849800	H	10.669030	1.595240	-2.663160
H	-11.967060	0.366910	-2.479350	H	10.469900	2.994040	-1.611900
C	-13.533590	-0.396690	1.866110	C	11.505840	-1.340630	-0.152590
H	-14.353470	-0.749920	2.497770	C	12.026590	1.352450	-0.004250
H	-12.681980	-0.191620	2.522180	C	11.149660	-2.243080	-1.191500
H	-13.840600	0.557460	1.425780	C	12.336470	-1.818950	0.891190
C	-10.594990	-2.411930	-1.862660	C	13.204480	1.419170	-0.796820
H	-9.703430	-2.726560	-1.310270	C	11.814060	2.368920	0.961390
H	-10.747370	-3.121810	-2.680640	C	11.620470	-3.559000	-1.174430
H	-10.368000	-1.440020	-2.310390	C	10.270780	-1.845530	-2.360930
N	-12.879660	5.448650	0.147580	C	12.771350	-3.152810	0.903200
N	-14.918930	-4.537190	-0.505700	C	12.787090	-0.948630	2.048000
C	-13.707330	5.816290	-1.060530	C	14.114100	2.466240	-0.623950
H	-14.600260	5.194400	-1.088460	C	13.533590	0.396690	-1.866110
H	-13.990250	6.863020	-0.958450	C	12.754250	3.395910	1.134250
H	-13.108670	5.680650	-1.959780	C	10.594990	2.411930	1.862660
C	-13.731900	5.688350	1.379090	C	12.417060	-4.012210	-0.126850
H	-13.137940	5.498720	2.270430	H	11.341230	-4.213480	-1.992370
H	-14.067670	6.725530	1.366970	H	10.582950	-0.900830	-2.816640
H	-14.582950	5.009220	1.340900	H	9.227770	-1.723840	-2.051600
C	-11.675420	6.370340	0.172380	H	10.300320	-2.610650	-3.141840
H	-11.090100	6.176390	1.068040	H	13.386880	-3.478920	1.730410
H	-11.079280	6.174160	-0.718090	H	13.558000	-0.237060	1.733780
H	-12.032550	7.400020	0.176250	H	13.208760	-1.561160	2.849800
C	-14.538820	-5.546920	-1.562030	H	11.967060	-0.366910	2.479350
H	-13.600850	-6.024120	-1.282810	C	13.891830	3.443670	0.341570
H	-15.333640	-6.290070	-1.605980	H	14.995170	2.489420	-1.255220

H	14.353470	0.749920	-2.497770	H	13.108670	-5.680650	1.959780
H	12.681980	0.191620	-2.522180	H	13.137940	-5.498720	-2.270430
H	13.840600	-0.557460	-1.425780	H	14.067670	-6.725530	-1.366970
H	12.557940	4.140630	1.893320	H	14.582950	-5.009220	-1.340900
H	9.703430	2.726560	1.310270	H	11.090100	-6.176390	-1.068040
H	10.747370	3.121810	2.680640	H	11.079280	-6.174160	0.718090
H	10.368000	1.440020	2.310390	H	12.032550	-7.400020	-0.176250
N	12.879660	-5.448650	-0.147580	H	13.600850	6.024120	1.282810
N	14.918930	4.537190	0.505700	H	15.333640	6.290070	1.605980
C	13.707330	-5.816290	1.060530	H	14.450910	5.045340	2.524040
C	13.731900	-5.688350	-1.379090	H	16.574300	3.231960	0.142080
C	11.675420	-6.370340	-0.172380	H	16.101820	3.400100	1.857110
C	14.538820	5.546920	1.562030	H	16.971650	4.729930	1.027690
C	16.245490	3.925140	0.913160	H	14.118660	5.714320	-1.073300
C	15.083560	5.286990	-0.802250	H	15.421640	4.599210	-1.573680
H	14.600260	-5.194400	1.088460	H	15.824220	6.073020	-0.653640
H	13.990250	-6.863020	0.958450				

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