Electronic Supporting Information (ESI) for

Indolo[2,3-b]carbazoles with Tunable Ground States: How Clar's Aromatic Sextet Determines The Singlet Biradical Character

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1. Experimental Section

1.1. General

All reagents were purchased from commercial suppliers and used as received without further purification. Anhydrous dichloromethane (DCM) was distilled from CaH_2. Anhydrous 2-Me THF was distilled from Na-benzophenone before use. The ^1H NMR and ^{13}C NMR spectra were recorded in solution of $CDCl_3$ or 1,1,2,2-tetrachloroethane-d_4 on Bruker DPX 300 or DRX 500 NMR spectrometers with tetramethylsilane (TMS) as the internal standard. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, m = multiplet. High resolution (HR) EI mass spectra were recorded on Agilent 5975C DIP/MS mass spectrometer. MALDI-TOF mass spectra were recorded on a Bruker Autoflex instrument using anthracene-1,8,9-triol as matrix. UV-vis-NIR absorption spectra were recorded on a Shimadzu UV-1700 spectrometer. The electrochemical measurements were carried out in anhydrous DCM with 0.1 M tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) as the supporting electrolyte at a scan rate of 0.05 V/s at room temperature under the protection of nitrogen. A gold disk was used as working electrode, platinum wire was used as counting electrode, and Ag/AgCl (3M KCl solution) was used as reference electrode. The potential was calibrated against the ferrocene/ferrocenium couple. Continuous wave X-band ESR spectra were obtained with a Bruker ELEXSYS E500 spectrometer using a variable temperature Bruker liquid nitrogen cryostat.

Picosecond Time-resolved Fluorescence. Time-resolved fluorescence decays were obtained by using a time-correlated single photon counting (TCSPC) technique. A mode-locked Ti:sapphire oscillator (MaiTai-BB, SpectraPhysics) was used as the excitation light source, which provides a fwhm (full width at half maximum) of 80 fs with a high repetition rate of 80 MHz. In order to minimize artifacts such as thermal lensing and accumulation effect, the repetition rate was reduced down to 800 kHz using a home-made acousto-optic pulse selector. The picked fundamental pulses were frequency-doubled by a BBO nonlinear crystal (Eksma) of 1 mm thickness. The fluorescence was collected by a microchannel plate photomultiplier (MCP-PMT, R3809U-51, Hamamatsu) with a thermoelectric cooler (C4878, Hamamatsu). Time-resolved fluorescence signals were calculated by a TCSPC board (SPC-130, Becker & Hickel GmbH). The overall instrumental response function (IRF) was determined to be less than 30 ps (fwhm) in all spectral regions. The polarization of the photoexcitation pulses was set to be vertical to the laboratory frame by both a half-wave retarder and a Glan laser polarizer and sheet polarizers were used in the fluorescence collection path at magic angle (54.7°) to obtain polarization-independent population decays when measuring the fluorescence decay profiles.

Femtosecond Time-resolved Transient Absorption. The femtosecond time-resolved transient absorption (fs-TA) spectrometer consists of an optical parametric amplifier (OPA; Palitra, Quantronix) pumped by a Ti:sapphire regenerative amplifier system (Integra-C, Quantronix) operating at 1 kHz repetition rate and an optical detection system. The generated OPA pulses have a pulsewidth of ~ 100 fs and an average power of 1 mW in the range of 280-2700 nm, which are used as pump pulses. White light continuum (WLC) probe pulses were generated using a sapphire window (3 mm thick) by focusing a small portion of the fundamental 800 nm pulses which was picked off by a quartz plate before entering the OPA. The time delay between pump and probe beams was carefully controlled by making the pump beam travel along a variable optical delay (ILS250, Newport). Intensities of the spectrally dispersed WLC probe pulses are monitored by a High Speed Spectrometer (Ultrafast Systems) for both visible and near-infrared measurements. To obtain the time-resolved transient absorption difference signal (ΔA) at a specific time, the pump pulses were chopped at 500 Hz and absorption spectra intensities were saved alternately with or without pump pulse. Typically, 4000 pulses excite the samples to obtain the fs-TA spectra at each delay time. The polarization angle between pump and probe beam was set at the magic angle (54.7°) using a Glan-laser polarizer with a

half-wave retarder in order to prevent polarization-dependent signals. Cross-correlation *fwhm* in pump-probe experiments was less than 200 fs and chirp of WLC probe pulses was measured to be 800 fs in the 400-800 nm region. To minimize chirp, all reflection optics in the probe beam path and a quartz cell of 2 mm path length were used. After fs-TA experiments, the absorption spectra of all compounds were carefully examined to detect if there were artifacts due to degradation and photo-oxidation of samples. The three-dimensional data sets of ΔA versus time and wavelength were subjected to singular value decomposition and global fitting to obtain the kinetic time constants and their associated spectra using Surface Xplorer software (Ultrafast Systems).

Two-photon absorption. The two-photon absorption spectrum was measured in the NIR region using the open-aperture Z-scan method with 130 fs pulses from an optical parametric amplifier (Light Conversion, TOPAS) operating at a repetition rate of 1 kHz generated from a Ti:sapphire regenerative amplifier system (Spectra-Physics, Hurricane). After passing through a 10 cm focal length lens, the laser beam was focused and passed through a 1 mm quartz cell. Since the position of the sample cell could be controlled along the laser beam direction (*z* axis) using the motorcontrolled delay stage, the local power density within the sample cell could be simply controlled under constant laser intensity. The transmitted laser beam from the sample cell was then detected by the same photodiode as used for reference monitoring. The on-axis peak intensity of the incident pulses at the focal point, I_0, ranged from 40 to 60 GW cm^{-2}. For a Gaussian beam profile, the nonlinear absorption coefficient can be obtained by curve fitting of the observed open-aperture traces $T(z)$ with the following equation:

$$T(z)=1-\frac{\beta I_0(1-e^{-\alpha_0 l})}{2\alpha_0[1+(z/z_0)^2]}$$

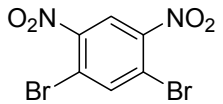
where α_0 is the linear absorption coefficient, l is the sample length, and z_0 is the diffraction length of the incident beam. After the nonlinear absorption coefficient has been obtained, the TPA cross section $\sigma^{(2)}$ of one solute molecule (in units of GM, where 1 GM = 10^{-50}cm^4 s photon^{-1} molecule^{-1}) can be determined by using the following relationship:

$$\beta=\frac{10^{-3}\sigma^{(2)}N_A d}{h\nu}$$

where N_A is the Avogadro constant, d is the concentration of the compound in solution, h is the Planck constant, and v is the frequency of the incident laser beam.

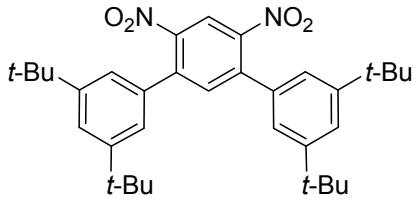
1.2. Detailed synthetic procedures and characterization data

1,5-Dibromo-2,4-dinitrobenzene (4)



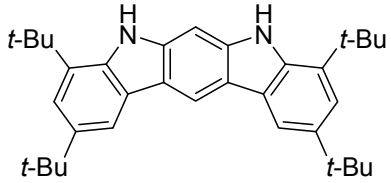
To a mixture of KNO_3 (5.6 g, 55.4 mmol) in concentrated H_2SO_4 (20 mL) was added 1,3-dibromobenzene (**3**, 6.4 g, 27.1 mmol). The temperature rose within several minutes. This mixture was then stirred at 130 °C for 2 h. The resulting yellow solution was poured into crushed ice. A yellow solid was precipitated and collected by suction filtration. Recrystallization from 95% ethanol to give pure compound **4** as yellow needles (5.1 g, 15.7 mmol) in 58% yield. ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 8.45 (s, 1H), 8.23 (s, 1H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 141.3, 122.8, 119.8 ppm. HR-MS (EI): *m*/*z* 325.8360, calcd. for $C_6H_2Br_2N_2O_4$: 325.8361.

1,5-Dinitro-2,4-bis(3,5-di-*tert*-butylphenyl)benzene (5)



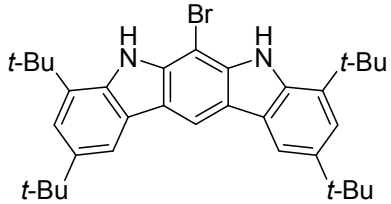
Compound **4** (0.48 g, 1.5 mmol), 2-(3,5-di-*tert*-butylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1.03 g, 3.3 mmol), aqueous K_2CO_3 solution of 2 M (4.0 mL, 8.0 mmol), and $Pd(PPh_3)_4$ (0.085 g, 0.007 mmol) in 1,2-dimethoxyethane (8 mL) was stirred at 90 °C overnight. After cooling to room temperature, the reaction was quenched by water. The resulting mixture was extracted with DCM and dried over anhydrous Na_2SO_4. The solvent was removed and the residue was purified through column chromatography (silica gel, DCM/hexane = 1/4 (v/v)) to give a yellow residue **5** (0.67 g, 1.2 mmol) in 83% yield. ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 8.38 (s, 1H), 7.65 (s, 1H), 7.56 (t, ^4J = 1.8 Hz, 2H), 7.23 (d, ^4J = 1.8 Hz, 4H), 1.38 (s, 36H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 151.6, 147.5, 140.8, 135.4, 134.6, 123.3, 122.2, 120.2, 35.0, 31.4 ppm. HR-MS (EI): *m*/*z* = 544.3324, calcd. for $C_{34}H_{44}O_4N_2$: 544.3301.

2,4,8,10-Tetra-*tert*-butyl-5,7-dihydroindolo[2,3-*b*]carbazole (6)



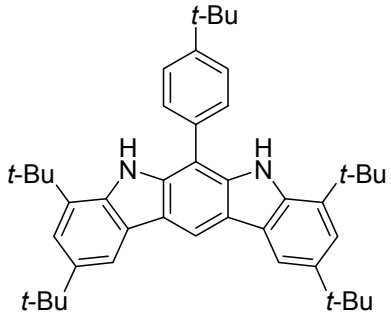
Compound **5** (0.37 g, 0.68 mmol), PPh_3 (1.80 g, 6.86 mmol), and *o*-dichlorobenzene (1 mL) was stirred at 170 °C for 2 days. The TLC showed the reaction was completed. The resulting mixture was then purified through column chromatography (silica gel, DCM/hexane = 3/4 (v/v)) to give a pale yellow solid **6** (0.19 g, 0.40 mmol) in 58% yield. ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 8.72 (s, 1H), 8.10 (d, ^4J = 1.5 Hz, 2H), 8.01 (s, 2H), 7.43 (d, ^4J = 1.5 Hz, 2H), 7.35 (s, 1H), 1.62 (s, 18H), 1.50 (s, 18H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 142.1, 139.8, 135.7, 131.6, 124.5, 119.5, 118.5, 113.8, 110.7, 90.2, 34.9, 34.8, 32.1, 30.4 ppm. HR-MS (EI): *m*/*z* = 480.3520, calcd. for $C_{34}H_{44}N_2$: 480.3504.

2,4,8,10-Tetra-*tert*-butyl-5,7-dihydro-6-bromoindolo[2,3-*b*]carbazole (7)



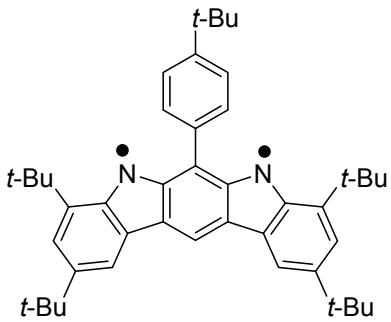
Compound **6** (20.0 mg, 0.042 mmol) was dissolved in DCM (5 mL). NBS (7.5 mg, 0.042 mmol) was added and the resulting solution was stirred for 1 h. Solvent was removed and the residue was purified through column chromatography (silica gel, dichloromethane/hexane = 1/10 (v/v)) to give a yellow solid **7** (16.5 mg, 0.030 mmol) in 79% yield. ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 8.79 (s, 1H), 8.23 (s, 2H), 8.19 (d, ^4J = 1.7 Hz, 2H), 7.57 (d, ^4J = 1.7 Hz, 2H), 1.74 (s, 18H), 1.61 (s, 18H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 142.8, 137.7, 135.3, 132.2, 125.2, 120.1, 119.3, 114.3, 109.9, 83.8, 34.9, 34.9, 32.1, 30.5 ppm. HR-MS (MALDI-TOF): *m*/*z* = 558.2599, 560.2594, calcd. for $C_{34}H_{43}BrN_2$: 558.2610, 560.2589.

2,4,8,10-Tetra-*tert*-butyl-5,7-dihydro-6-(4-*tert*-butylphenyl)indolo[2,3-*b*]carbazole (8)



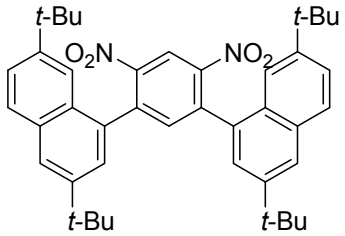
Compound **7** (143 mg, 0.25 mmol), 4-*tert*-butyl-phenylboronic acid (68 mg, 0.38 mmol), aqueous K_2CO_3 solution of 2 M (4.0 mL, 8.0 mmol), and $Pd(PPh_3)_4$ (15 mg, 0.013 mmol) in a mixed solvent of toluene (4.0 mL) and ethanol (2.0 mL) was stirred at 90 °C overnight. After cooling to room temperature, the reaction was quenched by water. The resulting mixture was extracted with DCM and dried over anhydrous Na_2SO_4. The solvent was removed and the residue was purified through column chromatography (silica gel, DCM/hexane = 1/5 (v/v)) to give a white solid **8** (120 mg, 0.20 mmol) in 77% yield. ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 8.73 (s, 1H), 8.26 (s, 2H), 8.14 (d, ^4J = 1.5 Hz, 2H), 7.85 (d, J = 8.4 Hz, 2H), 7.75 (d, J = 8.4 Hz, 2H), 7.44 (d, ^4J = 1.5 Hz, 2H), 1.58 (s, 18H), 1.52 (s, 18H), 1.51 (s, 9H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 150.6, 142.1, 137.3, 135.5, 133.0, 131.6, 127.9, 127.0, 124.8, 119.6, 118.7, 113.9, 109.9, 104.6, 34.9, 34.9, 34.8, 32.1, 31.4, 30.5 ppm. HR-MS (EI): m/z = 612.4458, calcd. for $C_{44}H_{56}N_2$: 612.4444.

Synthesis of 2,4,8,10-Tetra-*tert*-butyl-6-(4-*tert*-butylphenyl)indolo[2,3-*b*]carbazole (1)



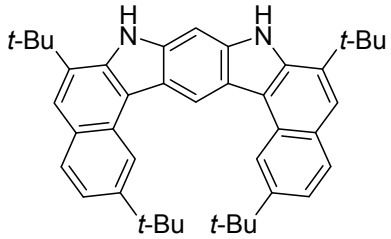
To a solution of **8** (2 mg, 0.0033 mmol) in anhydrous 2-MeTHF (0.5 mL) was added 20 equiv. *t*-BuOK (7.4 mg, 0.066 mmol), and an orange-yellow solution (dianion **9**) was obtained after stirring for 30 minutes at room temperature under nitrogen atmosphere. The solution was carefully transferred to an ESR tube containing 5 equiv. I_2 under nitrogen protection. The mixture was shook in a dry ice bath (-78 ^{o}C) for 30 minutes and resulted in a dark brown solution, which was submitted for VT ESR measurements from 150 K to room temperature under nitrogen atmosphere (see detailed data in later part).

1,5-Dinitro-2,4-bis(3,7-di-*tert*-butylnaphthalenyl)benzene (10)



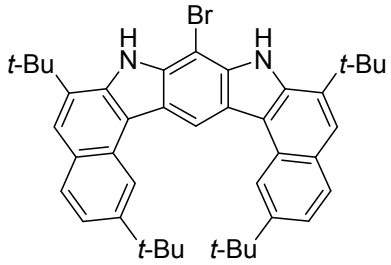
Compound **4** (1 g, 3.1 mmol), 3,7-di-*tert*-butyl-1-naphthylboronic acid (1.9 g, 6.7 mmol), aqueous K_2CO_3 solution of 2 M (8.0 mL, 16.0 mmol), and $Pd(PPh_3)_4$ (0.18 g, 0.015 mmol) in 1,2-dimethoxyethane (15 mL) was stirred at 90 °C overnight under nitrogen atmosphere. After cooling to room temperature, the reaction was quenched by water. The resulting mixture was extracted with DCM and dried over anhydrous Na_2SO_4. The solvent was removed and the residue was purified through column chromatography (silica gel, DCM/hexane = 1/3 (v/v)) to give a yellow compound **10** (1.9 g, 2.9 mmol) in 95% yield. This compound contains a pair of diastereoisomers, thus two sets of peaks were shown on NMR spectra. ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 8.81-8.80 (m, 1H), 7.88-7.77 (m, 5H), 7.65-7.38 (m, 6H), 1.45-1.27 (m, 36H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 149.5, 149.3, 148.7, 148.5, 147.5, 147.4, 140.0, 138.3, 137.8, 132.9, 132.7, 131.7, 131.6, 128.9, 128.6, 128.5, 128.4, 125.7, 125.3, 124.4, 124.2, 120.6, 120.3, 118.4, 118.3, 35.0, 34.9, 34.8, 31.2, 31.2, 31.1, 31.0 ppm. HR-MS (EI): *m*/*z* = 644.3637, calcd. for $C_{42}H_{48}O_4N_2$: 644.3614.

2,6,10,14-Tetra-*tert*-butyl-7,9-dihydrobenzo[*g*]benz[4,5]indolo[2,3-*b*]carbazole (11)



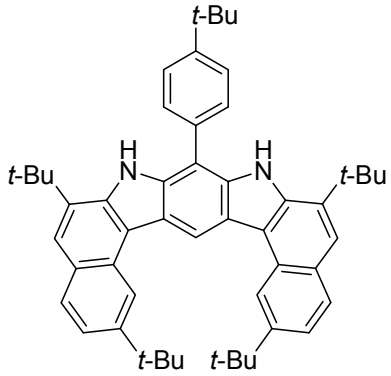
Compound **10** (1.9 g, 2.9 mmol), PPh_3 (3.8 g, 14.5 mmol), and *o*-dichlorobenzene (3 mL) was stirred at 170 °C for 1 day. The TLC showed the reaction was completed. The resulting mixture was then purified through column chromatography (silica gel, DCM/hexane = 1/1 (v/v)) to give a pale yellow solid **11** (0.24 g, 0.42 mmol) in 14% yield. Since the solubility of compound **11** in almost all general solvents is poor, even the NMR test at high temperature (80 °C in 1,1,2,2-tetrachloroethane-d^2) could not give excellent spectra. ^{1}H NMR (CD_2Cl_4, 500 MHz, 80 °C) δ: 9.65 (s, 1H), 9.03 (s, 2H), 8.57 (s, 2H), 8.03 (d, *J* = 8.5 Hz, 2H), 7.82 (s, 3H), 7.66 (d, *J* = 8.5 Hz 2H), 1.78 (s, 18H), 1.72 (s, 18H) ppm. ^{13}C NMR (CD_2Cl_4, 125 MHz, 80 °C) δ: 149.3, 137.6, 136.8, 133.2, 129.0, 128.8, 127.4, 122.5, 121.0, 119.9, 118.3, 91.4, 35.0, 34.4, 32.2, 30.5 ppm. HR-MS (EI): *m*/*z* = 580.3831, calcd. for $C_{42}H_{48}N_2$: 580.3817.

2,6,10,14-Tetra-*tert*-butyl-7,9-dihydro-8-bromobenzo[*g*]benz[4,5]indolo[2,3-*b*]carbazole (14)



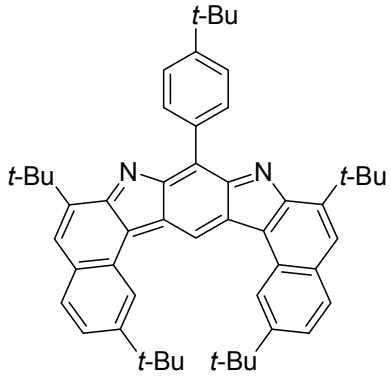
Compound **11** (83.2 mg, 0.14 mmol) was dissolved in DCM (50 mL). NBS (25.5 mg, 0.14 mmol) was added and the resulting solution was stirred for 2 h. The solvent was removed and the residue was purified through column chromatography (silica gel, dichloromethane/hexane = 1/6 (v/v)) to give a yellow solid **14** (83.4 mg, 0.13 mmol) in 88% yield. ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 9.59 (s, 1H), 8.99 (d, ^{4}J = 1.8 Hz, 2H), 8.72 (s, 2H), 8.00 (d, J = 8.5 Hz, 2H), 7.81 (s, 2H), 7.64 (dd, ^{3}J = 8.5 Hz, ^{4}J = 1.8 Hz 2H), 1.75 (s, 18H), 1.68 (s, 18H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 149.4, 136.5, 135.4, 133.2, 129.1, 129.0, 127.7, 122.9, 121.4, 120.6, 118.5, 117.7, 114.0, 85.1, 35.3, 34.7, 32.4, 30.5 ppm. HR-MS (MALDI-TOF): m/z = 658.2932, 660.2980, calcd. for $C_{42}H_{47}BrN_2$: 658.2917, 660.2897.

2,6,10,14-Tetra-*tert*-butyl-7,9-dihydro-8-(4-*tert*-butylphenyl)benzo[*g*]benz[4,5]indolo[2,3-*b*]carbazole (15)



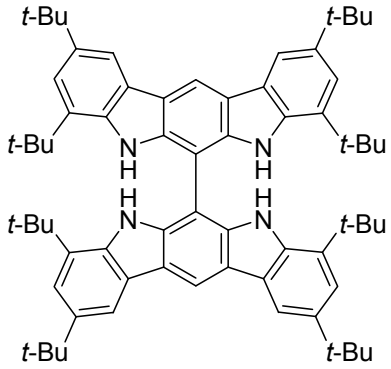
Compound **14** (83.4 mg, 0.13 mmol), 4-*tert*-butyl-phenylboronic acid (33.8 mg, 0.19 mmol), aqueous K_2CO_3 solution of 2 M (5.0 mL, 10.0 mmol), and $Pd(PPh_3)_4$ (7.0 mg, 0.006 mmol) in a mixed solvent of toluene (5.0 mL) and ethanol (2.5 mL) was stirred at 90 °C overnight under nitrogen atmosphere. After cooling to room temperature, the reaction was quenched by water. The resulting mixture was extracted with DCM and dried over anhydrous Na_2SO_4. The solvent was removed and the residue was purified through column chromatography (silica gel, dichloromethane/hexane = 1/4 (v/v)) to give a white solid **15** (77.7 mg, 0.11 mmol) in 86% yield. ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 9.67 (s, 1H), 9.09 (d, ^{4}J = 1.7 Hz, 2H), 8.83 (s, 2H), 8.01 (d, J = 8.5 Hz, 2H), 7.96 (d, J = 8.4 Hz, 2H), 7.82 (d, J = 8.4 Hz, 2H), 7.79 (s, 2H), 7.64 (dd, ^{3}J = 8.5 Hz, ^{4}J = 1.7 Hz, 2H), 1.71 (s, 18H), 1.66 (s, 18H), 1.54 (s, 9H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 151.2, 149.1, 136.5, 135.0, 133.1, 132.5, 129.0, 128.9, 128.4, 127.5, 127.1, 122.3, 121.0, 120.0, 118.5, 117.0, 113.9, 105.2, 35.3, 34.9, 34.6, 32.4, 31.4, 30.5 ppm. HR-MS (EI): m/z = 712.4770, calcd. for $C_{52}H_{60}N_2$: 712.4757.

2,6,10,14-Tetra-*tert*-butyl-8-(4-*tert*-butylphenyl)benzo[*g*]benz[4,5]indolo[2,3-*b*]carbazole (2)



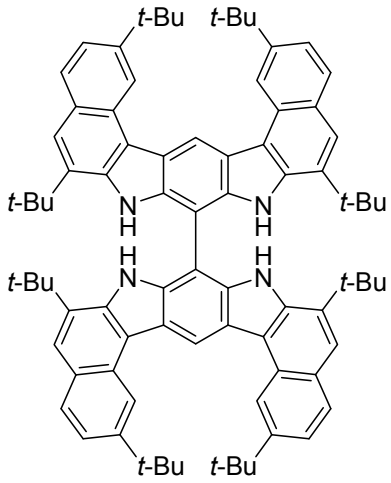
Compound **15** (5.0 mg, 0.0070 mmol) was refluxed with PbO_2 (25.0 mg, 0.1045 mmol) in dry ethyl acetate for 2 days. The solid was filtered off and then the solvent was removed using argon flow to give **2** as a deep blue solid in nearly quantitative yield. ^{1}H NMR ($CDCl_3$, 500 MHz) δ: 7.61 (d, J = 8.5 Hz, 2H), 7.28 (d, J = 8.5 Hz, 2H), 7.13-7.09 (m, 4H), 7.01 (d, J = 8.4 Hz, 2H), 6.51 (s, 2H), 6.31 (s, 1H), 1.32 (s, 9H), 1.29 (s, 18H), 1.25 (s, 18H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 166.4, 164.7, 152.7, 150.4, 143.8, 139.5, 136.3, 134.5, 134.0, 129.8, 129.2, 128.4, 128.1, 126.6, 123.7, 121.3, 34.7, 34.7, 34.6, 31.4, 31.2, 30.0 ppm. MALDI-TOF MS: m/z = 712.35 (M+2H) which is corresponding to the dihydro compound **15** due to hydrogenation during the measurement. Elemental analysis: calcd for $C_{52}H_{58}N_2$, C87.84, H 8.22, N 3.94; found C87.61, H 8.35, N 3.86.

6,6'-Bis(2,4,8,10-tetra-*tert*-butyl-5,7-dihydroindolo[2,3-*b*]carbazole) (16)



Compound **6** (40.0 mg, 0.083 mmol) and PbO_2 (300 mg, 1.254 mmol) in chloroform (10 mL) was stirred at 70 °C overnight. The mixture was simply filtered. Solvent was removed and the residue was purified through column chromatography (silica gel, DCM/hexane = 1/5 (v/v)) to give a yellow solid **16** (26.2 mg, 0.027 mmol) in 65% yield. It is noteworthy that the prolonged reaction time (3 days) led to the decomposition of part of **16** instead of the formation the corresponding diquinoid **17** or dihydrazine product. ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 8.96 (s, 2H), 8.22 (d, ^4J = 1.7 Hz, 4H), 7.77 (s, 4H), 7.40 (d, ^4J = 1.7 Hz, 4H), 1.52 (s, 36H), 1.27 (s, 36H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 142.6, 137.9, 135.7, 132.4, 124.9, 120.1, 118.9, 113.7, 111.2, 96.1, 34.9, 34.8, 32.1, 30.5, ppm. HR-MS (MALDI-TOF): m/z = 958.6879, calcd. for $C_{68}H_{86}N_4$: 958.6852.

8,8'-Bis(2,6,10,14-tetra-*tert*-butyl-7,9-dihydrobenzo[*g*]benz[4,5]indolo[2,3-*b*]carbazole) (18)



Compound **11** (50.0 mg, 0.086 mmol) and PbO_2 (300 mg, 1.254 mmol) in chloroform (10 mL) was stirred at 70 °C overnight. The mixture was simply filtered. The solvent was removed and the residue was purified through column chromatography (silica gel, DCM/hexane = 1/5 (v/v)) to give a yellow solid **18** (31.3 mg, 0.027 mmol) in 63% yield. It is noteworthy that the prolonged reaction time (3 days) led to the decomposition of part of **18** instead of the formation the corresponding diquinoid **19** or dihydrazine product. ^{1}H NMR ($CDCl_3$, 300 MHz) δ: 10.03 (s, 2H), 9.25 (d, ^{4}J = 1.6 Hz, 4H), 8.46 (s, 4H), 8.05 (d, J = 8.6 Hz, 4H), 7.78 (s, 4H), 7.71 (dd, ^{3}J = 8.6 Hz, ^{4}J = 1.6 Hz, 4H), 1.79 (s, 36H), 1.32 (s, 36H) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ: 149.5, 136.9, 135.6, 133.4, 129.2, 128.9, 127.7, 123.0, 121.3, 120.4, 118.5, 117.4, 115.7, 96.4, 35.4, 34.6, 32.5, 30.6 ppm. HR-MS (MALDI-TOF): m/z = 1158.7503, calcd. for $C_{84}H_{94}N_4$: 1158.7478.

2. VT ESR spectra of 1

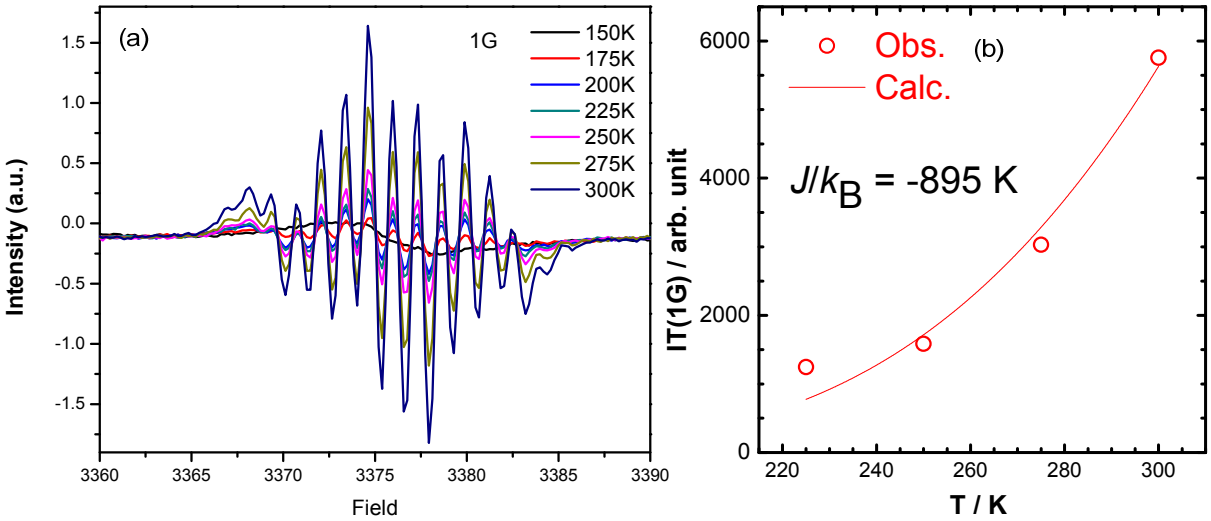


Fig. S1. (a) VT ESR spectra of the freshly prepared solution of **1** upon warm up from 150K to 300K (modulation amplitude of 1 G). (b) Fitting of the VT ESR data by Bleaney-Bowers equation. Due to uncertainty of the ESR intensity change at about 150 K (melting point of 2-Me THF), only the data above 200 K was used for simulation.

3. TCSPC, TA and Z-scan data

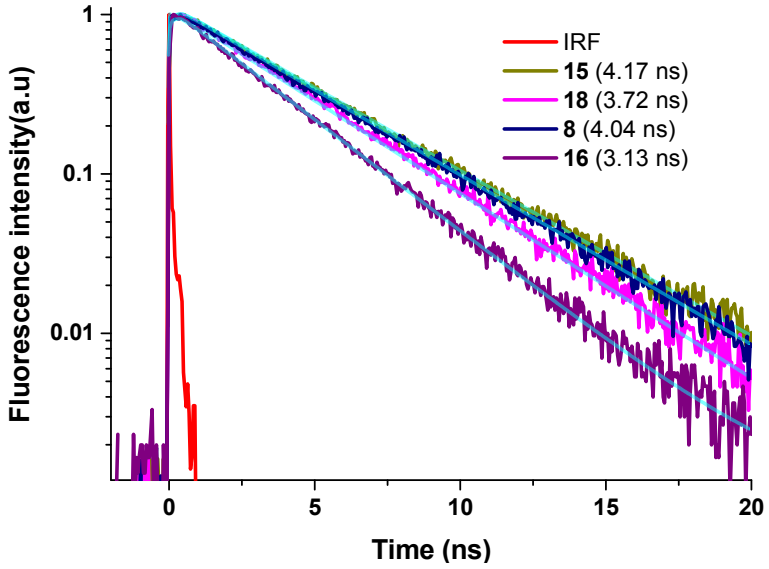


Fig. S2. Time-resolved fluorescence decay profiles of **8**, **15**, **16** and **18** in toluene obtained by using TCSPC technique with the photoexcitation at 370 nm with the best fit curves (cyan lines). Temporal profile for instrumental response function is plotted for comparison (red line, fwhm of ~ 30 ps)

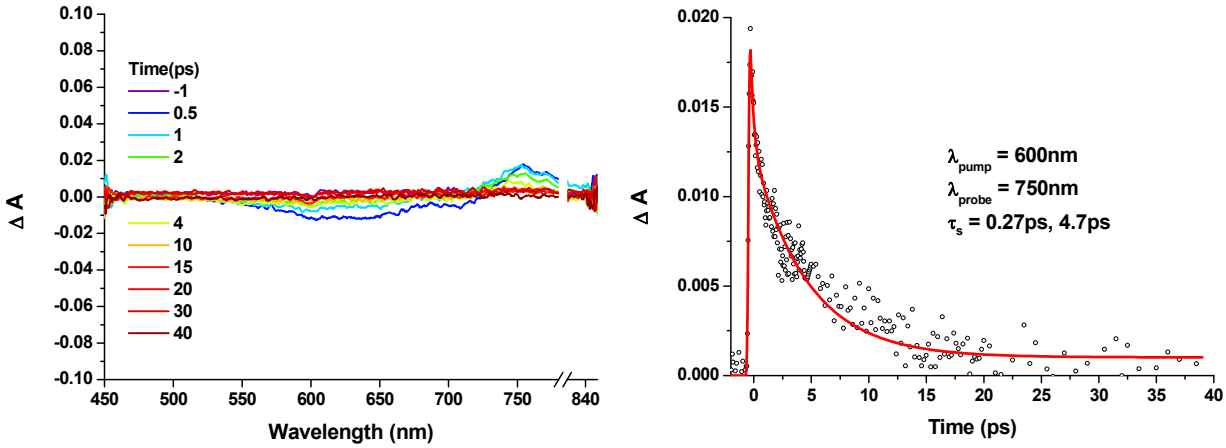


Fig. S3. Transient absorption spectrum and decay curve of **2** in toluene.

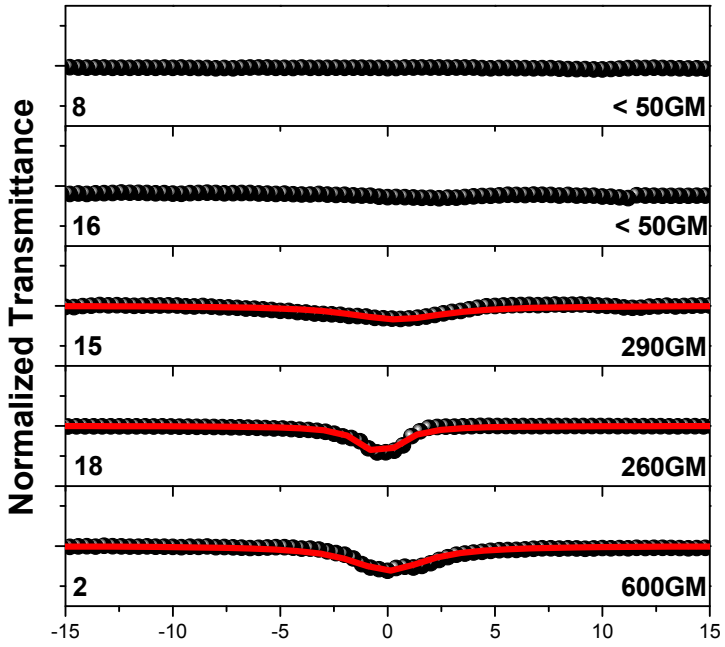


Fig. S4. Two-photon absorption cross-section of **2**, **8**, **15**, **16** and **18** in toluene obtained by using Z-scan technique with the photoexcitation at 800 nm with the best fit curves (red lines)

4. VT NMR spectra of 2

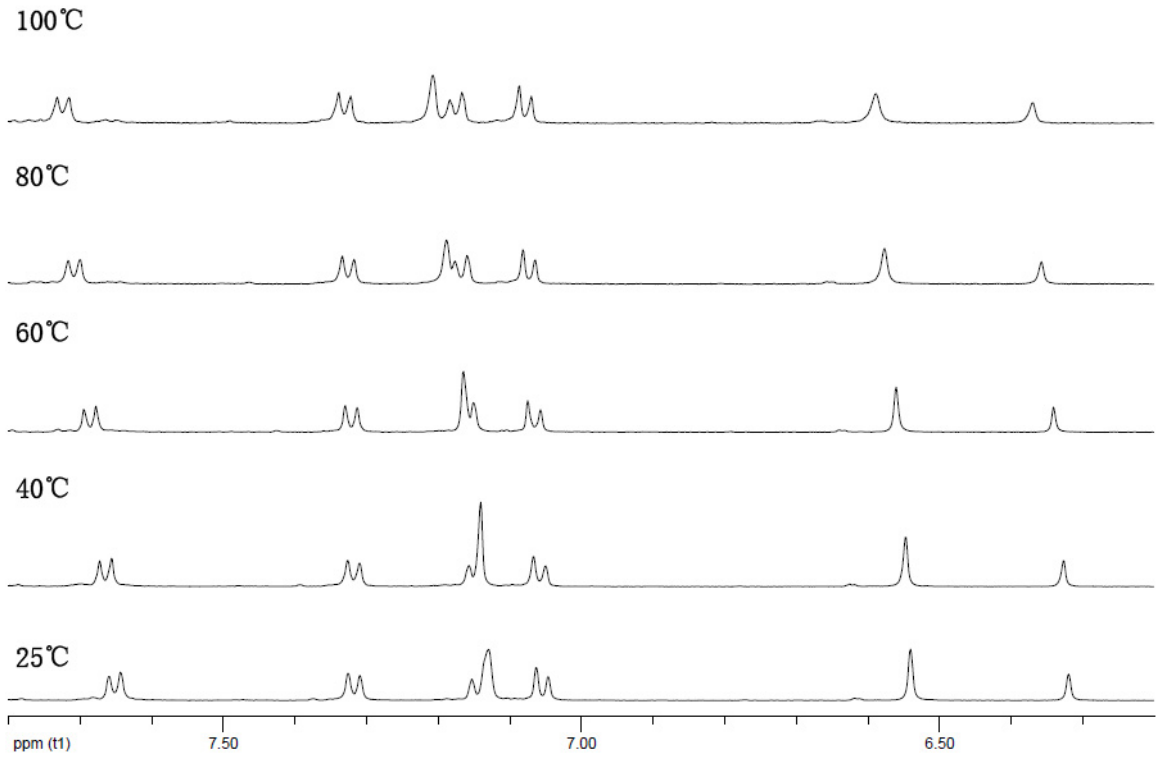


Fig. S5. VT ^{1}H NMR spectra (aromatic region) of **2** in 1,1,2,2-tetrachloroethane-d_2.

5. Decay of 2 in different solvents

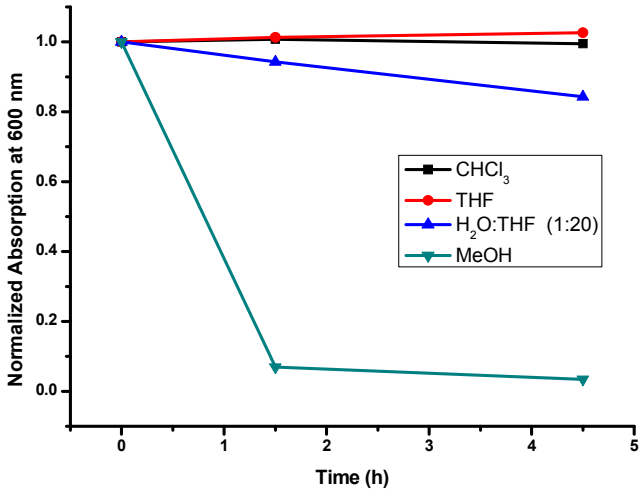


Fig. S6. The decay of **2** in different solvents indicated by the optical density at 600 nm *vs* time.

6. X-ray crystallographic structures of 8, 11, and 15

*6.1 Data for compound **8***

Singlet crystals of compound **8** were obtained through evaporation from $CHCl_3$.

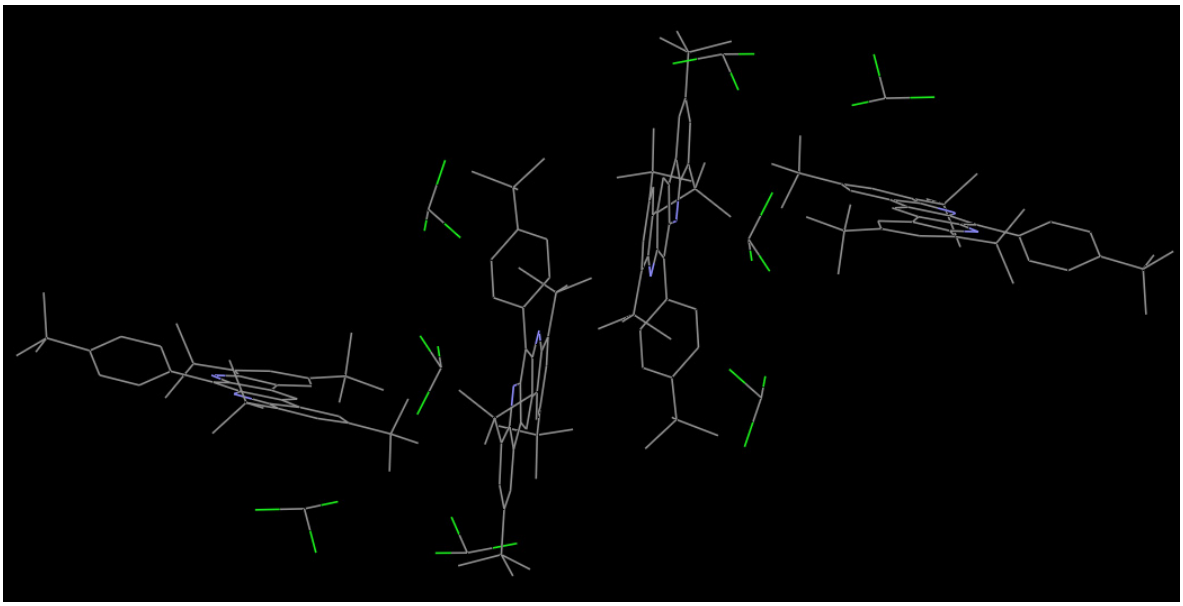


Fig. S7. The 3D packing structure of **8** in the single crystals.

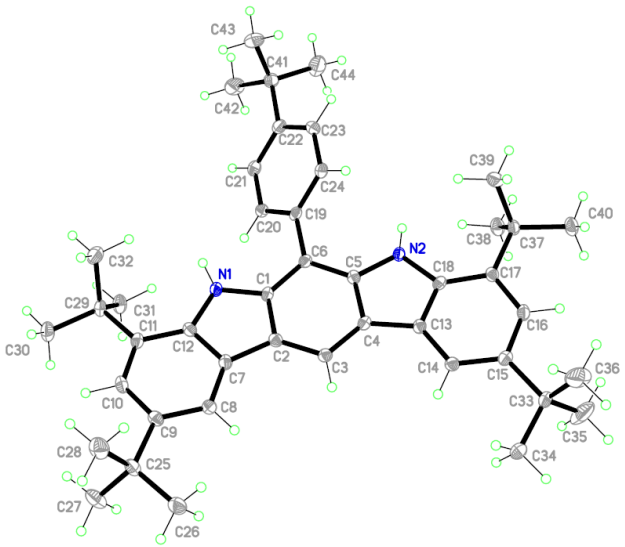


Table S1. Crystal data and structure refinement for **8**.

Empirical formula	C46 H58 Cl6 N2
Formula weight	851.64
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic

Space group	P2(1)/c
Unit cell dimensions	a = 13.6043(18) Å □= 90°.
	b = 29.340(4) Å □= 101.006(3)°.
	c = 11.7173(15) Å □ = 90°.
Volume	4590.9(10) $Å^3$
Z	4
Density (calculated)	1.232 Mg/m^3
Absorption coefficient	0.407 mm^{-1}
F(000)	1800
Crystal size	0.51 x 0.50 x 0.42 mm^3
Theta range for data collection	1.39 to 27.50°.
Index ranges	-17<=h<=11, -37<=k<=38, -15<=l<=14
Reflections collected	32323
Independent reflections	10529 [R(int) = 0.0324]
Completeness to theta = 27.50°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8476 and 0.8193
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10529 / 0 / 510
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0489, wR2 = 0.1210
R indices (all data)	R1 = 0.0632, wR2 = 0.1279
Largest diff. peak and hole	0.682 and -0.606 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	5844(1)	780(1)	10943(1)	14(1)
N(2)	2775(1)	1129(1)	8012(1)	13(1)
C(1)	5207(1)	964(1)	9986(1)	13(1)
C(2)	5776(1)	1265(1)	9418(1)	14(1)
C(3)	5331(1)	1496(1)	8421(1)	14(1)
C(4)	4316(1)	1422(1)	8013(1)	13(1)
C(5)	3760(1)	1128(1)	8610(1)	13(1)
C(6)	4178(1)	889(1)	9625(1)	13(1)
C(7)	6780(1)	1272(1)	10105(1)	14(1)
C(8)	7626(1)	1528(1)	10005(1)	15(1)

C(9)	8495(1)	1477(1)	10835(1)	16(1)
C(10)	8497(1)	1153(1)	11725(1)	16(1)
C(11)	7680(1)	885(1)	11853(1)	14(1)
C(12)	6800(1)	967(1)	11032(1)	14(1)
C(13)	3625(1)	1606(1)	7033(1)	13(1)
C(14)	3762(1)	1915(1)	6171(1)	14(1)
C(15)	2960(1)	2028(1)	5302(1)	15(1)
C(16)	2015(1)	1838(1)	5354(1)	16(1)
C(17)	1832(1)	1537(1)	6210(1)	14(1)
C(18)	2679(1)	1416(1)	7046(1)	13(1)
C(19)	3577(1)	601(1)	10278(1)	13(1)
C(20)	3920(1)	180(1)	10752(1)	15(1)
C(21)	3345(1)	-90(1)	11349(1)	16(1)
C(22)	2401(1)	50(1)	11500(1)	17(1)
C(23)	2059(1)	472(1)	11030(1)	18(1)
C(24)	2632(1)	743(1)	10439(1)	16(1)
C(25)	9435(1)	1767(1)	10830(2)	18(1)
C(26)	9346(1)	2052(1)	9721(2)	24(1)
C(27)	10364(1)	1462(1)	10922(2)	27(1)
C(28)	9581(2)	2094(1)	11875(2)	26(1)
C(29)	7730(1)	526(1)	12815(1)	16(1)
C(30)	8798(1)	457(1)	13493(2)	23(1)
C(31)	7375(1)	63(1)	12269(2)	20(1)
C(32)	7072(1)	675(1)	13679(2)	22(1)
C(33)	3062(1)	2356(1)	4315(2)	20(1)
C(34)	4151(1)	2471(1)	4305(2)	25(1)
C(35)	2630(2)	2139(1)	3133(2)	49(1)
C(36)	2500(2)	2797(1)	4470(2)	48(1)
C(37)	780(1)	1355(1)	6240(1)	16(1)
C(38)	760(1)	834(1)	6104(2)	20(1)
C(39)	476(1)	1493(1)	7388(2)	20(1)
C(40)	-12(1)	1552(1)	5253(2)	22(1)
C(41)	1748(1)	-230(1)	12173(2)	20(1)
C(42)	2254(2)	-676(1)	12641(2)	30(1)
C(43)	1551(2)	52(1)	13208(2)	28(1)
C(44)	751(2)	-342(1)	11364(2)	36(1)
C(1S)	6680(2)	2030(1)	2412(2)	29(1)
Cl(1)	4043(1)	791(1)	3462(1)	62(1)
Cl(2)	5490(1)	1213(1)	5269(1)	34(1)

Cl(3)	4305(1)	461(1)	5815(1)	104(1)
C(2S)	4326(2)	940(1)	4941(2)	35(1)
Cl(4)	7169(1)	2068(1)	3910(1)	63(1)
Cl(5)	5451(1)	1822(1)	2178(1)	37(1)
Cl(6)	6731(1)	2565(1)	1751(1)	51(1)

Table S3. Bond lengths [Å] and angles [°] for **8**.

N(1)-C(1)	1.389(2)
N(1)-C(12)	1.396(2)
N(2)-C(5)	1.389(2)
N(2)-C(18)	1.397(2)
C(1)-C(6)	1.399(2)
C(1)-C(2)	1.420(2)
C(2)-C(3)	1.387(2)
C(2)-C(7)	1.447(2)
C(3)-C(4)	1.388(2)
C(4)-C(5)	1.417(2)
C(4)-C(13)	1.444(2)
C(5)-C(6)	1.403(2)
C(6)-C(19)	1.487(2)
C(7)-C(8)	1.398(2)
C(7)-C(12)	1.404(2)
C(8)-C(9)	1.388(2)
C(9)-C(10)	1.411(2)
C(9)-C(25)	1.537(2)
C(10)-C(11)	1.392(2)
C(11)-C(12)	1.406(2)
C(11)-C(29)	1.535(2)
C(13)-C(14)	1.396(2)
C(13)-C(18)	1.406(2)
C(14)-C(15)	1.383(2)
C(15)-C(16)	1.413(2)
C(15)-C(33)	1.533(2)
C(16)-C(17)	1.393(2)
C(17)-C(18)	1.408(2)
C(17)-C(37)	1.534(2)
C(19)-C(20)	1.397(2)

C(19)-C(24)	1.398(2)
C(20)-C(21)	1.391(2)
C(21)-C(22)	1.390(2)
C(22)-C(23)	1.399(2)
C(22)-C(41)	1.533(2)
C(23)-C(24)	1.387(2)
C(25)-C(26)	1.530(2)
C(25)-C(27)	1.536(2)
C(25)-C(28)	1.539(2)
C(29)-C(30)	1.530(2)
C(29)-C(32)	1.537(2)
C(29)-C(31)	1.540(2)
C(33)-C(34)	1.521(2)
C(33)-C(36)	1.530(3)
C(33)-C(35)	1.536(3)
C(37)-C(38)	1.535(2)
C(37)-C(39)	1.535(2)
C(37)-C(40)	1.536(2)
C(41)-C(42)	1.530(3)
C(41)-C(43)	1.532(3)
C(41)-C(44)	1.535(3)
C(1S)-Cl(5)	1.752(2)
C(1S)-Cl(4)	1.758(2)
C(1S)-Cl(6)	1.758(2)
Cl(1)-C(2S)	1.757(2)
Cl(2)-C(2S)	1.750(2)
Cl(3)-C(2S)	1.742(2)

C(1)-N(1)-C(12)	109.70(13)
C(5)-N(2)-C(18)	110.02(13)
N(1)-C(1)-C(6)	128.13(14)
N(1)-C(1)-C(2)	107.88(14)
C(6)-C(1)-C(2)	123.97(14)
C(3)-C(2)-C(1)	120.64(15)
C(3)-C(2)-C(7)	132.45(15)
C(1)-C(2)-C(7)	106.86(14)
C(2)-C(3)-C(4)	117.25(15)
C(3)-C(4)-C(5)	121.01(14)
C(3)-C(4)-C(13)	131.96(15)

C(5)-C(4)-C(13)	107.00(14)
N(2)-C(5)-C(6)	128.65(15)
N(2)-C(5)-C(4)	107.71(13)
C(6)-C(5)-C(4)	123.64(15)
C(1)-C(6)-C(5)	113.45(14)
C(1)-C(6)-C(19)	123.39(14)
C(5)-C(6)-C(19)	123.11(14)
C(8)-C(7)-C(12)	120.83(15)
C(8)-C(7)-C(2)	131.82(15)
C(12)-C(7)-C(2)	107.30(14)
C(9)-C(8)-C(7)	119.22(15)
C(8)-C(9)-C(10)	118.18(15)
C(8)-C(9)-C(25)	122.33(15)
C(10)-C(9)-C(25)	119.48(14)
C(11)-C(10)-C(9)	124.81(15)
C(10)-C(11)-C(12)	115.02(15)
C(10)-C(11)-C(29)	122.84(14)
C(12)-C(11)-C(29)	122.13(15)
N(1)-C(12)-C(7)	108.20(14)
N(1)-C(12)-C(11)	130.05(15)
C(7)-C(12)-C(11)	121.75(15)
C(14)-C(13)-C(18)	120.99(14)
C(14)-C(13)-C(4)	131.45(15)
C(18)-C(13)-C(4)	107.57(14)
C(15)-C(14)-C(13)	119.45(15)
C(14)-C(15)-C(16)	118.12(15)
C(14)-C(15)-C(33)	122.22(15)
C(16)-C(15)-C(33)	119.64(14)
C(17)-C(16)-C(15)	124.71(15)
C(16)-C(17)-C(18)	115.19(15)
C(16)-C(17)-C(37)	122.21(14)
C(18)-C(17)-C(37)	122.60(14)
N(2)-C(18)-C(13)	107.69(14)
N(2)-C(18)-C(17)	130.81(15)
C(13)-C(18)-C(17)	121.45(14)
C(20)-C(19)-C(24)	117.14(15)
C(20)-C(19)-C(6)	122.16(15)
C(24)-C(19)-C(6)	120.71(14)
C(21)-C(20)-C(19)	121.61(15)

C(22)-C(21)-C(20)	121.27(15)
C(21)-C(22)-C(23)	117.13(15)
C(21)-C(22)-C(41)	123.26(15)
C(23)-C(22)-C(41)	119.59(15)
C(24)-C(23)-C(22)	121.80(16)
C(23)-C(24)-C(19)	121.05(15)
C(26)-C(25)-C(27)	107.98(15)
C(26)-C(25)-C(9)	112.03(14)
C(27)-C(25)-C(9)	110.54(14)
C(26)-C(25)-C(28)	108.18(15)
C(27)-C(25)-C(28)	109.15(15)
C(9)-C(25)-C(28)	108.88(14)
C(30)-C(29)-C(11)	112.05(14)
C(30)-C(29)-C(32)	108.09(14)
C(11)-C(29)-C(32)	109.84(13)
C(30)-C(29)-C(31)	106.88(14)
C(11)-C(29)-C(31)	109.50(13)
C(32)-C(29)-C(31)	110.44(14)
C(34)-C(33)-C(36)	108.83(17)
C(34)-C(33)-C(15)	111.93(14)
C(36)-C(33)-C(15)	108.82(15)
C(34)-C(33)-C(35)	106.95(16)
C(36)-C(33)-C(35)	110.15(19)
C(15)-C(33)-C(35)	110.14(16)
C(17)-C(37)-C(38)	110.04(14)
C(17)-C(37)-C(39)	109.66(13)
C(38)-C(37)-C(39)	110.56(14)
C(17)-C(37)-C(40)	111.99(13)
C(38)-C(37)-C(40)	107.54(14)
C(39)-C(37)-C(40)	107.00(14)
C(42)-C(41)-C(43)	108.21(15)
C(42)-C(41)-C(22)	112.06(15)
C(43)-C(41)-C(22)	108.94(15)
C(42)-C(41)-C(44)	108.80(16)
C(43)-C(41)-C(44)	109.71(17)
C(22)-C(41)-C(44)	109.10(14)
Cl(5)-C(1S)-Cl(4)	110.23(11)
Cl(5)-C(1S)-Cl(6)	111.05(11)
Cl(4)-C(1S)-Cl(6)	110.16(11)

Cl(3)-C(2S)-Cl(2)	110.84(14)
Cl(3)-C(2S)-Cl(1)	110.77(12)
Cl(2)-C(2S)-Cl(1)	110.41(12)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	13(1)	16(1)	13(1)	4(1)	1(1)	0(1)
N(2)	12(1)	15(1)	12(1)	3(1)	0(1)	-2(1)
C(1)	14(1)	13(1)	11(1)	0(1)	1(1)	1(1)
C(2)	13(1)	14(1)	14(1)	-1(1)	2(1)	0(1)
C(3)	14(1)	14(1)	14(1)	0(1)	3(1)	-1(1)
C(4)	16(1)	13(1)	11(1)	0(1)	2(1)	1(1)
C(5)	13(1)	13(1)	13(1)	-2(1)	1(1)	0(1)
C(6)	14(1)	14(1)	11(1)	0(1)	3(1)	1(1)
C(7)	14(1)	15(1)	13(1)	-1(1)	1(1)	2(1)
C(8)	14(1)	17(1)	14(1)	1(1)	3(1)	1(1)
C(9)	13(1)	16(1)	18(1)	-2(1)	3(1)	1(1)
C(10)	13(1)	19(1)	16(1)	-1(1)	-2(1)	2(1)
C(11)	16(1)	15(1)	12(1)	-1(1)	0(1)	2(1)
C(12)	12(1)	15(1)	15(1)	-2(1)	2(1)	1(1)
C(13)	14(1)	14(1)	11(1)	-2(1)	1(1)	1(1)
C(14)	14(1)	14(1)	14(1)	1(1)	4(1)	0(1)
C(15)	17(1)	15(1)	13(1)	2(1)	3(1)	1(1)
C(16)	15(1)	18(1)	14(1)	1(1)	-1(1)	2(1)
C(17)	13(1)	15(1)	13(1)	-2(1)	1(1)	0(1)
C(18)	17(1)	12(1)	11(1)	0(1)	3(1)	0(1)
C(19)	15(1)	15(1)	9(1)	0(1)	1(1)	-2(1)
C(20)	14(1)	17(1)	13(1)	0(1)	2(1)	1(1)
C(21)	20(1)	14(1)	14(1)	1(1)	2(1)	1(1)
C(22)	18(1)	19(1)	13(1)	1(1)	2(1)	-3(1)
C(23)	13(1)	23(1)	19(1)	3(1)	5(1)	2(1)
C(24)	17(1)	17(1)	14(1)	4(1)	2(1)	3(1)
C(25)	13(1)	18(1)	23(1)	2(1)	1(1)	0(1)

C(26)	17(1)	26(1)	27(1)	6(1)	4(1)	-4(1)
C(27)	14(1)	24(1)	43(1)	4(1)	6(1)	1(1)
C(28)	24(1)	24(1)	28(1)	-4(1)	1(1)	-7(1)
C(29)	16(1)	16(1)	14(1)	1(1)	-2(1)	1(1)
C(30)	21(1)	22(1)	21(1)	5(1)	-4(1)	-1(1)
C(31)	22(1)	15(1)	20(1)	1(1)	-3(1)	0(1)
C(32)	26(1)	25(1)	16(1)	2(1)	4(1)	2(1)
C(33)	17(1)	26(1)	18(1)	10(1)	2(1)	0(1)
C(34)	22(1)	30(1)	25(1)	15(1)	6(1)	0(1)
C(35)	49(2)	78(2)	17(1)	12(1)	-3(1)	-33(1)
C(36)	48(1)	39(1)	68(2)	36(1)	35(1)	22(1)
C(37)	13(1)	17(1)	16(1)	3(1)	0(1)	0(1)
C(38)	17(1)	19(1)	22(1)	1(1)	-2(1)	-3(1)
C(39)	15(1)	24(1)	22(1)	0(1)	5(1)	-1(1)
C(40)	15(1)	24(1)	25(1)	7(1)	-3(1)	-3(1)
C(41)	17(1)	25(1)	20(1)	6(1)	5(1)	-4(1)
C(42)	32(1)	27(1)	34(1)	13(1)	13(1)	-2(1)
C(43)	28(1)	33(1)	26(1)	5(1)	13(1)	-3(1)
C(44)	28(1)	49(1)	28(1)	13(1)	-2(1)	-19(1)
C(1S)	36(1)	25(1)	25(1)	-2(1)	7(1)	2(1)
Cl(1)	52(1)	89(1)	45(1)	-36(1)	11(1)	-23(1)
Cl(2)	29(1)	42(1)	32(1)	-11(1)	6(1)	5(1)
Cl(3)	202(1)	41(1)	88(1)	4(1)	73(1)	-31(1)
C(2S)	44(1)	30(1)	36(1)	-12(1)	20(1)	-9(1)
Cl(4)	85(1)	70(1)	28(1)	-3(1)	-5(1)	-42(1)
Cl(5)	33(1)	44(1)	35(1)	-9(1)	8(1)	0(1)
Cl(6)	56(1)	37(1)	67(1)	21(1)	32(1)	15(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8**.

	x	y	z	U(eq)
H(1N)	5642(16)	626(7)	11473(19)	23(5)
H(2N)	2304(17)	960(8)	8176(19)	28(6)
H(3)	5704	1698	8032	16
H(8)	7607	1734	9376	18

H(10)	9100	1114	12277	20
H(14)	4401	2048	6182	17
H(16)	1465	1921	4762	19
H(20)	4563	75	10665	18
H(21)	3601	-374	11659	19
H(23)	1416	576	11118	22
H(24)	2378	1029	10138	19
H(26A)	9220	1850	9041	35
H(26B)	9970	2220	9734	35
H(26C)	8790	2268	9676	35
H(27A)	10270	1249	10266	40
H(27B)	10462	1290	11652	40
H(27C)	10954	1652	10907	40
H(28A)	10186	2277	11887	39
H(28B)	9650	1918	12596	39
H(28C)	8999	2297	11807	39
H(30A)	9234	368	12955	34
H(30B)	8801	218	14076	34
H(30C)	9042	743	13881	34
H(31A)	6680	88	11856	30
H(31B)	7419	-168	12883	30
H(31C)	7801	-28	11721	30
H(32A)	7319	965	14038	34
H(32B)	7097	442	14284	34
H(32C)	6379	713	13266	34
H(34A)	4435	2641	5012	38
H(34B)	4189	2658	3622	38
H(34C)	4530	2189	4275	38
H(35A)	2696	2352	2509	74
H(35B)	1920	2067	3096	74
H(35C)	2996	1858	3042	74
H(36A)	2796	2938	5214	73
H(36B)	1794	2727	4459	73
H(36C)	2551	3008	3834	73
H(38A)	1213	696	6764	30
H(38B)	976	752	5379	30
H(38C)	78	722	6081	30
H(39A)	-195	1375	7406	30
H(39B)	473	1826	7450	30

H(39C)	956	1366	8041	30
H(40A)	-673	1432	5311	33
H(40B)	149	1466	4502	33
H(40C)	-17	1885	5317	33
H(42A)	2381	-862	11991	45
H(42B)	1816	-842	13069	45
H(42C)	2890	-608	13163	45
H(43A)	1120	-121	13632	42
H(43B)	1220	338	12925	42
H(43C)	2189	119	13728	42
H(44A)	880	-518	10698	54
H(44B)	406	-58	11088	54
H(44C)	330	-521	11789	54
H(1S)	7101	1812	2058	34
H(2S)	3803	1158	5101	42

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*6.2 Data for compound **11***

Singlet crystals of compound **11** were obtained through diffusion of DCM and hexane.

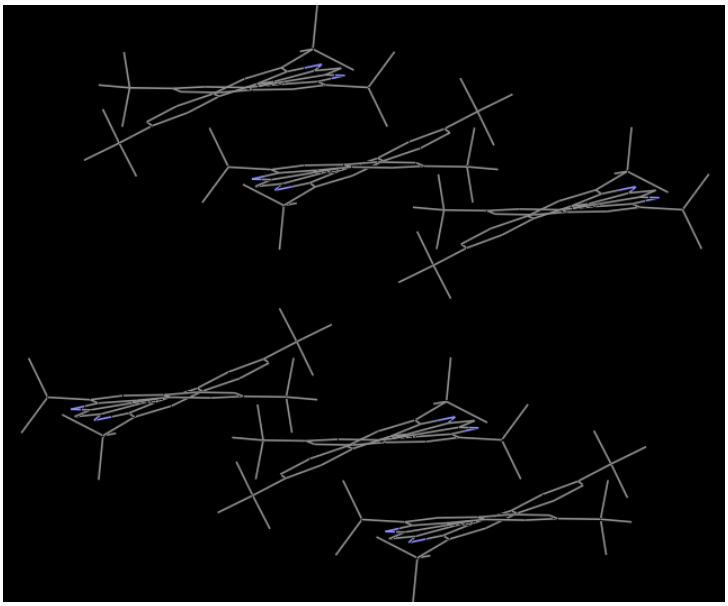


Fig. S8. The 3D packing structure of **11** in the single crystals.

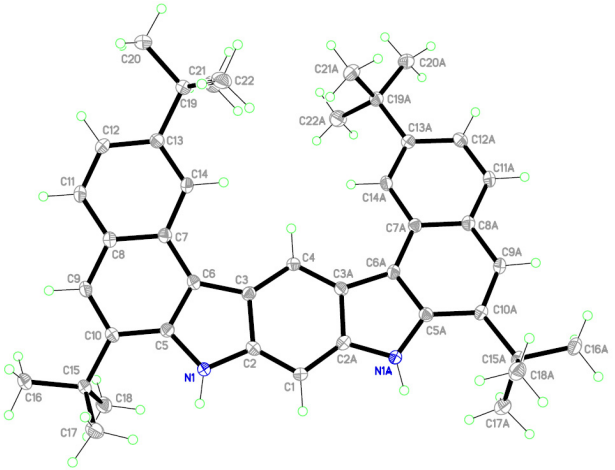


Table S6. Crystal data and structure refinement for **11**.

Empirical formula	C42 H48 N2	
Formula weight	580.82	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 18.183(5) Å	□= 90°.
	b = 17.083(5) Å	□= 97.513(5)°.
	c = 10.329(3) Å	□ = 90°.
Volume	3181.0(15) Å^3	
Z	4	
Density (calculated)	1.213 Mg/m^3	
Absorption coefficient	0.069 mm^{-1}	
F(000)	1256	
Crystal size	0.60 x 0.20 x 0.16 mm^3	
Theta range for data collection	2.26 to 27.50°.	
Index ranges	-23<=h<=17, -22<=k<=22, -13<=l<=13	
Reflections collected	11189	
Independent reflections	3649 [R(int) = 0.0416]	
Completeness to theta = 27.50°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9890 and 0.9595	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3649 / 0 / 210	
Goodness-of-fit on F^2	1.016	
Final R indices [I>2sigma(I)]	R1 = 0.0488, wR2 = 0.1163	
R indices (all data)	R1 = 0.0676, wR2 = 0.1260	

Largest diff. peak and hole 0.405 and -0.225 e.Å^{-3}

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4027(1)	-753(1)	8957(1)	16(1)
C(1)	5000	-917(1)	7500	14(1)
C(2)	4548(1)	-482(1)	8205(1)	15(1)
C(3)	4563(1)	348(1)	8281(1)	14(1)
C(4)	5000	764(1)	7500	14(1)
C(5)	3712(1)	-130(1)	9550(1)	14(1)
C(6)	4049(1)	563(1)	9186(1)	14(1)
C(7)	3866(1)	1289(1)	9750(1)	14(1)
C(8)	3316(1)	1275(1)	10608(1)	15(1)
C(9)	2966(1)	558(1)	10874(1)	16(1)
C(10)	3144(1)	-150(1)	10381(1)	14(1)
C(11)	3131(1)	1980(1)	11192(1)	18(1)
C(12)	3481(1)	2668(1)	10979(1)	18(1)
C(13)	4044(1)	2697(1)	10159(1)	15(1)
C(14)	4218(1)	2012(1)	9552(1)	15(1)
C(15)	2711(1)	-899(1)	10620(1)	16(1)
C(16)	2173(1)	-763(1)	11626(2)	22(1)
C(17)	3221(1)	-1578(1)	11146(2)	22(1)
C(18)	2251(1)	-1135(1)	9325(1)	20(1)
C(19)	4440(1)	3466(1)	9904(1)	18(1)
C(20)	4231(1)	4134(1)	10782(2)	23(1)
C(21)	4204(1)	3707(1)	8475(2)	23(1)
C(22)	5282(1)	3350(1)	10150(2)	25(1)

Table S8. Bond lengths [Å] and angles [°] for **11**.

N(1)-C(2)	1.3811(19)
N(1)-C(5)	1.3880(18)
N(1)-H(1N)	0.88(2)
C(1)-C(2)#1	1.3833(18)
C(1)-C(2)	1.3833(18)

C(1)-H(1)	0.9500
C(2)-C(3)	1.421(2)
C(3)-C(4)	1.3970(17)
C(3)-C(6)	1.453(2)
C(4)-C(3)#1	1.3970(17)
C(4)-H(4)	0.9500
C(5)-C(6)	1.4068(19)
C(5)-C(10)	1.427(2)
C(6)-C(7)	1.4267(19)
C(7)-C(8)	1.421(2)
C(7)-C(14)	1.419(2)
C(8)-C(11)	1.408(2)
C(8)-C(9)	1.424(2)
C(9)-C(10)	1.368(2)
C(9)-H(9)	0.9500
C(10)-C(15)	1.540(2)
C(11)-C(12)	1.368(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.412(2)
C(12)-H(12)	0.9500
C(13)-C(14)	1.383(2)
C(13)-C(19)	1.537(2)
C(14)-H(14)	0.9500
C(15)-C(16)	1.535(2)
C(15)-C(18)	1.536(2)
C(15)-C(17)	1.539(2)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(22)	1.533(2)
C(19)-C(21)	1.538(2)
C(19)-C(20)	1.536(2)
C(20)-H(20A)	0.9800

C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800

C(2)-N(1)-C(5)	110.09(12)
C(2)-N(1)-H(1N)	120.8(14)
C(5)-N(1)-H(1N)	129.1(14)
C(2)#1-C(1)-C(2)	115.06(18)
C(2)#1-C(1)-H(1)	122.5
C(2)-C(1)-H(1)	122.5
C(1)-C(2)-N(1)	127.91(13)
C(1)-C(2)-C(3)	123.81(14)
N(1)-C(2)-C(3)	108.27(12)
C(4)-C(3)-C(2)	118.90(14)
C(4)-C(3)-C(6)	134.86(14)
C(2)-C(3)-C(6)	106.15(12)
C(3)#1-C(4)-C(3)	118.99(18)
C(3)#1-C(4)-H(4)	120.5
C(3)-C(4)-H(4)	120.5
N(1)-C(5)-C(6)	108.02(12)
N(1)-C(5)-C(10)	128.24(13)
C(6)-C(5)-C(10)	123.73(13)
C(5)-C(6)-C(7)	119.33(13)
C(5)-C(6)-C(3)	107.33(12)
C(7)-C(6)-C(3)	133.30(13)
C(8)-C(7)-C(14)	118.15(12)
C(8)-C(7)-C(6)	117.43(12)
C(14)-C(7)-C(6)	124.36(13)
C(11)-C(8)-C(7)	118.72(13)
C(11)-C(8)-C(9)	121.04(13)
C(7)-C(8)-C(9)	120.24(13)
C(10)-C(9)-C(8)	123.74(13)
C(10)-C(9)-H(9)	118.1
C(8)-C(9)-H(9)	118.1

C(9)-C(10)-C(5)	115.33(13)
C(9)-C(10)-C(15)	121.59(13)
C(5)-C(10)-C(15)	122.88(12)
C(12)-C(11)-C(8)	121.61(13)
C(12)-C(11)-H(11)	119.2
C(8)-C(11)-H(11)	119.2
C(11)-C(12)-C(13)	120.98(13)
C(11)-C(12)-H(12)	119.5
C(13)-C(12)-H(12)	119.5
C(14)-C(13)-C(12)	118.02(13)
C(14)-C(13)-C(19)	120.30(13)
C(12)-C(13)-C(19)	121.65(12)
C(13)-C(14)-C(7)	122.47(13)
C(13)-C(14)-H(14)	118.8
C(7)-C(14)-H(14)	118.8
C(16)-C(15)-C(18)	107.87(12)
C(16)-C(15)-C(10)	111.55(12)
C(18)-C(15)-C(10)	108.04(11)
C(16)-C(15)-C(17)	106.49(12)
C(18)-C(15)-C(17)	110.14(12)
C(10)-C(15)-C(17)	112.65(12)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

C(22)-C(19)-C(21)	109.94(13)
C(22)-C(19)-C(20)	108.46(12)
C(21)-C(19)-C(20)	107.96(13)
C(22)-C(19)-C(13)	109.95(12)
C(21)-C(19)-C(13)	108.36(12)
C(20)-C(19)-C(13)	112.14(12)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **11**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	18(1)	12(1)	18(1)	-1(1)	8(1)	-1(1)
C(1)	16(1)	11(1)	16(1)	0	4(1)	0
C(2)	15(1)	15(1)	15(1)	2(1)	2(1)	-2(1)
C(3)	13(1)	14(1)	16(1)	-1(1)	2(1)	1(1)
C(4)	13(1)	12(1)	16(1)	0	3(1)	0
C(5)	14(1)	14(1)	14(1)	-1(1)	2(1)	0(1)

C(6)	12(1)	16(1)	15(1)	1(1)	3(1)	-1(1)
C(7)	14(1)	15(1)	13(1)	0(1)	2(1)	0(1)
C(8)	15(1)	17(1)	14(1)	0(1)	4(1)	0(1)
C(9)	14(1)	18(1)	15(1)	1(1)	5(1)	-1(1)
C(10)	14(1)	16(1)	14(1)	2(1)	2(1)	-2(1)
C(11)	18(1)	20(1)	18(1)	0(1)	9(1)	1(1)
C(12)	21(1)	16(1)	19(1)	-3(1)	7(1)	2(1)
C(13)	15(1)	15(1)	15(1)	0(1)	2(1)	0(1)
C(14)	13(1)	17(1)	15(1)	-1(1)	5(1)	0(1)
C(15)	16(1)	15(1)	18(1)	1(1)	6(1)	-3(1)
C(16)	23(1)	20(1)	24(1)	-1(1)	11(1)	-6(1)
C(17)	22(1)	18(1)	26(1)	4(1)	6(1)	-2(1)
C(18)	21(1)	21(1)	20(1)	-1(1)	4(1)	-4(1)
C(19)	19(1)	15(1)	20(1)	-1(1)	6(1)	-2(1)
C(20)	28(1)	15(1)	29(1)	-2(1)	10(1)	-3(1)
C(21)	27(1)	19(1)	24(1)	3(1)	8(1)	-2(1)
C(22)	19(1)	20(1)	36(1)	-2(1)	5(1)	-4(1)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **11**.

	x	y	z	U(eq)
H(1)	5000	-1473	7500	17
H(4)	5000	1320	7500	16
H(9)	2587	572	11425	19
H(11)	2753	1978	11746	22
H(12)	3343	3134	11389	22
H(14)	4588	2027	8982	18
H(16A)	1826	-343	11320	32
H(16B)	2454	-613	12464	32
H(16C)	1896	-1245	11736	32
H(17A)	2919	-2018	11380	33
H(17B)	3549	-1403	11921	33
H(17C)	3521	-1744	10472	33
H(18A)	1913	-708	9019	30
H(18B)	1963	-1606	9459	30
H(18C)	2584	-1242	8673	30

H(20A)	3698	4238	10598	35
H(20B)	4507	4607	10609	35
H(20C)	4356	3984	11701	35
H(21A)	4344	3295	7894	35
H(21B)	4452	4197	8295	35
H(21C)	3665	3783	8326	35
H(22A)	5426	3173	11051	37
H(22B)	5531	3846	10013	37
H(22C)	5429	2955	9545	37
H(1N)	3929(11)	-1256(13)	9000(20)	41(6)

*6.3 Data for compound **15***

Singlet crystals of compound **15** were obtained through evaporation from toluene.

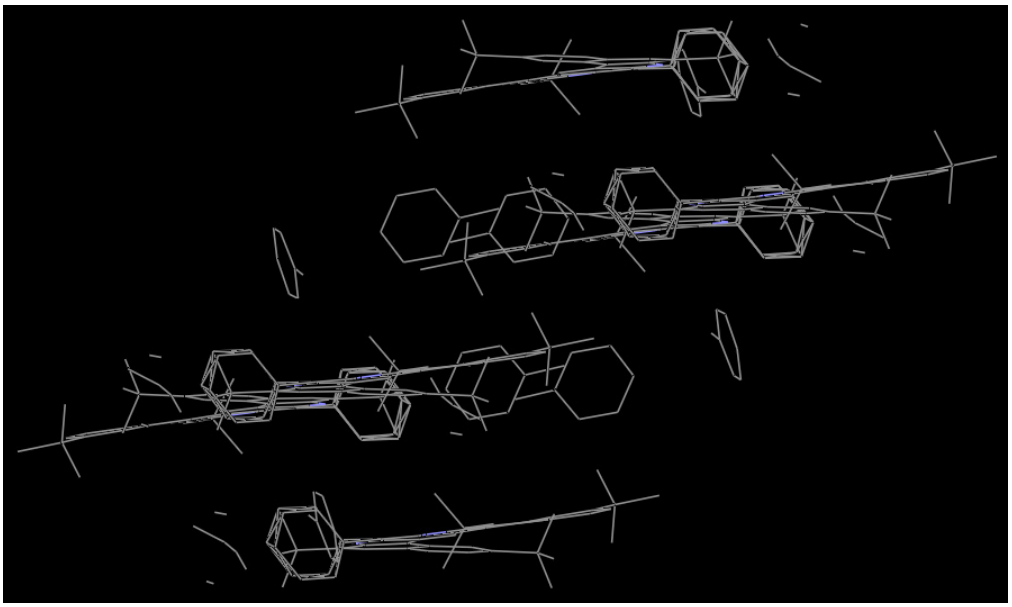


Fig. S9. The packing structure in the single crystals of **15**.

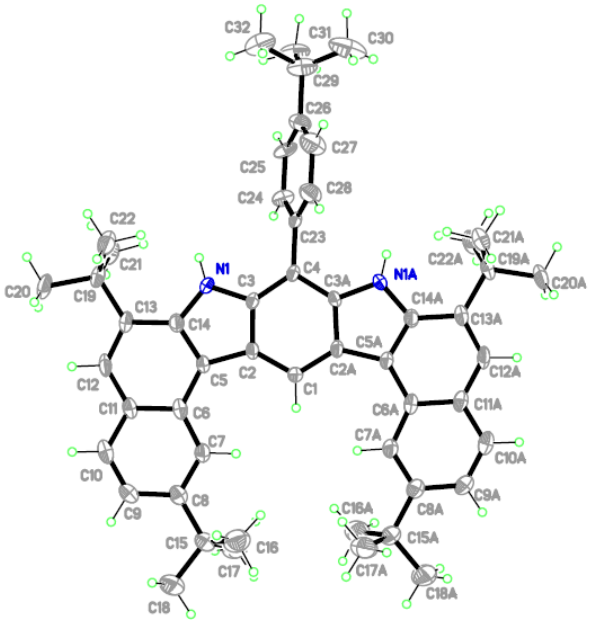


Table S11. Crystal data and structure refinement for **15**.

Empirical formula	C66 H76 N2	
Formula weight	897.29	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 25.799(6) Å	□= 90°.
	b = 18.171(4) Å	□= 103.053(4)°.
	c = 11.441(3) Å	□ = 90°.
Volume	5225(2) Å^3	
Z	4	
Density (calculated)	1.141 Mg/m^3	
Absorption coefficient	0.065 mm^{-1}	
F(000)	1944	
Crystal size	0.50 x 0.30 x 0.20 mm^3	
Theta range for data collection	1.62 to 24.99°.	
Index ranges	-25<=h<=30, -21<=k<=21, -13<=l<=13	
Reflections collected	15119	
Independent reflections	4603 [R(int) = 0.0838]	
Completeness to theta = 24.99°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9872 and 0.9684	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	4603 / 108 / 344
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0839, wR2 = 0.2355
R indices (all data)	R1 = 0.1196, wR2 = 0.2628
Largest diff. peak and hole	0.652 and -0.504 e.Å^{-3}

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **15**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(23)	5018(5)	-561(1)	2426(11)	21(1)
C(24)	5180(4)	-966(4)	3475(8)	28(2)
C(25)	5205(3)	-1729(4)	3424(6)	29(2)
C(26)	5068(4)	-2087(1)	2324(8)	34(3)
C(27)	4906(4)	-1682(4)	1275(6)	49(3)
C(28)	4880(4)	-919(4)	1325(8)	38(3)
C(29)	5076(4)	-2949(4)	2214(7)	51(3)
C(30)	5340(4)	-3178(4)	1245(8)	81(3)
C(31)	5339(5)	-3296(7)	3414(8)	49(3)
C(32)	4486(4)	-3246(8)	1897(12)	63(4)
N(1)	4204(1)	435(1)	3360(2)	24(1)
C(1)	5000	1863(2)	2500	22(1)
C(2)	4600(1)	1471(2)	2885(3)	21(1)
C(3)	4621(1)	689(2)	2903(3)	21(1)
C(4)	5000	270(2)	2500	21(1)
C(5)	4130(1)	1670(2)	3320(3)	22(1)
C(6)	3886(1)	2364(2)	3469(3)	26(1)
C(7)	4052(1)	3057(2)	3145(3)	27(1)
C(8)	3793(1)	3705(2)	3280(3)	31(1)
C(9)	3348(1)	3662(2)	3792(3)	40(1)
C(10)	3175(1)	3006(2)	4132(3)	41(1)
C(11)	3427(1)	2334(2)	3967(3)	31(1)
C(12)	3226(1)	1655(2)	4265(3)	33(1)
C(13)	3436(1)	984(2)	4090(3)	28(1)
C(14)	3902(1)	1014(2)	3604(3)	24(1)
C(15)	3989(1)	4439(2)	2884(3)	36(1)
C(16)	3994(2)	4401(2)	1555(4)	52(1)
C(17)	4547(2)	4586(2)	3625(4)	50(1)

C(18)	3635(2)	5090(2)	3052(4)	57(1)
C(19)	3195(1)	259(2)	4399(3)	31(1)
C(20)	2695(1)	404(2)	4890(3)	41(1)
C(21)	3598(1)	-150(2)	5367(3)	38(1)
C(22)	3018(1)	-212(2)	3265(3)	41(1)
C(1S)	8088(3)	7863(3)	8996(7)	94(2)
C(2S)	8097(2)	7639(3)	7864(6)	93(2)
C(3S)	8451(3)	7130(4)	7628(7)	103(2)
C(4S)	8821(3)	6832(4)	8495(10)	126(3)
C(5S)	8832(4)	7037(5)	9641(10)	149(4)
C(6S)	8452(4)	7533(4)	9911(6)	125(3)
C(7S)	7698(4)	8375(5)	9194(11)	184(4)

Table S13. Bond lengths [Å] and angles [°] for **15**.

C(23)-C(24)	1.3900
C(23)-C(28)	1.3900
C(23)-C(4)	1.513(4)
C(24)-C(25)	1.3900
C(24)-H(24)	0.9500
C(25)-C(26)	1.3900
C(25)-H(25)	0.9500
C(26)-C(27)	1.3900
C(26)-C(29)	1.573(7)
C(27)-C(28)	1.3900
C(27)-H(27)	0.9500
C(28)-H(28)	0.9500
C(29)-C(30)	1.485(10)
C(29)-C(31)	1.524(11)
C(29)-C(32)	1.579(12)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800

C(32)-H(32C)	0.9800
N(1)-C(14)	1.376(4)
N(1)-C(3)	1.377(4)
N(1)-H(1N)	0.82(3)
C(1)-C(2)#1	1.403(3)
C(1)-C(2)	1.403(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.423(4)
C(2)-C(5)	1.459(4)
C(3)-C(4)	1.396(3)
C(4)-C(3)#1	1.396(3)
C(4)-C(23)#1	1.513(4)
C(5)-C(14)	1.400(4)
C(5)-C(6)	1.437(4)
C(6)-C(7)	1.406(4)
C(6)-C(11)	1.425(4)
C(7)-C(8)	1.379(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.404(5)
C(8)-C(15)	1.530(5)
C(9)-C(10)	1.360(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.417(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.410(4)
C(12)-C(13)	1.367(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.436(4)
C(13)-C(19)	1.531(4)
C(15)-C(17)	1.521(5)
C(15)-C(16)	1.525(5)
C(15)-C(18)	1.532(5)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800

C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(21)	1.530(5)
C(19)-C(22)	1.535(5)
C(19)-C(20)	1.541(4)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(1S)-C(2S)	1.362(9)
C(1S)-C(6S)	1.376(10)
C(1S)-C(7S)	1.425(9)
C(2S)-C(3S)	1.370(9)
C(2S)-H(2S)	0.9500
C(3S)-C(4S)	1.326(10)
C(3S)-H(3S)	0.9500
C(4S)-C(5S)	1.357(12)
C(4S)-H(4S)	0.9500
C(5S)-C(6S)	1.416(12)
C(5S)-H(5S)	0.9500
C(6S)-H(6S)	0.9500
C(7S)-H(7S1)	0.9800
C(7S)-H(7S2)	0.9800
C(7S)-H(7S3)	0.9800

C(24)-C(23)-C(28)	120.0
C(24)-C(23)-C(4)	119.1(8)
C(28)-C(23)-C(4)	120.9(8)
C(25)-C(24)-C(23)	120.0
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(24)-C(25)-C(26)	120.0
C(24)-C(25)-H(25)	120.0
C(26)-C(25)-H(25)	120.0

C(27)-C(26)-C(25)	120.0
C(27)-C(26)-C(29)	117.7(7)
C(25)-C(26)-C(29)	122.3(7)
C(26)-C(27)-C(28)	120.0
C(26)-C(27)-H(27)	120.0
C(28)-C(27)-H(27)	120.0
C(27)-C(28)-C(23)	120.0
C(27)-C(28)-H(28)	120.0
C(23)-C(28)-H(28)	120.0
C(30)-C(29)-C(31)	111.8(7)
C(30)-C(29)-C(26)	110.8(6)
C(31)-C(29)-C(26)	110.6(8)
C(30)-C(29)-C(32)	108.3(7)
C(31)-C(29)-C(32)	106.0(5)
C(26)-C(29)-C(32)	109.2(8)
C(14)-N(1)-C(3)	110.4(2)
C(14)-N(1)-H(1N)	125(2)
C(3)-N(1)-H(1N)	124(2)
C(2)#1-C(1)-C(2)	119.0(4)
C(2)#1-C(1)-H(1)	120.5
C(2)-C(1)-H(1)	120.5
C(1)-C(2)-C(3)	118.9(3)
C(1)-C(2)-C(5)	135.2(3)
C(3)-C(2)-C(5)	105.9(2)
N(1)-C(3)-C(4)	127.4(3)
N(1)-C(3)-C(2)	108.1(2)
C(4)-C(3)-C(2)	124.5(3)
C(3)#1-C(4)-C(3)	113.9(3)
C(3)#1-C(4)-C(23)#1	126.5(4)
C(3)-C(4)-C(23)#1	119.5(4)
C(3)#1-C(4)-C(23)	119.5(4)
C(3)-C(4)-C(23)	126.5(4)
C(23)#1-C(4)-C(23)	8.0(7)
C(14)-C(5)-C(6)	120.2(2)
C(14)-C(5)-C(2)	107.1(2)
C(6)-C(5)-C(2)	132.8(3)
C(7)-C(6)-C(11)	118.0(3)
C(7)-C(6)-C(5)	125.9(3)
C(11)-C(6)-C(5)	116.0(3)

C(8)-C(7)-C(6)	123.5(3)
C(8)-C(7)-H(7)	118.3
C(6)-C(7)-H(7)	118.3
C(7)-C(8)-C(9)	117.4(3)
C(7)-C(8)-C(15)	120.7(3)
C(9)-C(8)-C(15)	121.9(3)
C(10)-C(9)-C(8)	121.4(3)
C(10)-C(9)-H(9)	119.3
C(8)-C(9)-H(9)	119.3
C(9)-C(10)-C(11)	121.8(3)
C(9)-C(10)-H(10)	119.1
C(11)-C(10)-H(10)	119.1
C(12)-C(11)-C(10)	121.1(3)
C(12)-C(11)-C(6)	121.0(3)
C(10)-C(11)-C(6)	117.9(3)
C(13)-C(12)-C(11)	124.4(3)
C(13)-C(12)-H(12)	117.8
C(11)-C(12)-H(12)	117.8
C(12)-C(13)-C(14)	114.7(3)
C(12)-C(13)-C(19)	122.6(3)
C(14)-C(13)-C(19)	122.8(3)
N(1)-C(14)-C(5)	108.5(2)
N(1)-C(14)-C(13)	127.8(3)
C(5)-C(14)-C(13)	123.7(3)
C(17)-C(15)-C(16)	110.1(3)
C(17)-C(15)-C(8)	108.8(3)
C(16)-C(15)-C(8)	109.4(3)
C(17)-C(15)-C(18)	108.1(3)
C(16)-C(15)-C(18)	107.4(3)
C(8)-C(15)-C(18)	113.0(3)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5

C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(21)-C(19)-C(13)	109.9(3)
C(21)-C(19)-C(22)	111.4(3)
C(13)-C(19)-C(22)	110.1(3)
C(21)-C(19)-C(20)	107.9(3)
C(13)-C(19)-C(20)	110.7(3)
C(22)-C(19)-C(20)	106.9(3)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(2S)-C(1S)-C(6S)	116.0(6)
C(2S)-C(1S)-C(7S)	120.7(8)
C(6S)-C(1S)-C(7S)	123.3(8)
C(1S)-C(2S)-C(3S)	123.0(6)
C(1S)-C(2S)-H(2S)	118.5
C(3S)-C(2S)-H(2S)	118.5

C(4S)-C(3S)-C(2S)	121.9(7)
C(4S)-C(3S)-H(3S)	119.1
C(2S)-C(3S)-H(3S)	119.1
C(3S)-C(4S)-C(5S)	117.7(8)
C(3S)-C(4S)-H(4S)	121.1
C(5S)-C(4S)-H(4S)	121.1
C(4S)-C(5S)-C(6S)	121.4(7)
C(4S)-C(5S)-H(5S)	119.3
C(6S)-C(5S)-H(5S)	119.3
C(1S)-C(6S)-C(5S)	119.9(7)
C(1S)-C(6S)-H(6S)	120.0
C(5S)-C(6S)-H(6S)	120.0
C(1S)-C(7S)-H(7S1)	109.5
C(1S)-C(7S)-H(7S2)	109.5
H(7S1)-C(7S)-H(7S2)	109.5
C(1S)-C(7S)-H(7S3)	109.5
H(7S1)-C(7S)-H(7S3)	109.5
H(7S2)-C(7S)-H(7S3)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+1/2

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **15**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(23)	17(1)	22(1)	26(1)	2(1)	10(1)	-2(1)
C(24)	37(5)	23(4)	23(4)	1(3)	1(4)	-5(4)
C(25)	34(4)	19(4)	27(4)	13(3)	-5(4)	-6(3)
C(26)	32(5)	26(3)	41(6)	-8(3)	4(4)	2(3)
C(27)	62(6)	40(5)	46(6)	0(4)	15(5)	13(4)
C(28)	53(6)	31(5)	34(5)	1(4)	18(4)	8(4)
C(29)	66(6)	25(3)	57(7)	3(3)	4(4)	-3(4)
C(30)	114(7)	38(4)	88(6)	-11(4)	15(6)	24(5)
C(31)	67(6)	22(4)	51(6)	6(4)	-2(5)	-1(5)
C(32)	71(7)	41(6)	75(7)	4(5)	14(5)	-15(5)
N(1)	24(1)	20(1)	31(2)	1(1)	14(1)	-4(1)
C(1)	21(2)	18(2)	30(2)	0	9(2)	0

C(2)	16(1)	25(2)	24(2)	1(1)	8(1)	1(1)
C(3)	17(1)	22(1)	26(1)	2(1)	10(1)	-2(1)
C(4)	17(1)	22(1)	26(1)	2(1)	10(1)	-2(1)
C(5)	18(1)	25(2)	25(2)	-1(1)	10(1)	1(1)
C(6)	19(2)	35(2)	24(2)	-2(1)	8(1)	2(1)
C(7)	21(2)	30(2)	32(2)	-1(1)	10(1)	0(1)
C(8)	26(2)	31(2)	35(2)	0(1)	9(1)	5(1)
C(9)	36(2)	30(2)	59(2)	-1(2)	21(2)	10(2)
C(10)	29(2)	46(2)	55(2)	-2(2)	23(2)	8(2)
C(11)	21(2)	36(2)	40(2)	-1(2)	14(1)	5(1)
C(12)	22(2)	43(2)	41(2)	0(2)	20(2)	2(1)
C(13)	21(2)	36(2)	29(2)	3(1)	12(1)	-2(1)
C(14)	21(2)	28(2)	26(2)	2(1)	10(1)	1(1)
C(15)	33(2)	29(2)	46(2)	3(2)	11(2)	8(1)
C(16)	64(3)	41(2)	53(3)	7(2)	16(2)	-1(2)
C(17)	42(2)	35(2)	68(3)	4(2)	4(2)	-2(2)
C(18)	47(2)	36(2)	90(3)	10(2)	20(2)	13(2)
C(19)	25(2)	40(2)	31(2)	3(1)	15(1)	-7(1)
C(20)	31(2)	51(2)	47(2)	6(2)	24(2)	-9(2)
C(21)	35(2)	44(2)	40(2)	6(2)	18(2)	-8(2)
C(22)	33(2)	49(2)	44(2)	-4(2)	17(2)	-13(2)
C(1S)	104(4)	68(3)	113(5)	-24(4)	31(4)	-19(3)
C(2S)	72(4)	88(4)	104(5)	11(4)	-14(3)	2(3)
C(3S)	104(5)	100(4)	106(5)	-7(4)	24(4)	-9(4)
C(4S)	82(4)	90(5)	189(8)	3(5)	-5(5)	10(4)
C(5S)	164(7)	87(5)	147(7)	32(5)	-66(6)	-22(5)
C(6S)	206(8)	79(4)	73(4)	-9(4)	-4(5)	-37(5)
C(7S)	160(7)	117(6)	308(12)	-48(7)	119(8)	-2(5)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **15**.

	x	y	z	U(eq)
H(24)	5274	-721	4227	34
H(25)	5317	-2006	4142	35
H(27)	4812	-1926	523	59

H(28)	4769	-642	608	46
H(30A)	5719	-3053	1473	121
H(30B)	5175	-2921	500	121
H(30C)	5300	-3710	1120	121
H(31A)	5376	-3828	3309	74
H(31B)	5118	-3207	3993	74
H(31C)	5691	-3078	3711	74
H(32A)	4295	-3032	1135	94
H(32B)	4307	-3106	2534	94
H(32C)	4489	-3783	1826	94
H(1N)	4128(13)	-3(18)	3400(30)	28
H(1)	5000	2385	2500	27
H(7)	4358	3080	2817	32
H(9)	3164	4100	3903	48
H(10)	2876	2998	4489	50
H(12)	2924	1664	4611	40
H(16A)	4241	4016	1428	78
H(16B)	4108	4876	1295	78
H(16C)	3635	4286	1089	78
H(17A)	4536	4644	4470	75
H(17B)	4686	5038	3340	75
H(17C)	4779	4172	3541	75
H(18A)	3276	5017	2554	85
H(18B)	3785	5546	2811	85
H(18C)	3617	5124	3897	85
H(20A)	2791	705	5618	61
H(20B)	2546	-66	5080	61
H(20C)	2429	666	4284	61
H(21A)	3908	-285	5052	57
H(21B)	3433	-596	5600	57
H(21C)	3711	169	6069	57
H(22A)	2755	61	2669	61
H(22B)	2859	-670	3468	61
H(22C)	3327	-326	2933	61
H(2S)	7846	7846	7209	111
H(3S)	8431	6986	6821	124
H(4S)	9070	6488	8320	151
H(5S)	9100	6843	10276	179
H(6S)	8449	7638	10723	150

H(7S1)	7684	8794	8650	277
H(7S2)	7793	8548	10027	277
H(7S3)	7349	8134	9043	277

7. ^{1}H, ^{13}C NMR, and HR mass spectra

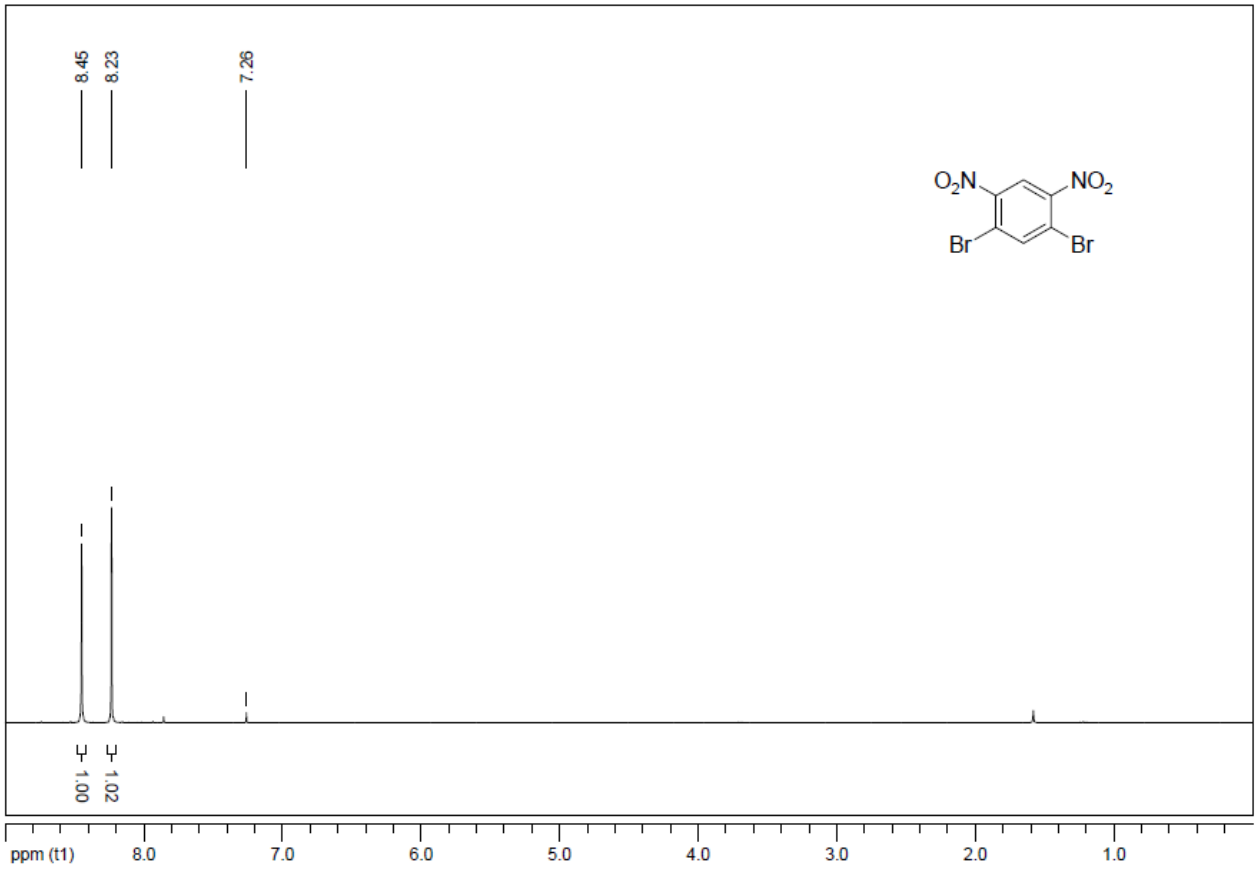


Fig. S10. ^{1}H NMR spectrum of compound **4** ($CDCl_3$, 300 MHz, rt).

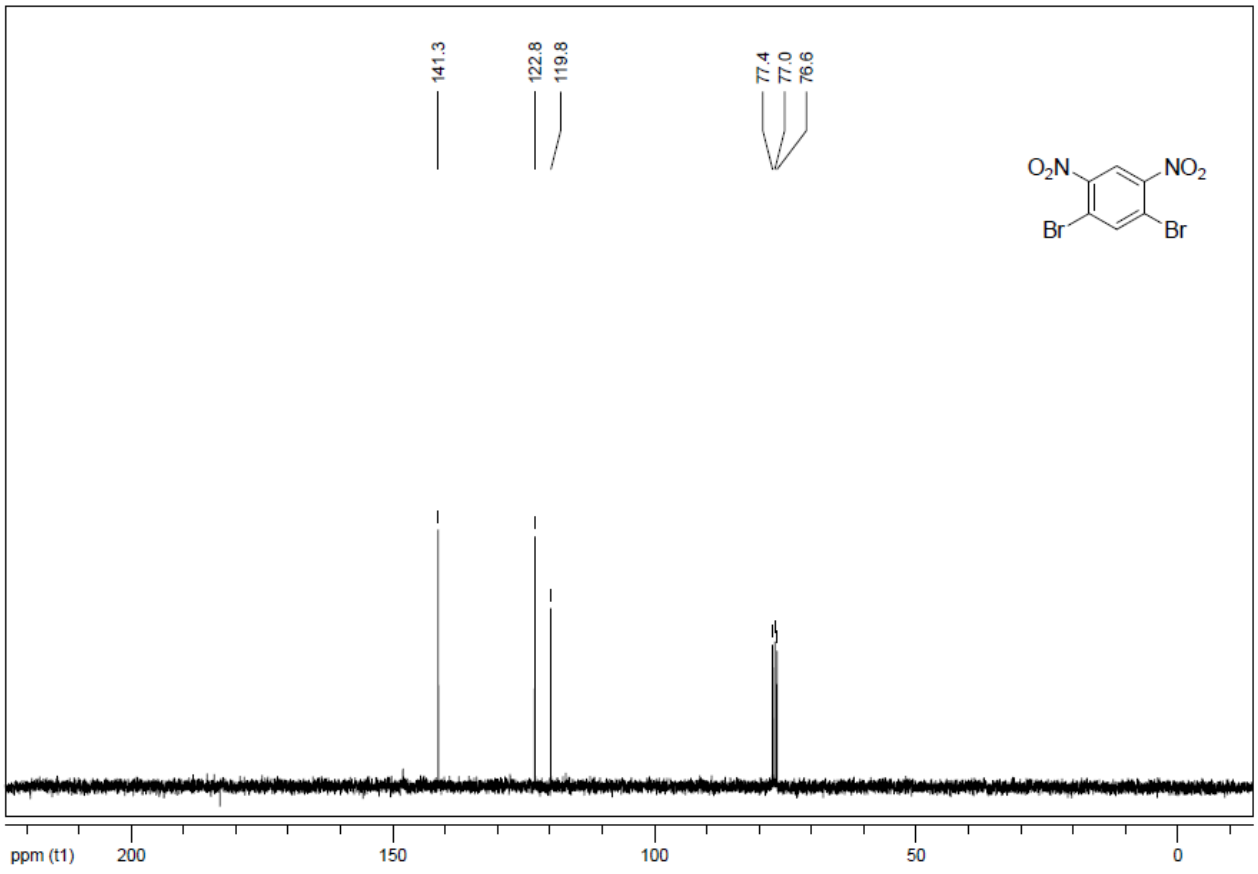
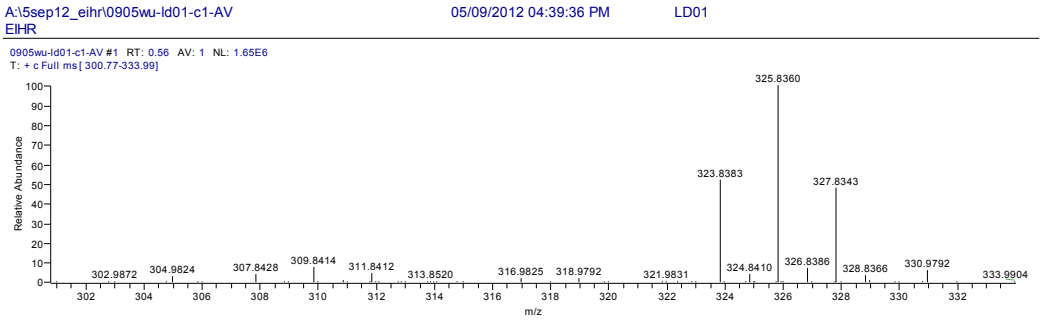


Fig. S11. ^{13}C NMR spectrum of compound **4** ($CDCl_3$, 75 MHz, rt).



0905wu-ld01-c1-AV#1 RT: 0.56
T: + c Full ms [300.77-333.99]
m/z= 323.35-328.18

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
323.8383	862073.0	52.13	323.8381	0.44	6.0	$C_6H_2O_4N_2{}^{79}Br_2$
325.8360	1653555.0	100.00	325.8361	-0.21	6.0	$C_6H_2O_4N_2{}^{79}Br_1{}^{81}Br_1$
327.8343	791568.0	47.87	327.8340	0.82	6.0	$C_6H_2O_4N_2{}^{81}Br_2$

Fig. S12. HR mass spectrum (EI) of compound **4.**

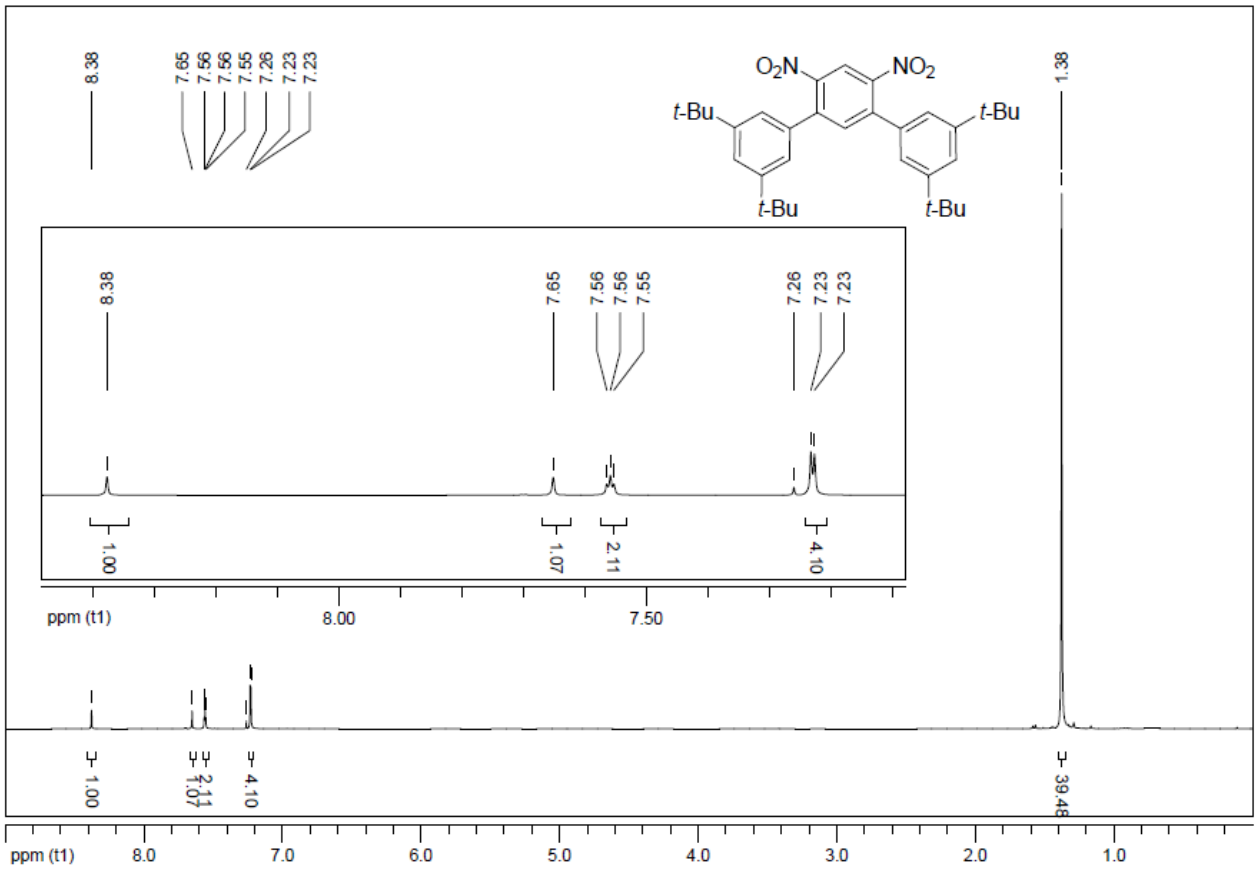


Fig. S13. ^{1}H NMR spectrum of compound **5** ($CDCl_3$, 300 MHz, rt).

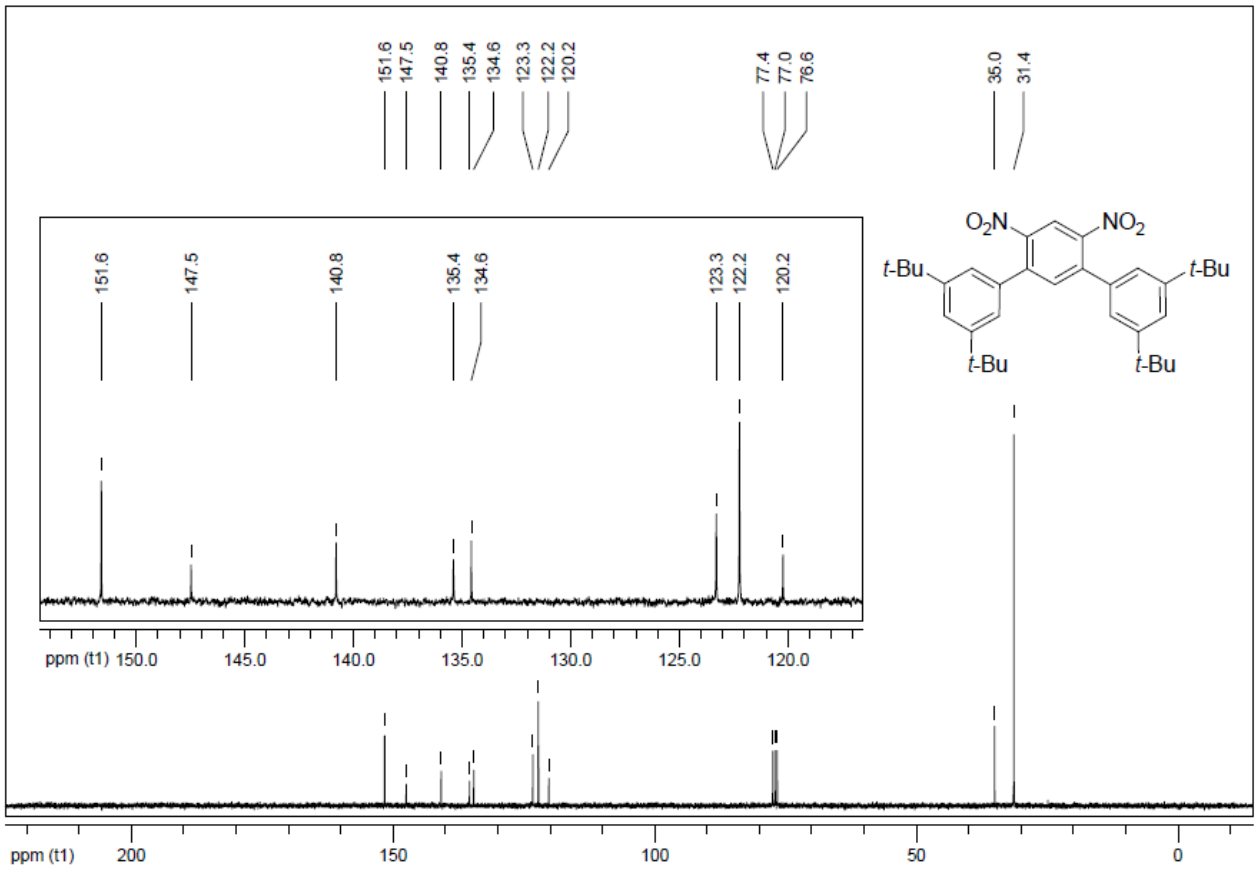
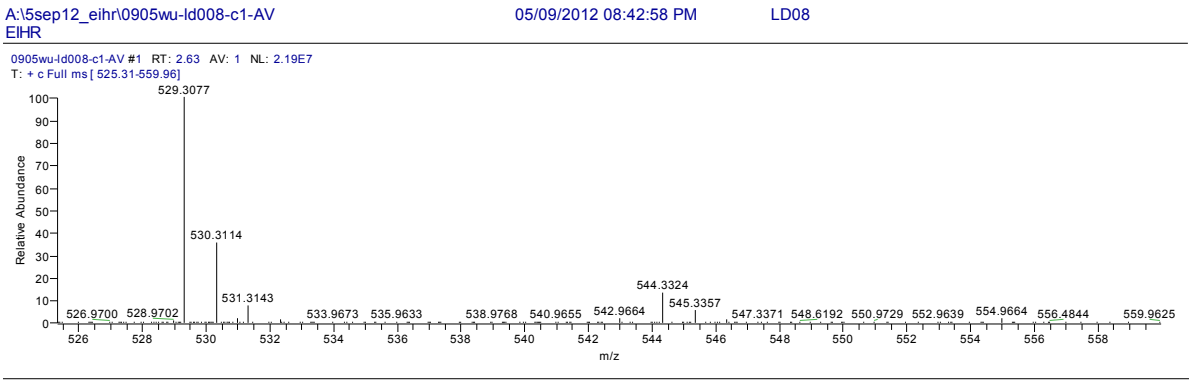


Fig. S14. ^{13}C NMR spectrum of compound **5** ($CDCl_3$, 75 MHz, rt).



0905wu-ld008-c1-AV#1 RT: 2.63
T: + c Full ms [525.31-559.96]
m/z= 544.24-544.64

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
544.3324	2918122.0	100.00	544.3341	-3.18	18.0	$C_{39}H_{44}O_2$
			544.3301	4.21	14.0	$C_{34}H_{44}O_4N_2$

Fig. S15. HR mass spectrum (EI) of compound **5.**

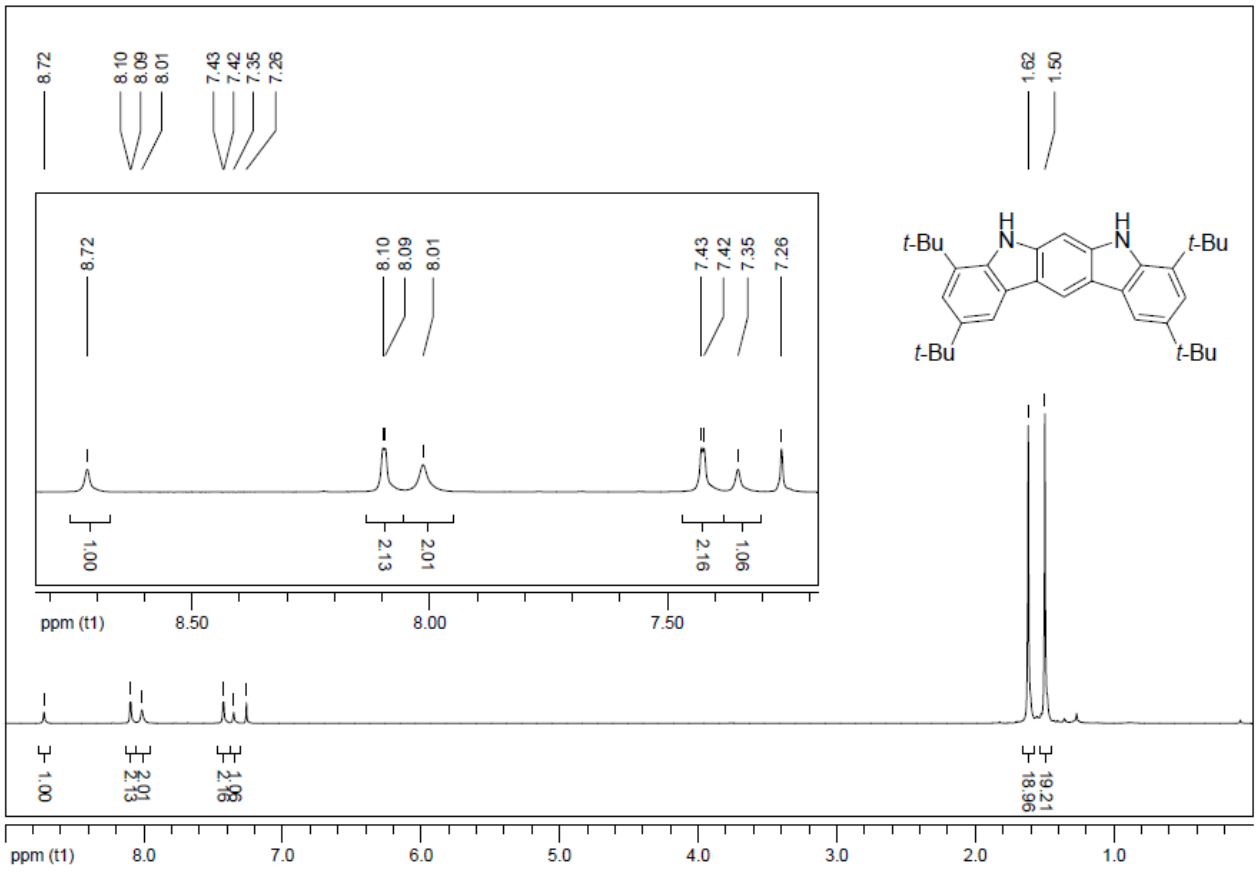


Fig. S16. ^{1}H NMR spectrum of compound **6** ($CDCl_3$, 300 MHz, rt).

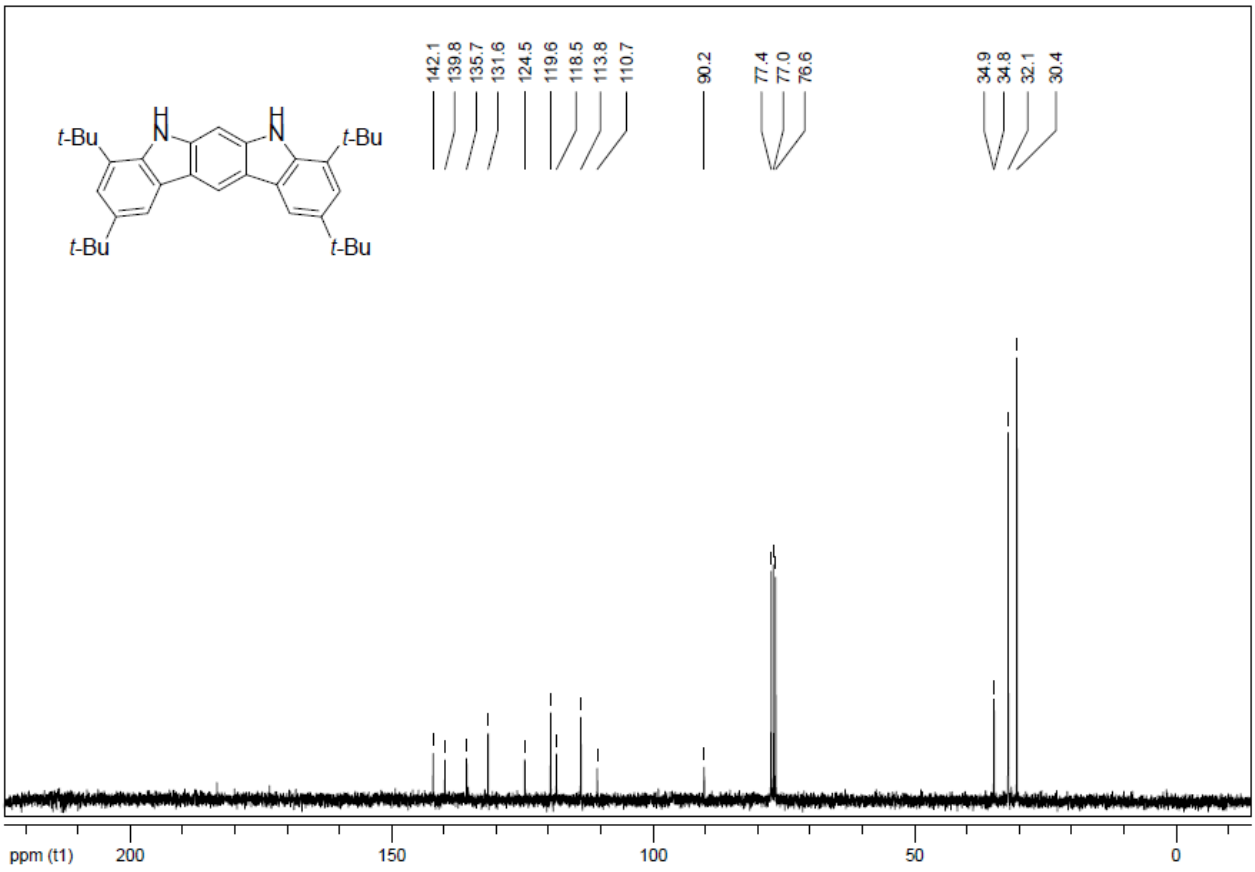
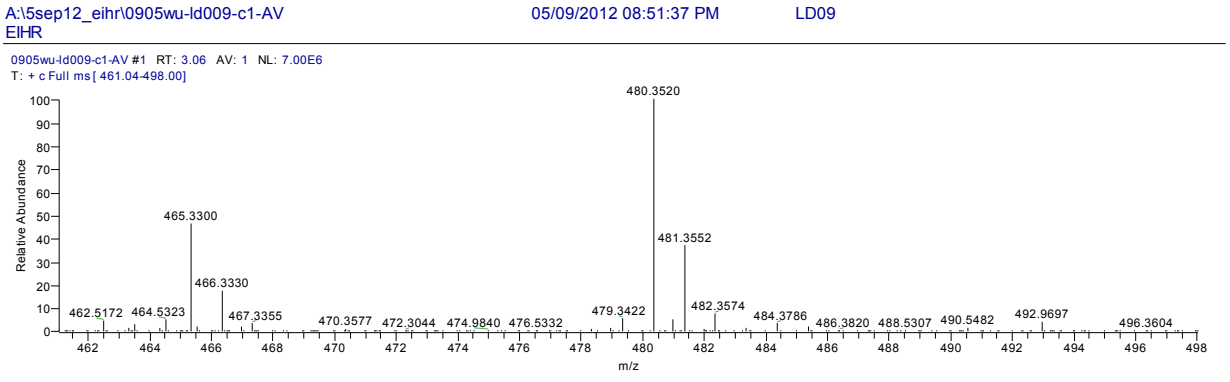


Fig. S17. ^{13}C NMR spectrum of compound **6** ($CDCl_3$, 75 MHz, rt).



0905wu-ld009-c1-AV#1 RT: 3.06
T: + c Full ms [461.04-498.00]
m/z= 480.18-480.57

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
480.3520	6999381.0	100.00	480.3504	3.30	14.0	$C_{34}H_{44}N_2$

Fig. S18. HR mass spectrum (EI) of compound **6.**

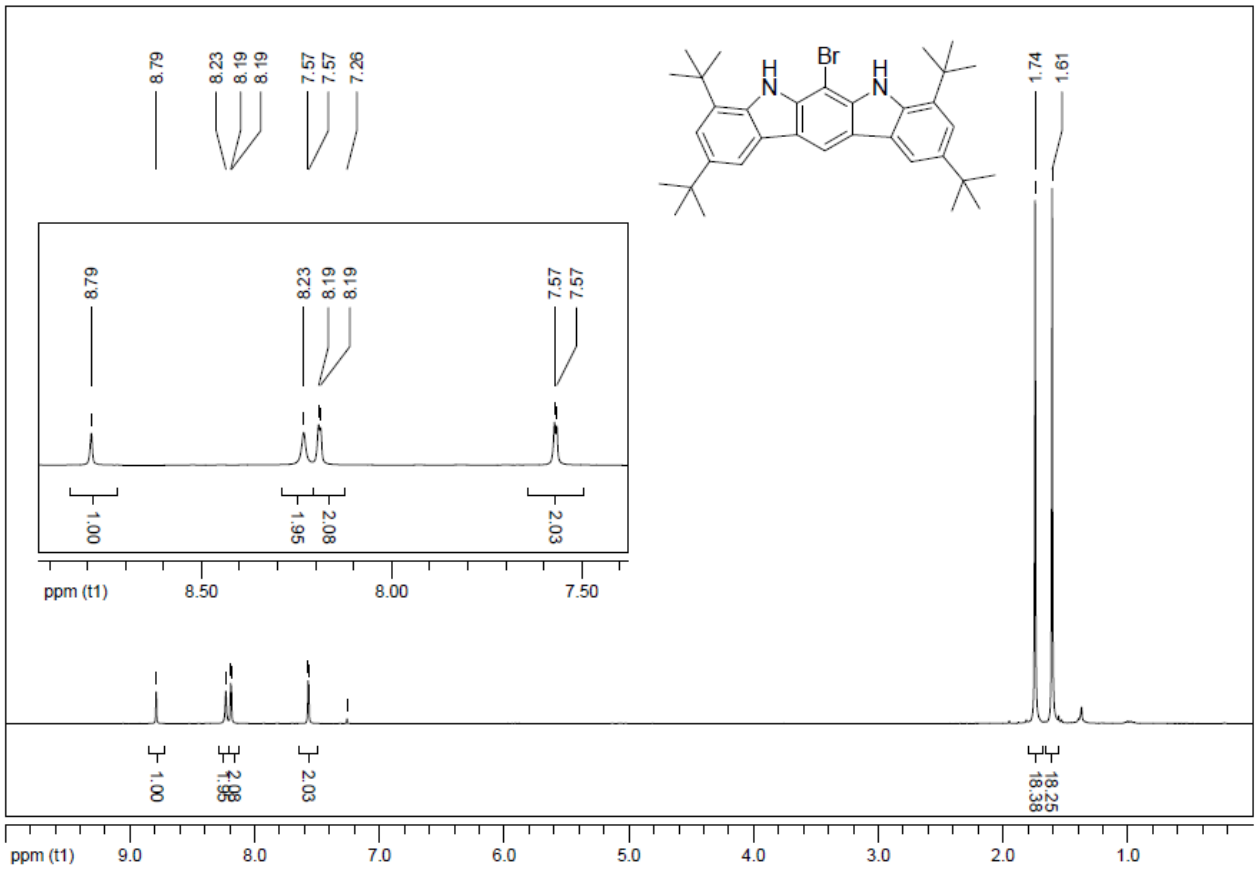


Fig. S19. ^{1}H NMR spectrum of compound **7** ($CDCl_3$, 300 MHz, rt).

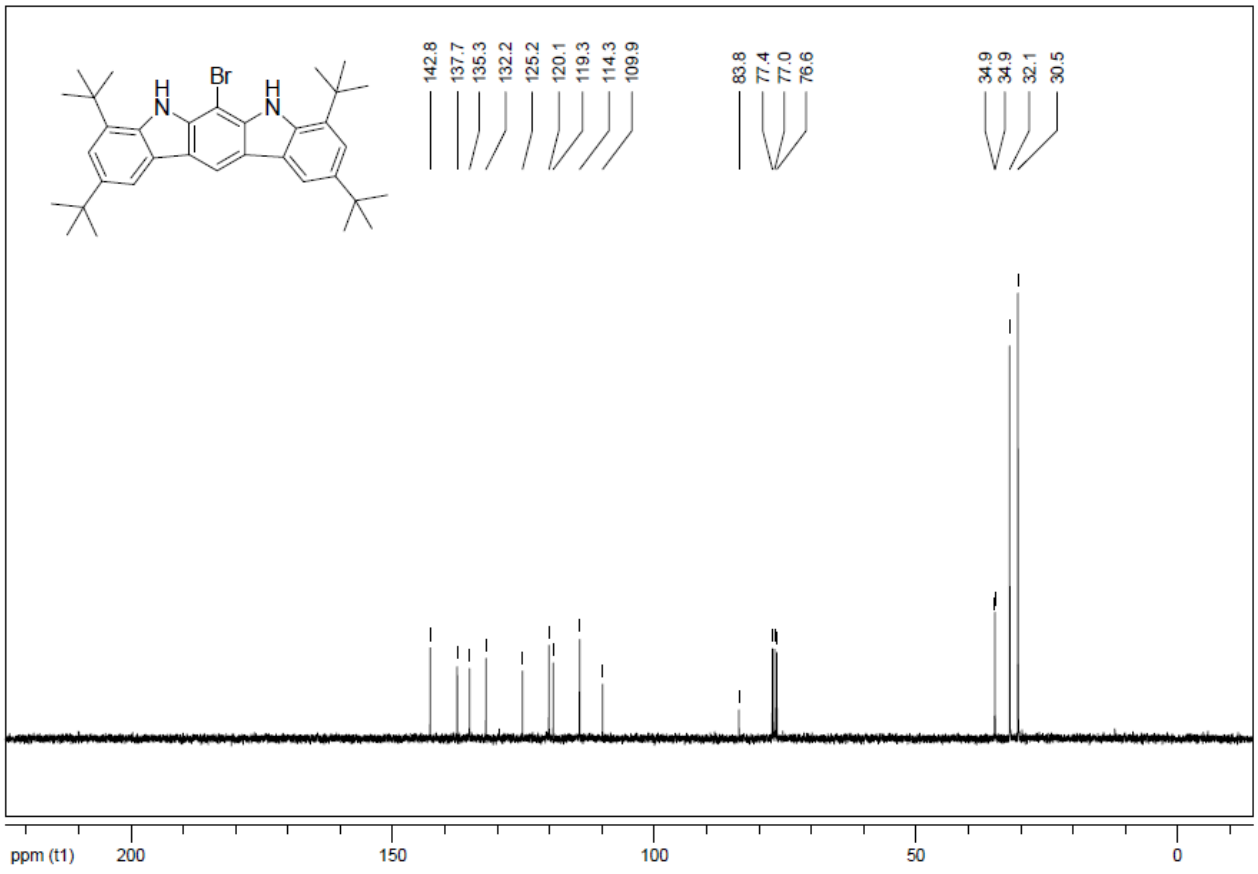
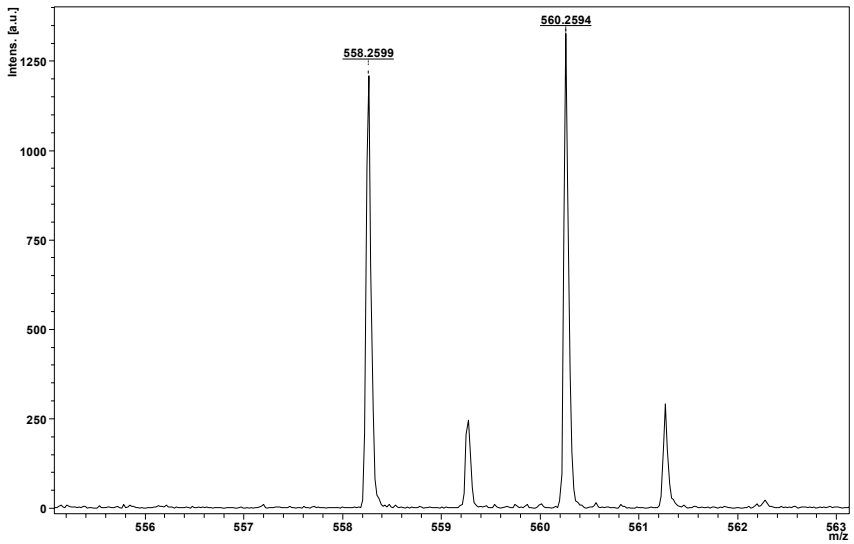


Fig. S20. ^{13}C NMR spectrum of compound **7** ($CDCl_3$, 75 MHz, rt).



Formula	Mass	Error (ppm)	DblEq	N rule	Electron Configuration
C 34 H 43 Br N 2	558.2610	1.8583	14.00	ok	odd
C 34 H 43 N 2 ^81Br	560.2589	0.8123	14.00	ok	odd

Fig. S21. HR mass spectrum MOLDI-TOF of compound **7.**

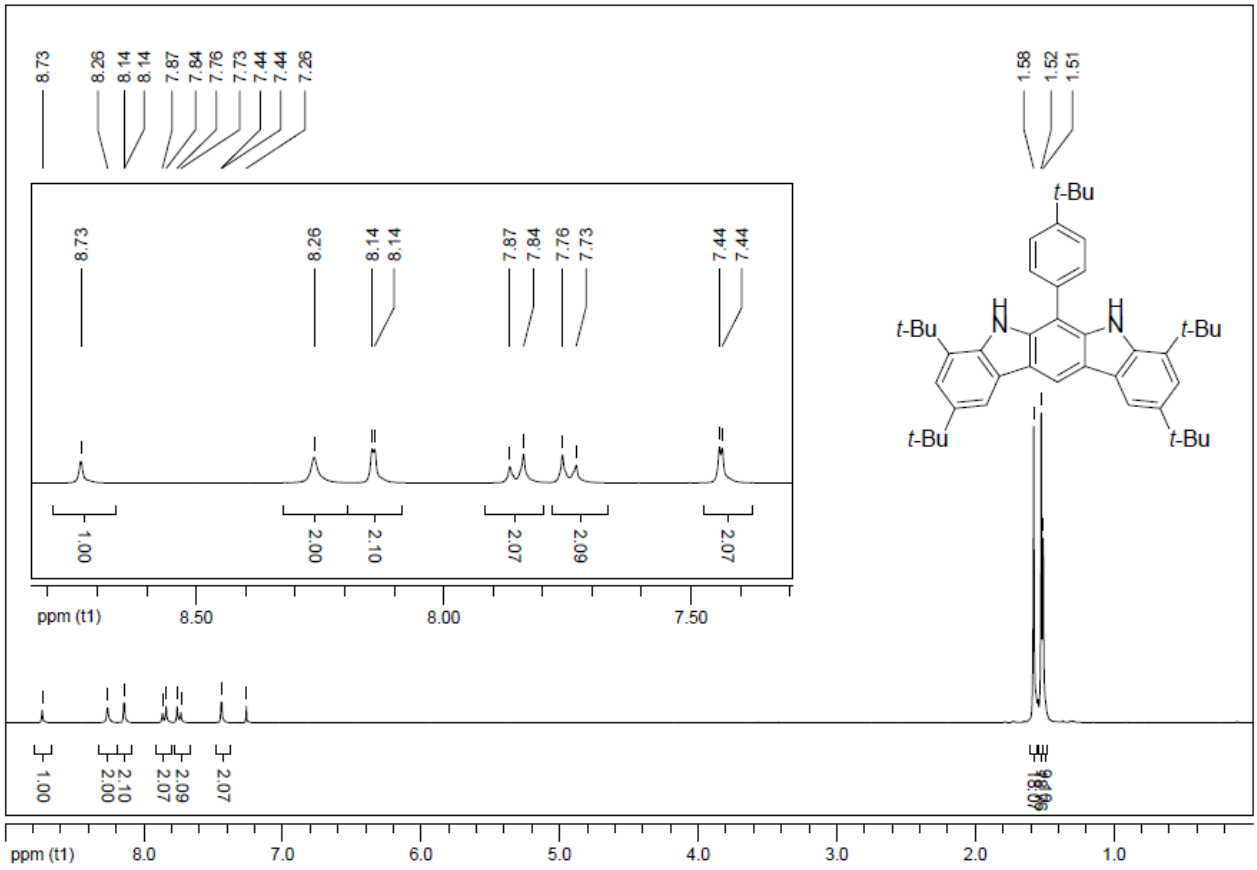


Fig. S22. ^{1}H NMR spectrum of compound **8** ($CDCl_3$, 300 MHz, rt).

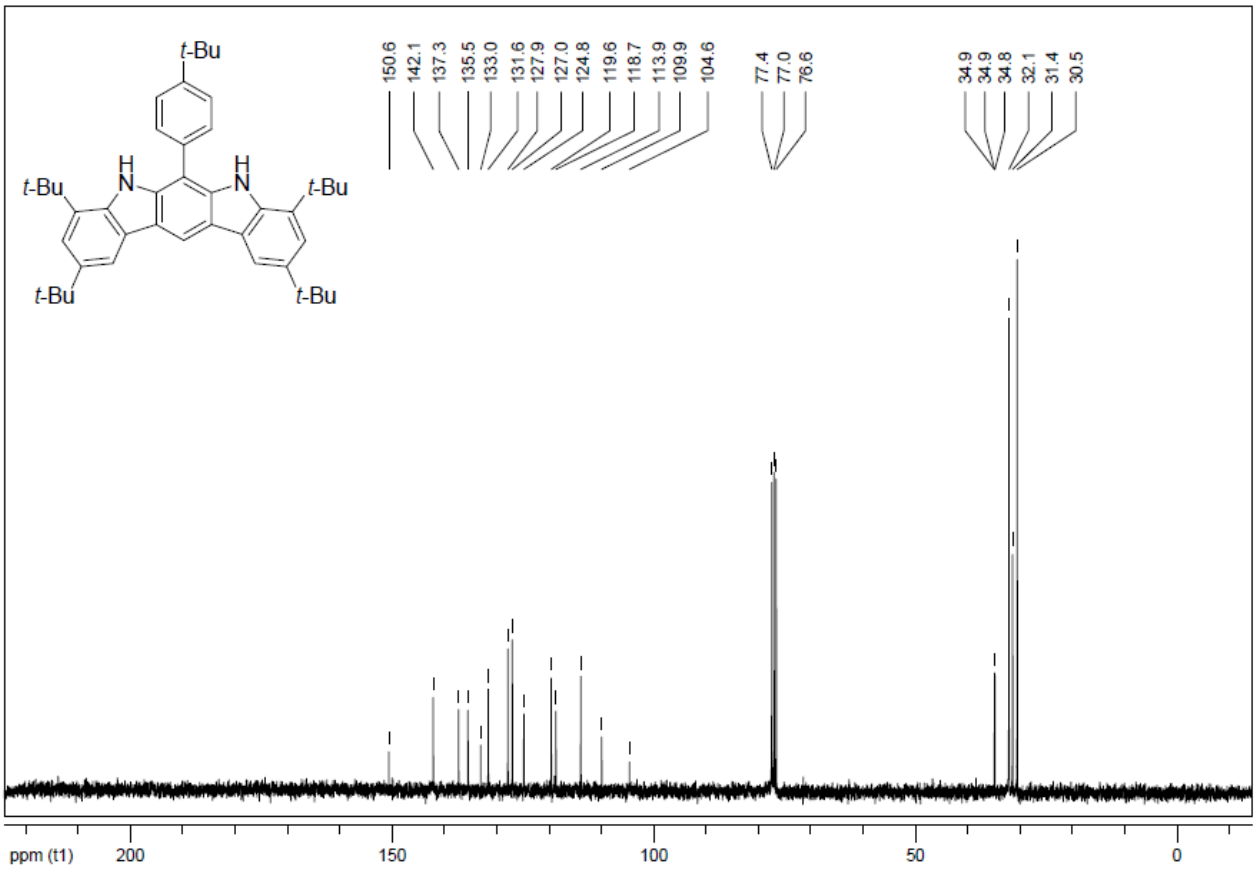
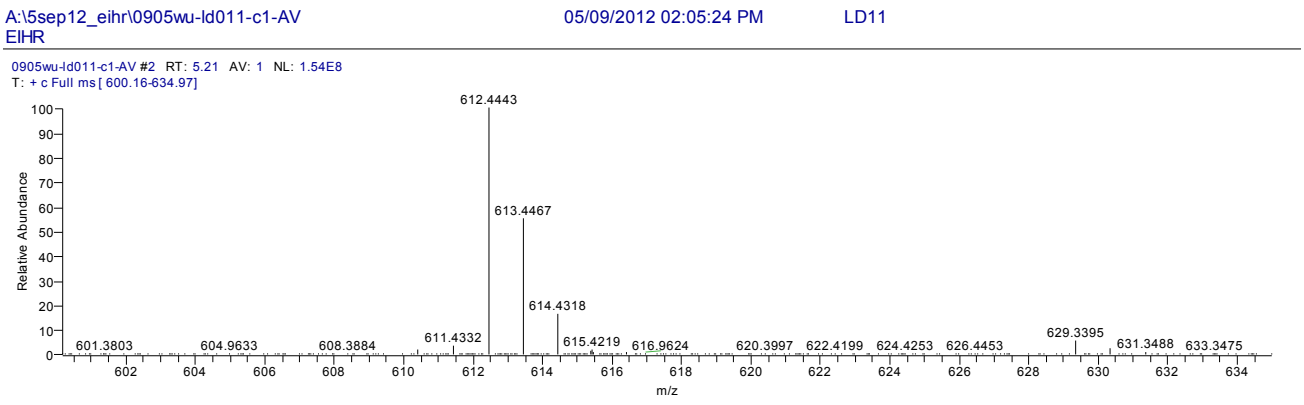


Fig. S23. ^{13}C NMR spectrum of compound **8** ($CDCl_3$, 75 MHz, rt).



0905wu-ld011-c1-AV#1 RT: 5.06
T: + c Full ms [600.04-634.97]
m/z= 612.25-612.66

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
612.4458	4875069.0	100.00	612.4444	2.32	18.0	$C_{44}H_{56}N_2$

Fig. S24. HR mass spectrum (EI) of compound **8.**

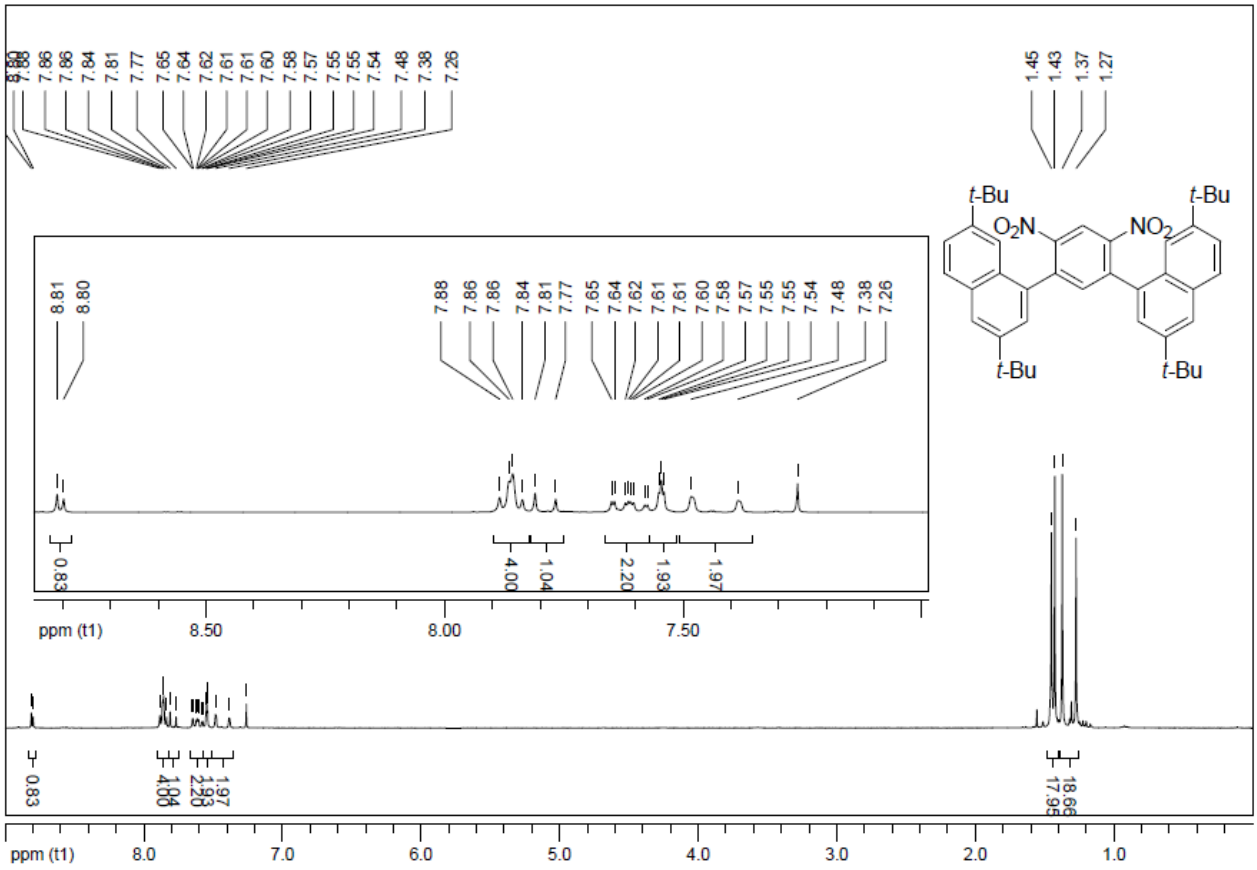


Fig. S25. ^{1}H NMR spectrum of compound **10** ($CDCl_3$, 300 MHz, rt).

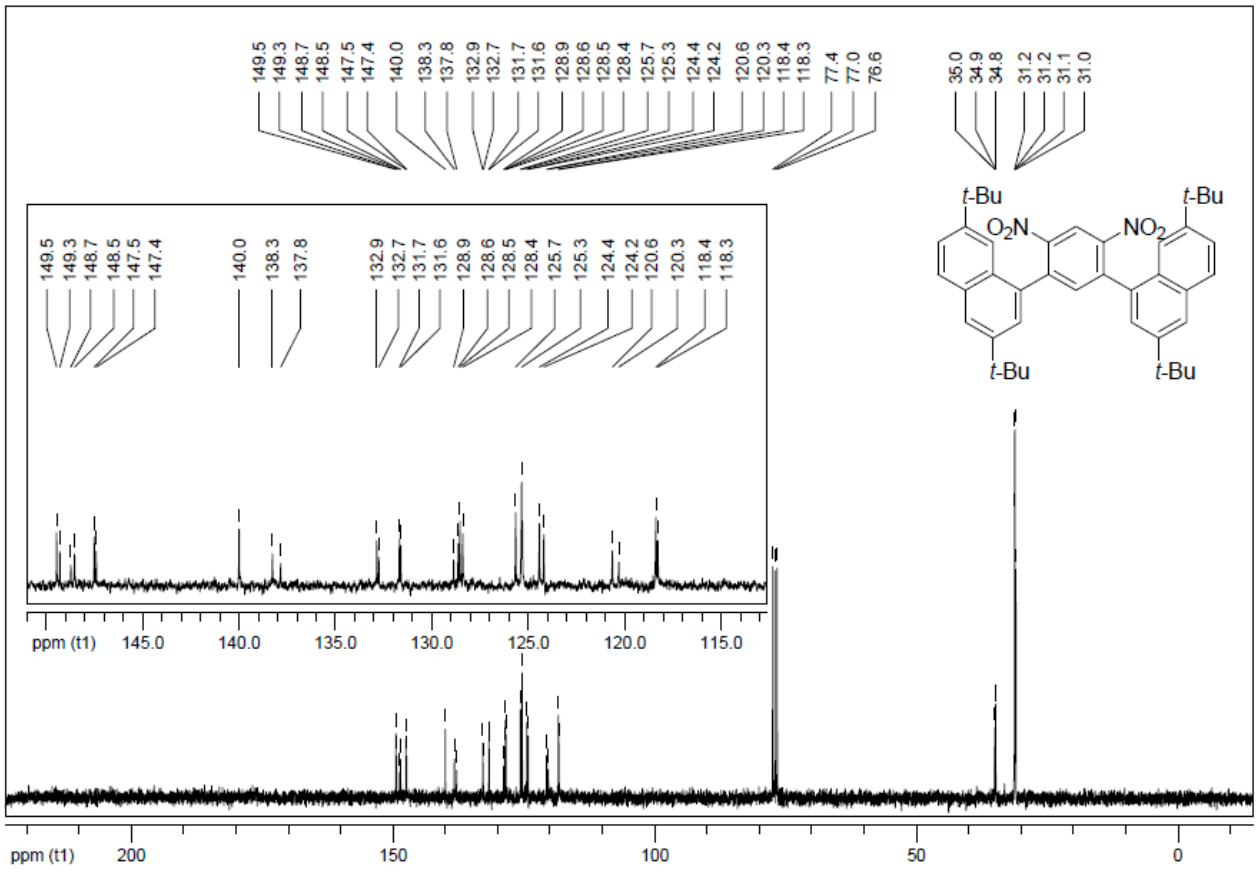
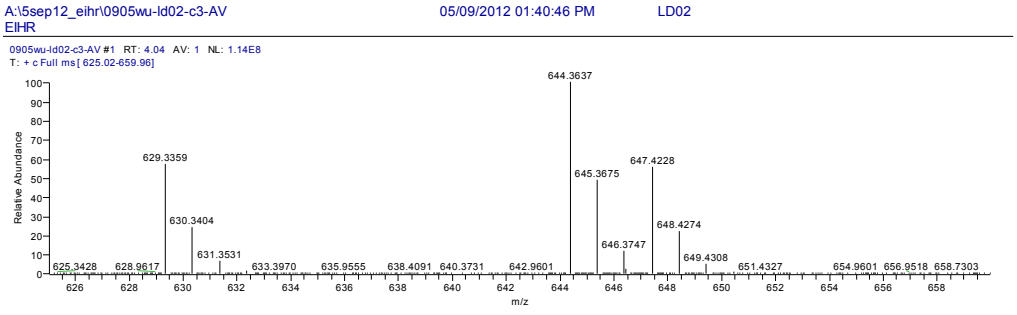


Fig. S26. ^{13}C NMR spectrum of compound **10** ($CDCl_3$, 75 MHz, rt).



0905wu-ld02-c3-AV#1 RT: 4.04
T: + c Full ms [625.02-659.96]
m/z= 644.09-644.77

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
644.3637	113663744.0	100.00	644.3654	-2.63	24.0	$C_{47}H_{48}O_2$
			644.3614	3.62	20.0	$C_{42}H_{48}O_4N_2$

Fig. S27. HR mass spectrum (EI) of compound **10**.

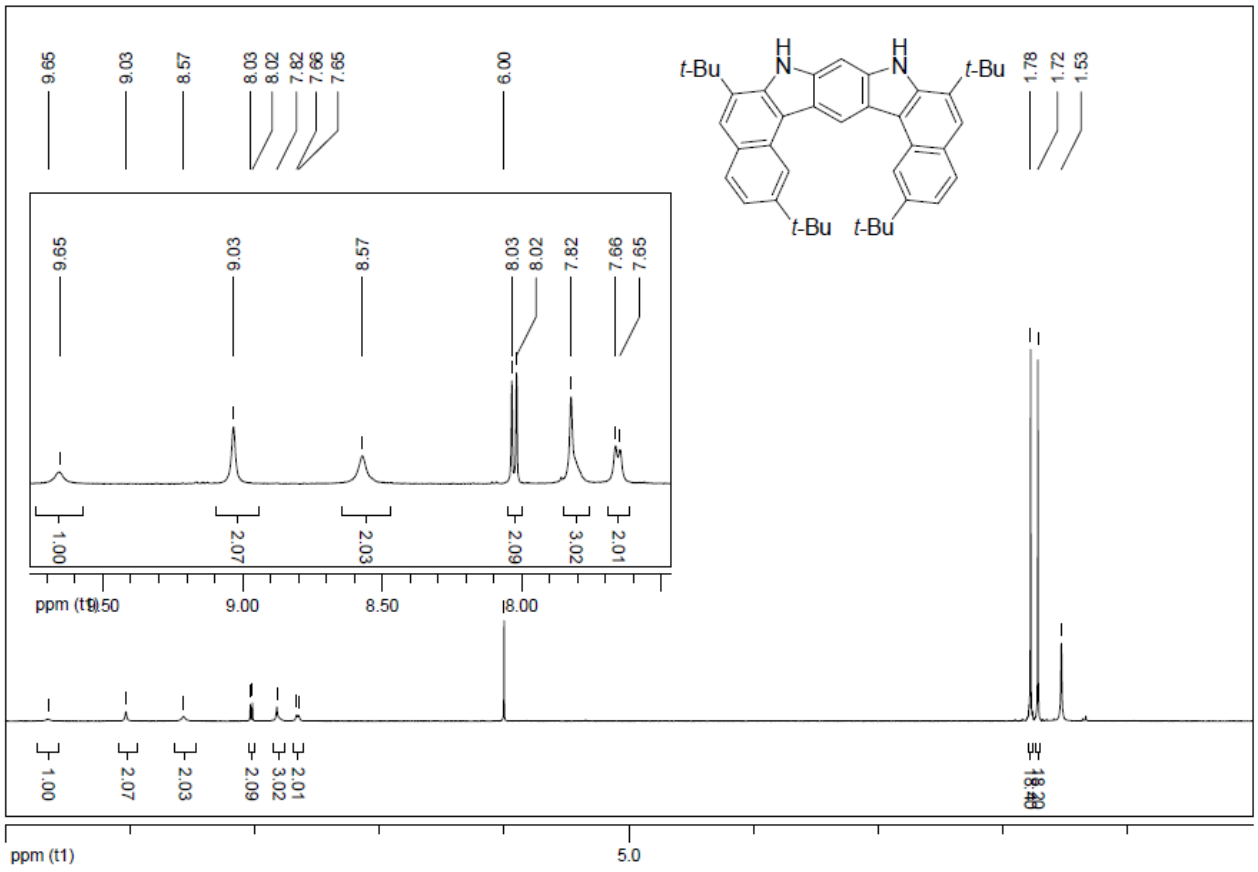


Fig. S28. ^{1}H NMR spectrum of compound **11** (1,1,2,2-tetrachloroethane-d^2, 500 MHz, 80 °C).

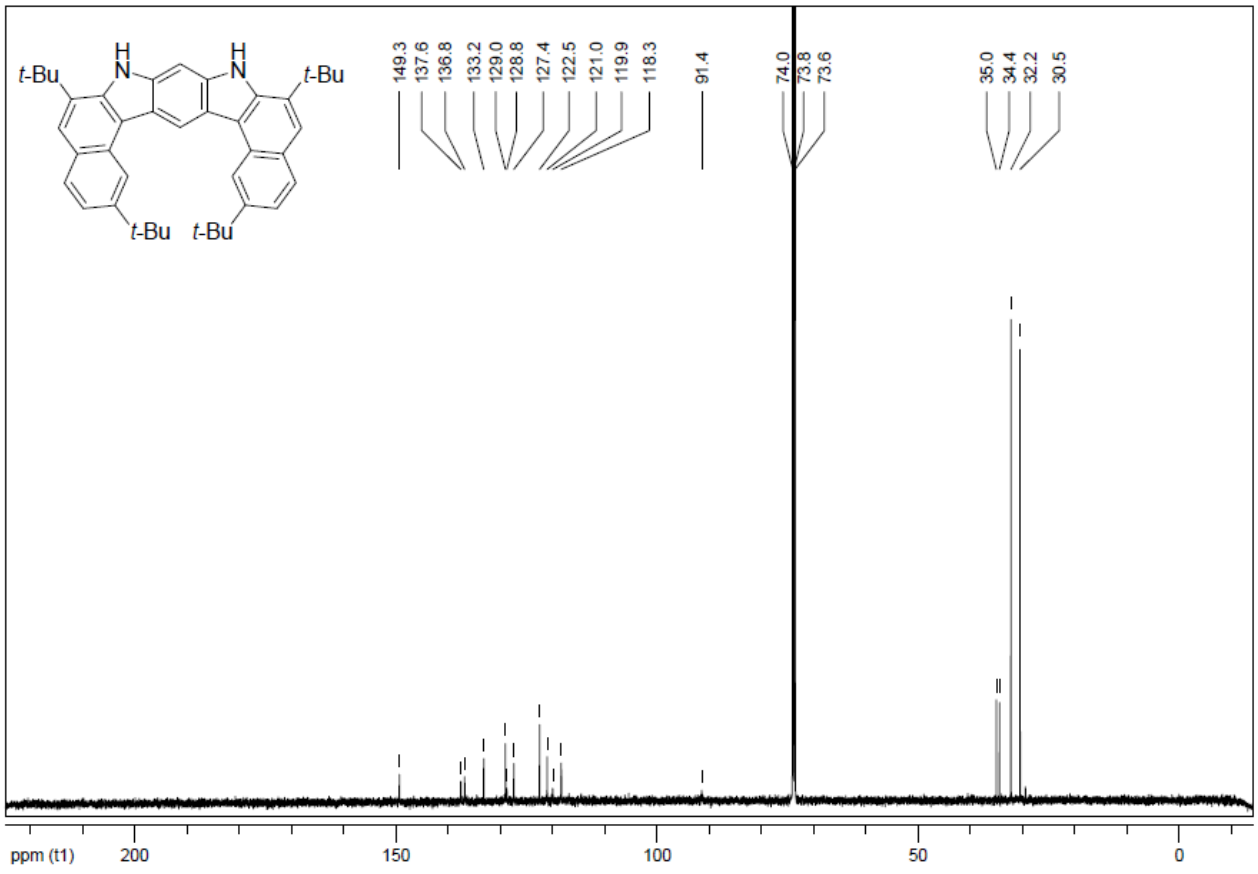
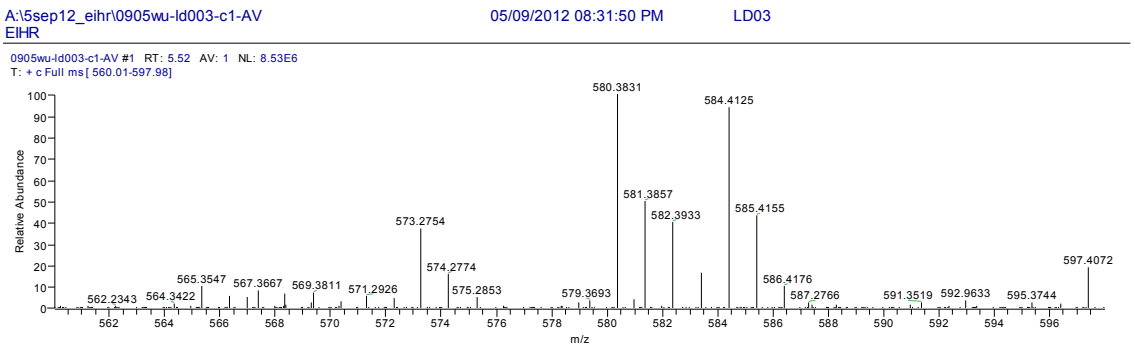


Fig. S29. ^{13}C NMR spectrum of compound **11** (1,1,2,2-tetrachloroethane-d^2, 125 MHz, 80 °C).



0905wu-ld003-c1-AV#1 RT: 5.52
T: + c Full ms [560.01-597.98]
m/z= 580.12-580.56

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
580.3831	8527360.0	100.00	580.3817	2.38	20.0	C 42 H 48 N 2

Fig. S30. HR mass spectrum (EI) of compound **11.**

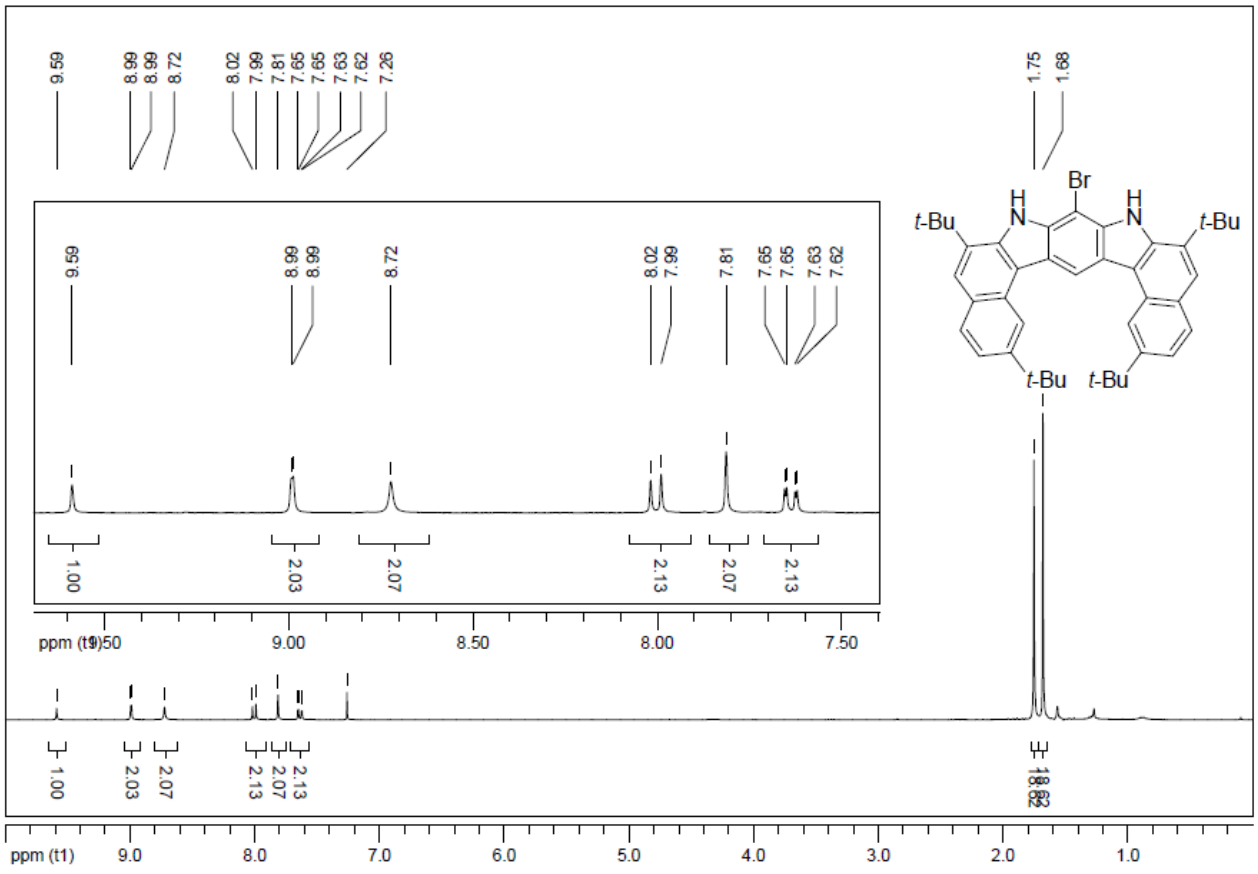


Fig. S31. ^{1}H NMR spectrum of compound **14** ($CDCl_3$, 300 MHz, rt).

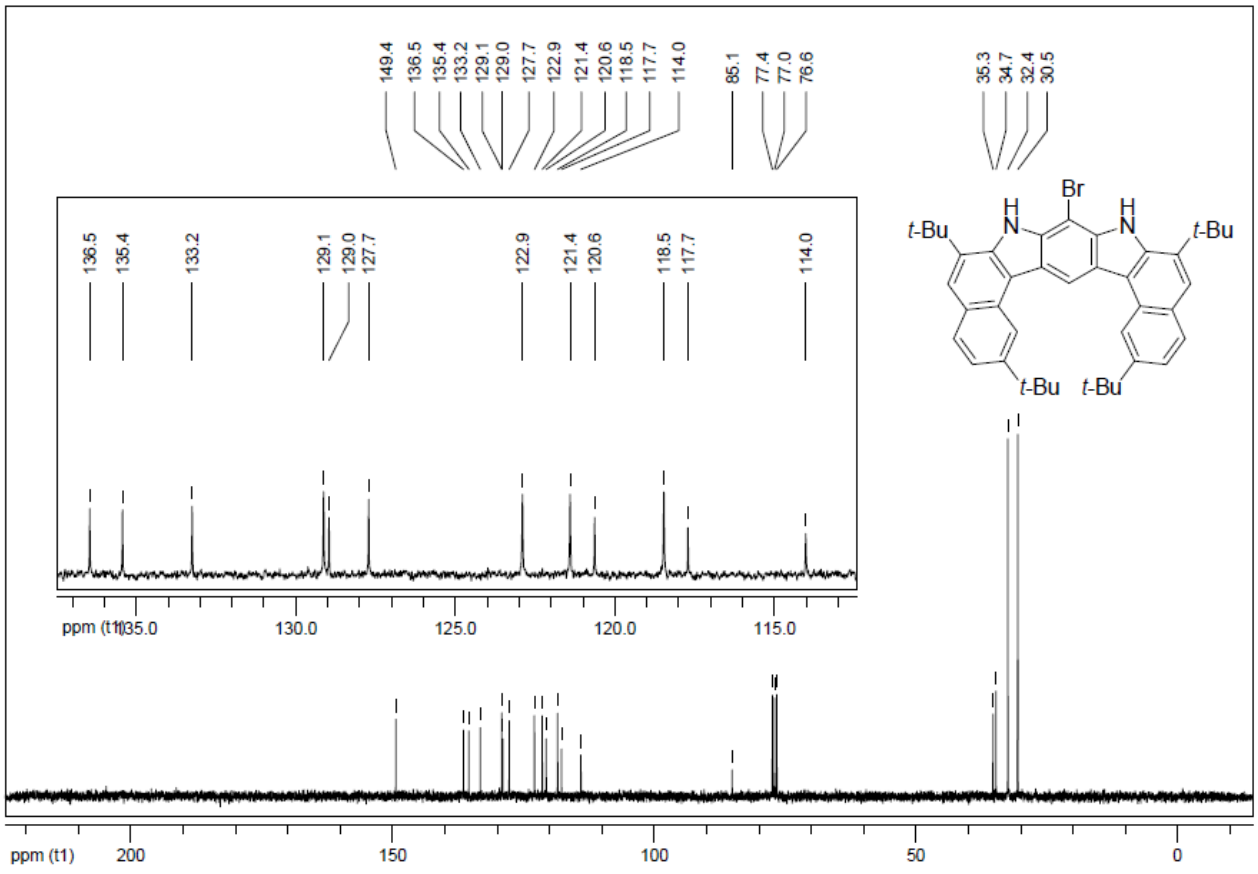
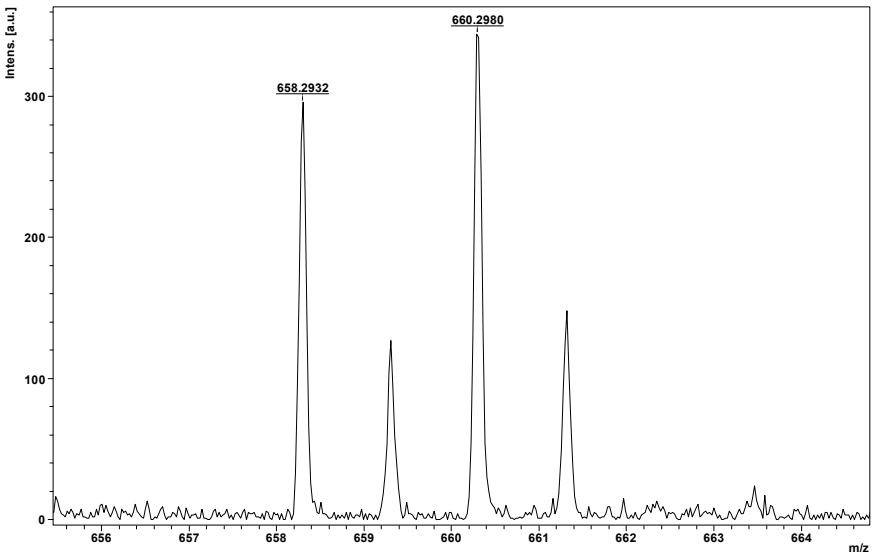


Fig. S32. ^{13}C NMR spectrum of compound **14** ($CDCl_3$, 75 MHz, rt).



Formula	Mass	Error (ppm)	DblEq	N rule	Electron Configuration
C 42 H 47 Br N 2	658.2917	2.2042	20.00	ok	odd
C 42 H 47 N 2 ^81Br	660.2897	12.6912	20.00	ok	odd

Fig. S33. HR mass spectrum (MOLDI-TOF) of compound **14.**

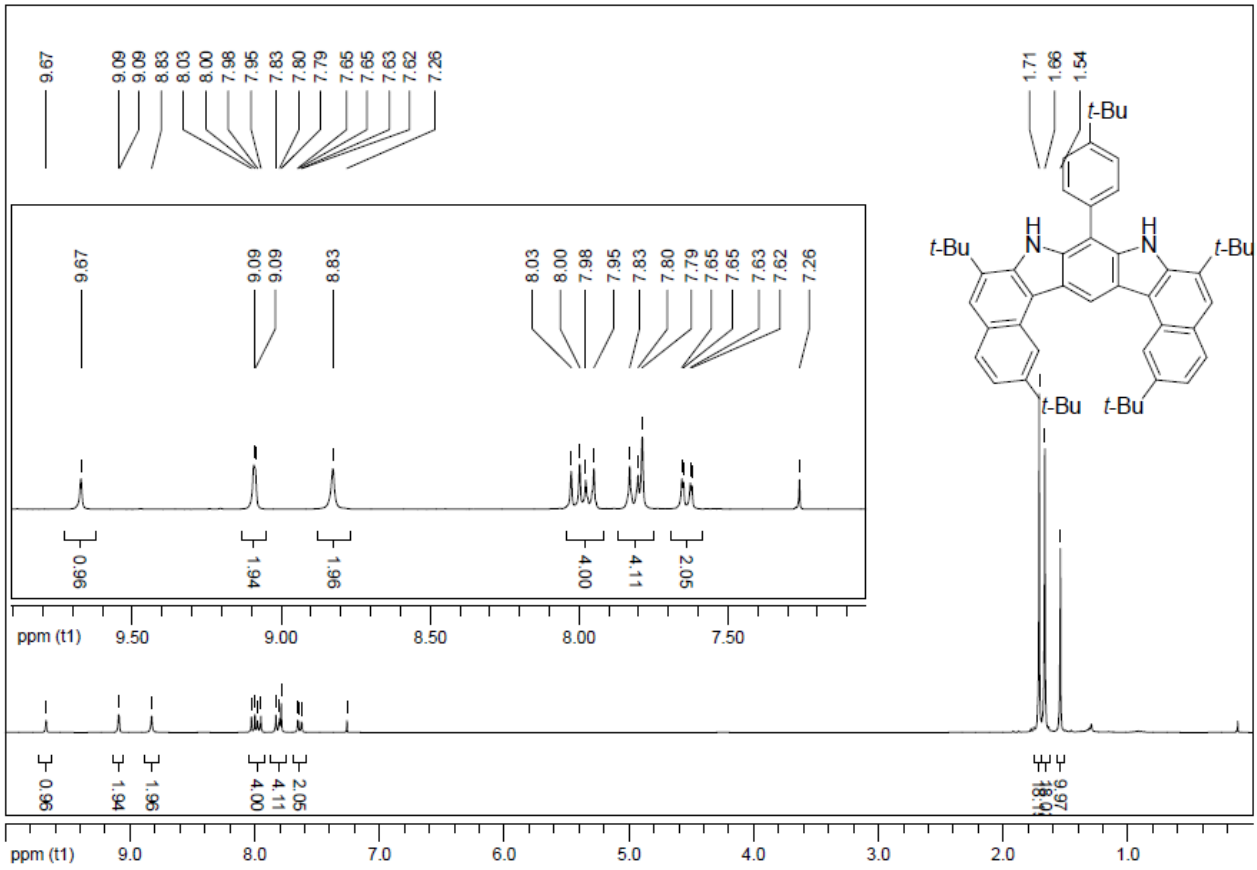


Fig. S34. ^{1}H NMR spectrum of compound **15** ($CDCl_3$, 300 MHz, rt).

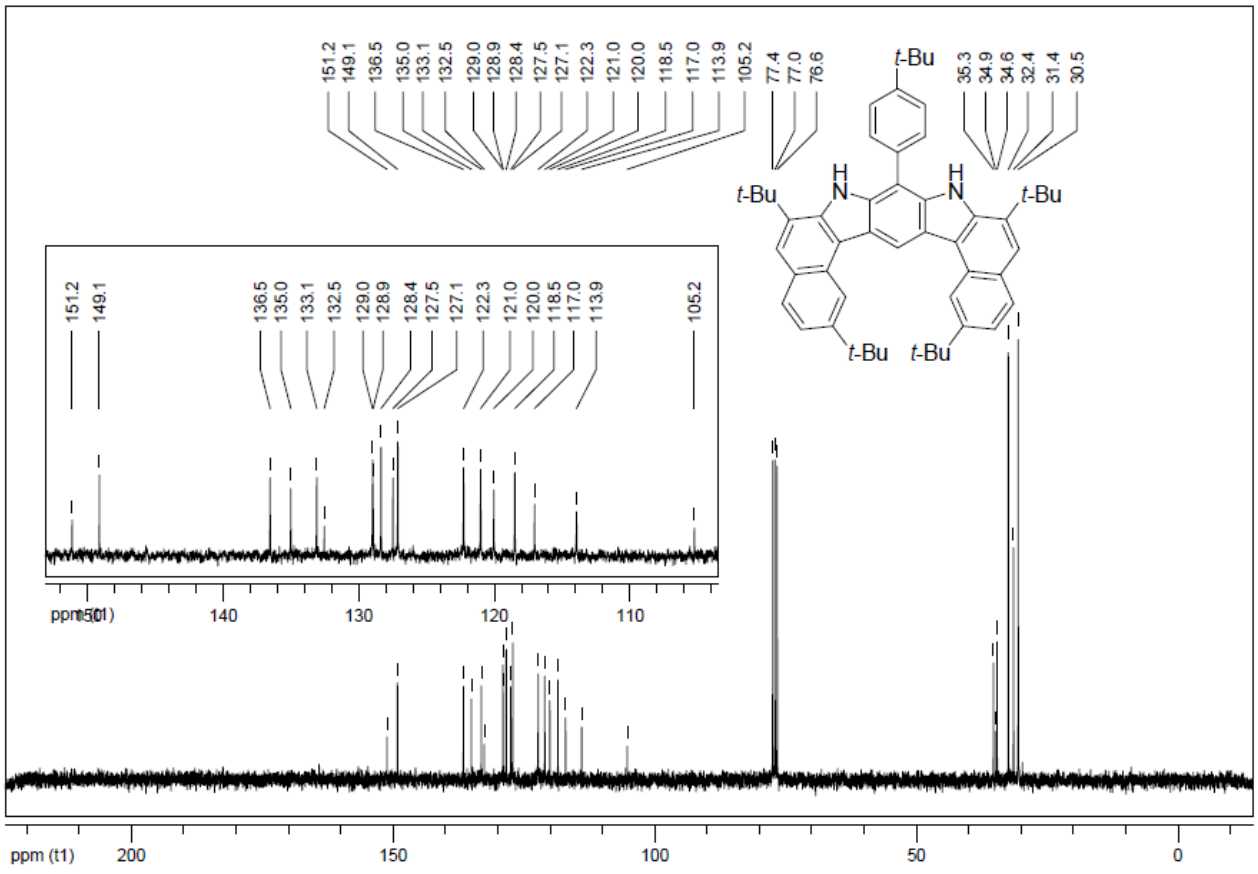
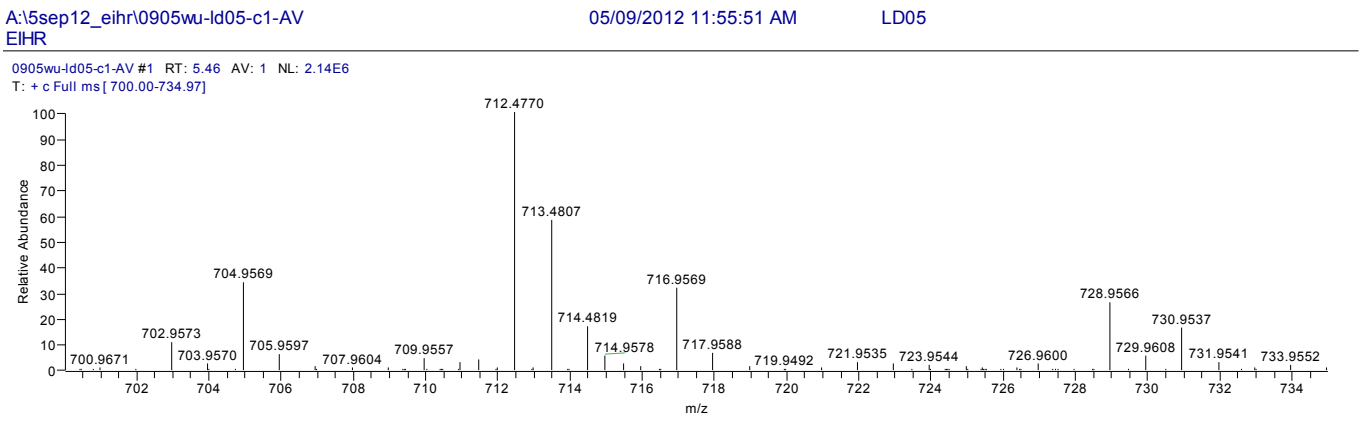


Fig. S35. ^{13}C NMR spectrum of compound **15** ($CDCl_3$, 75 MHz, rt).



0905wu-ld05-c1-AV#1 RT: 5.46
T: + c Full ms [700.00-734.97]
m/z= 712.19-712.70

m/z	Intensity	Relative	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
712.4770	2141363.0	100.00	712.4757	1.84	24.0	$C_{52}H_{60}N_2$

Fig. S36. HR mass spectrum (EI) of compound **15**.

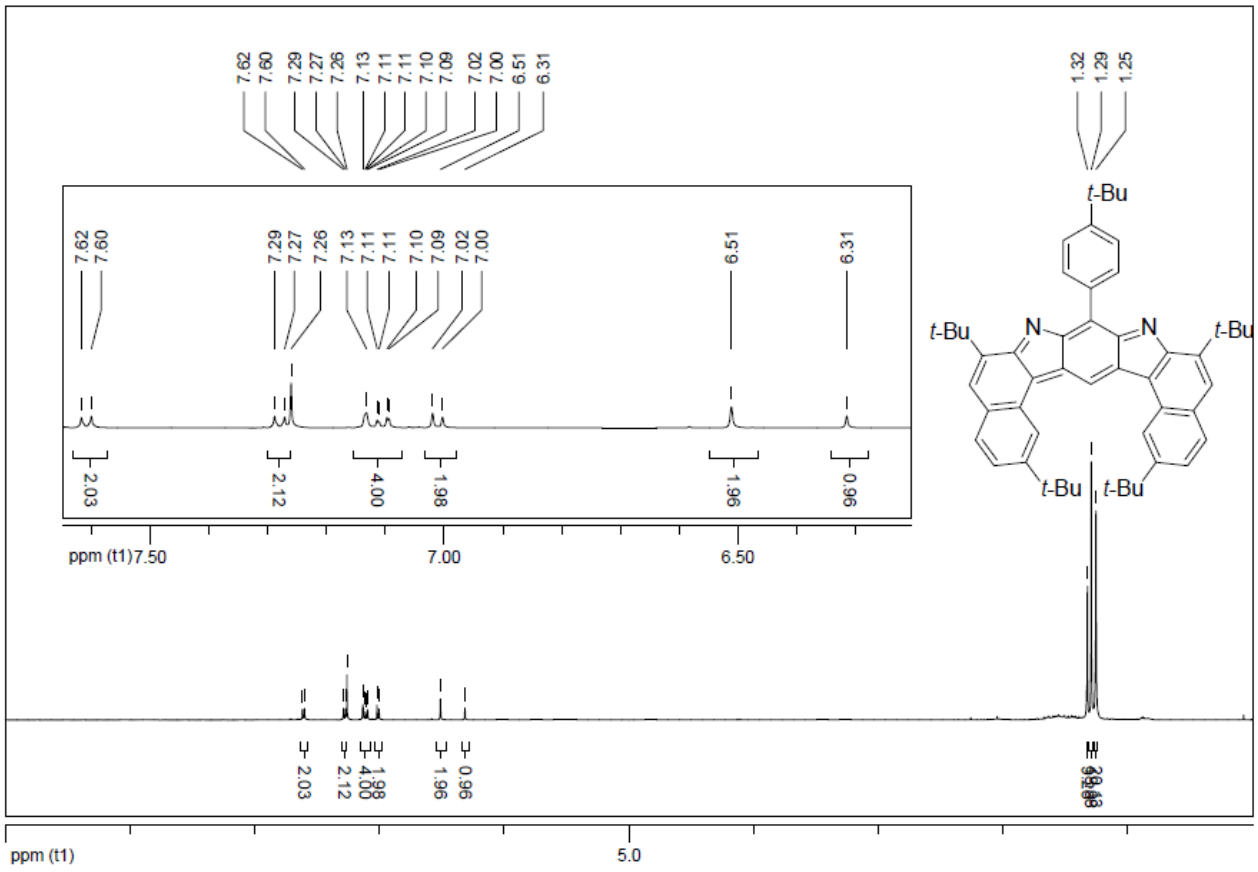


Fig. S37. ^{1}H NMR spectrum of compound **2** ($CDCl_3$, 500 MHz, rt).

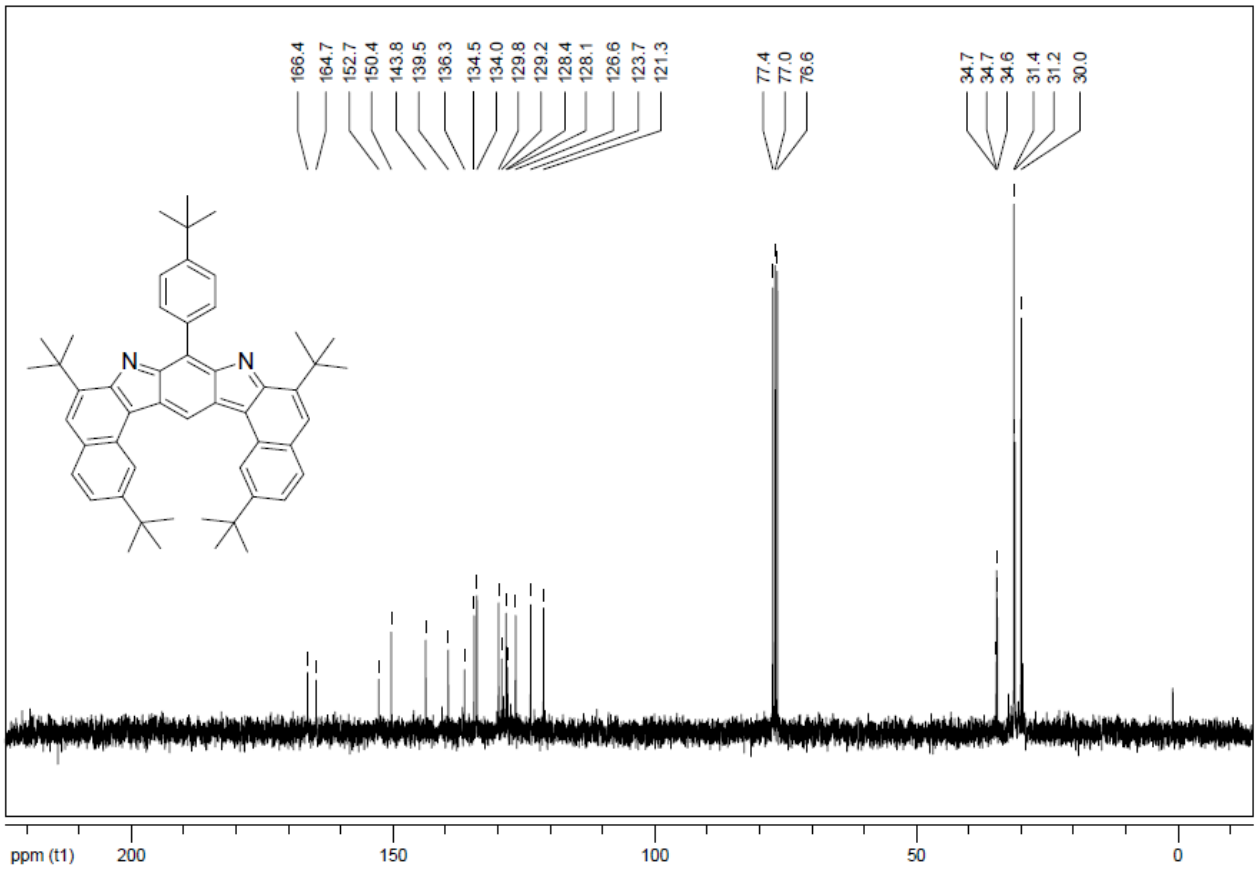


Fig. S38. ^{13}C NMR spectrum of compound **2** ($CDCl_3$, 75 MHz, rt).

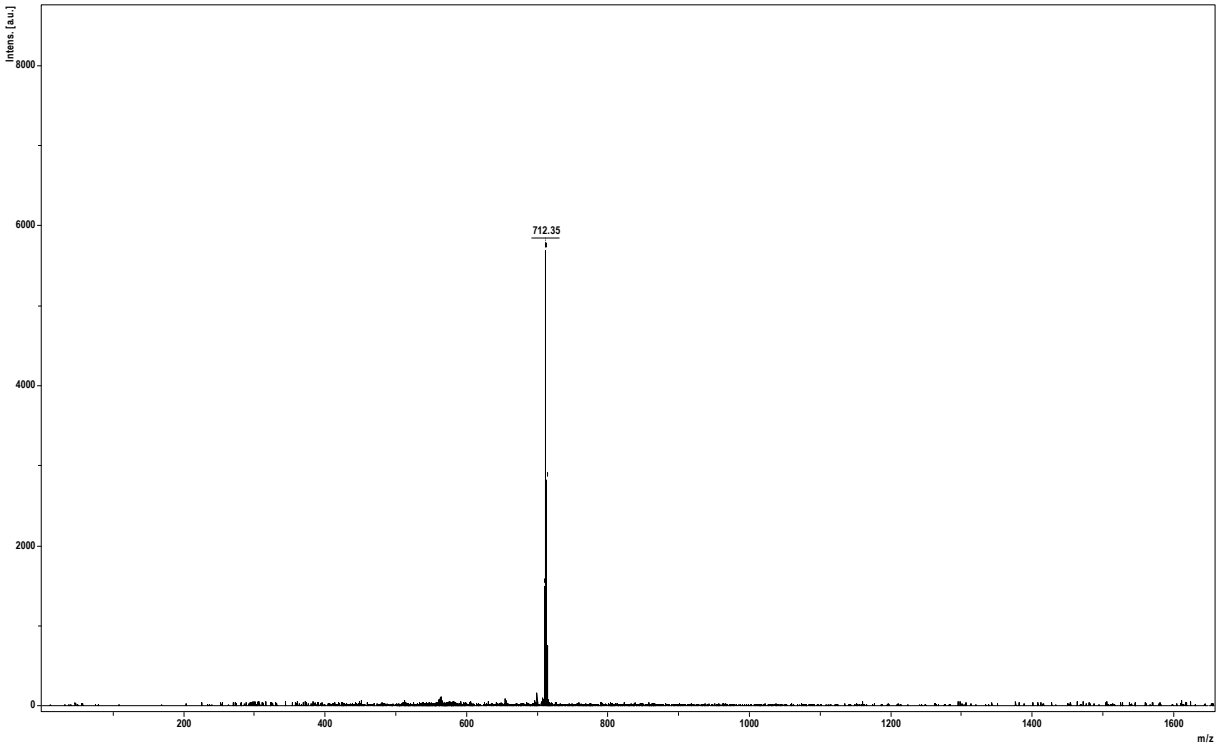


Fig. S39. MALDI-TOF mass spectrum of compound **2** (M+2H).

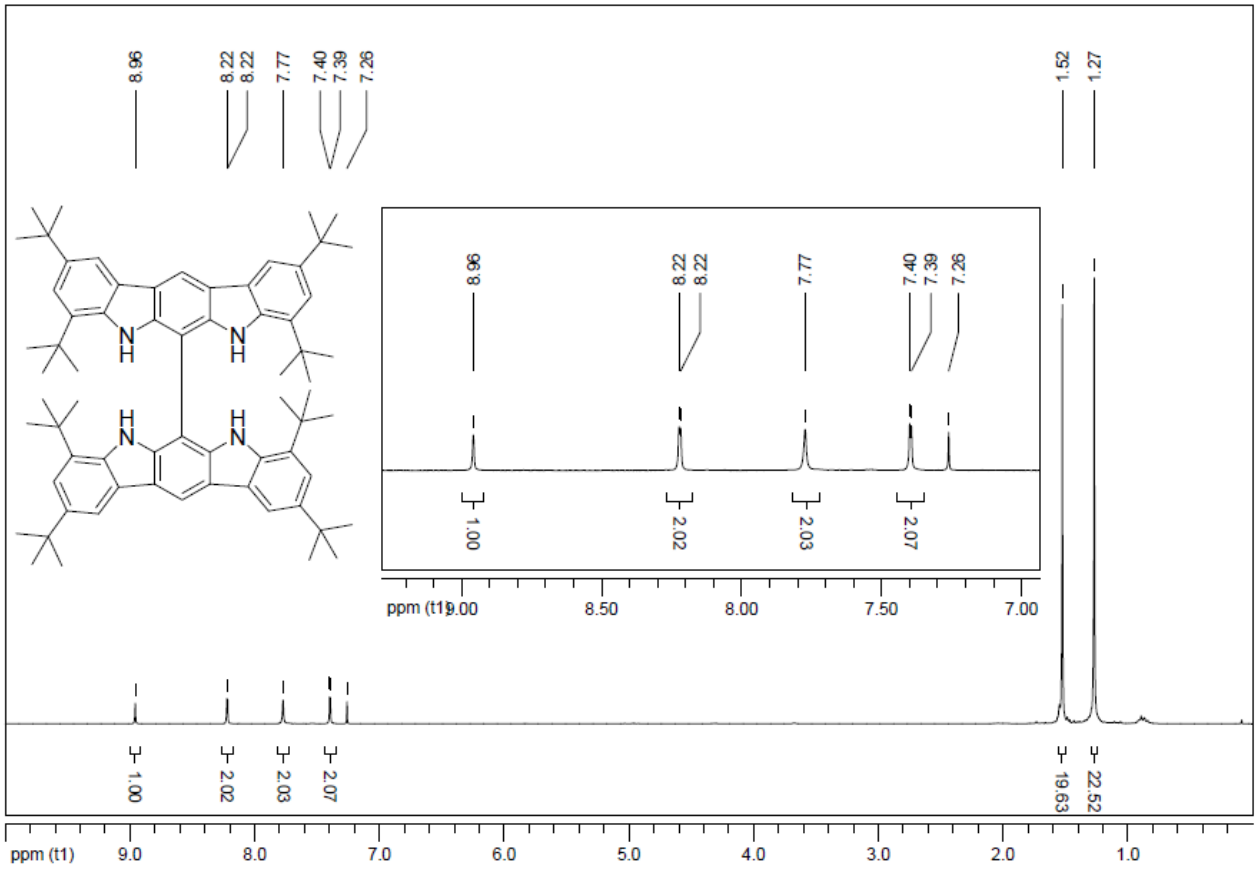


Fig. S40. ^{1}H NMR spectrum of compound **16** ($CDCl_3$, 300 MHz, rt).

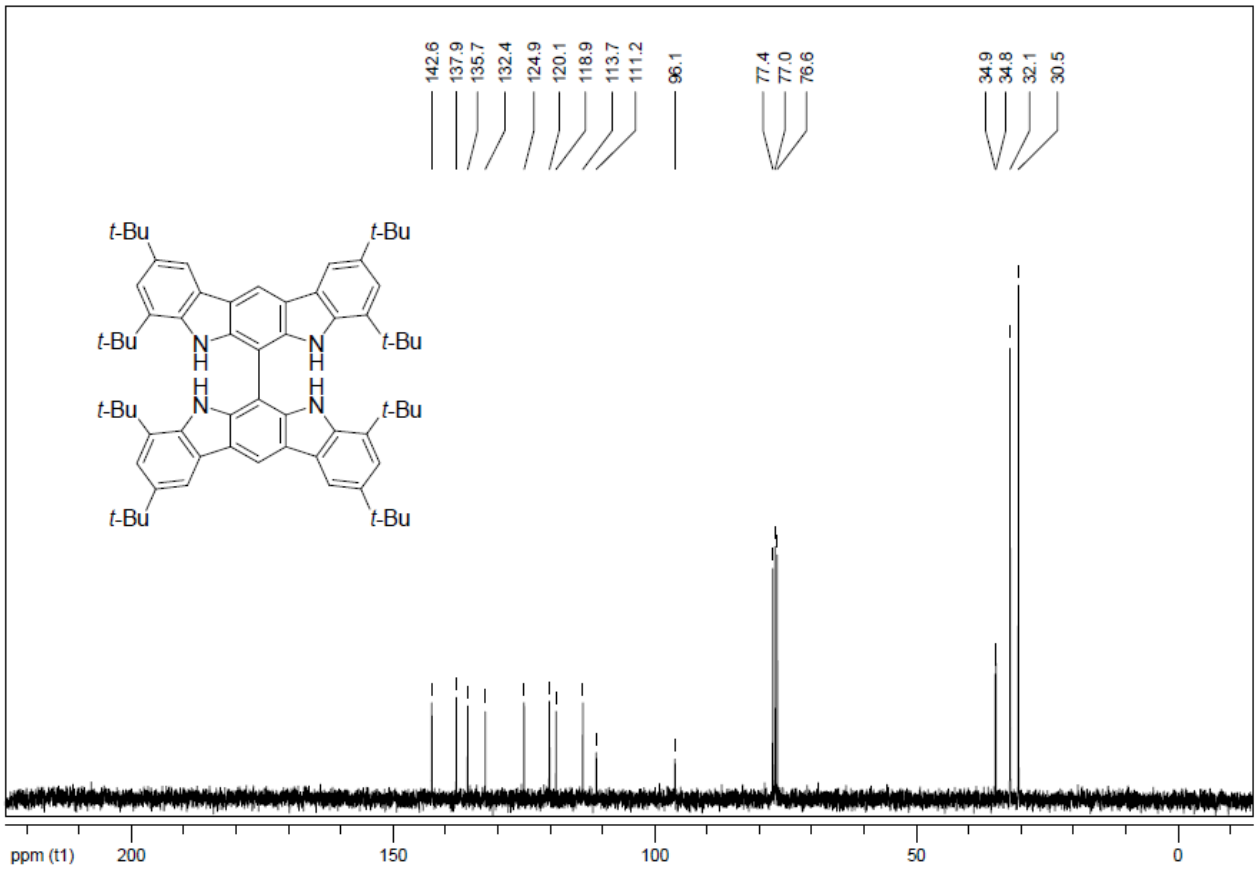
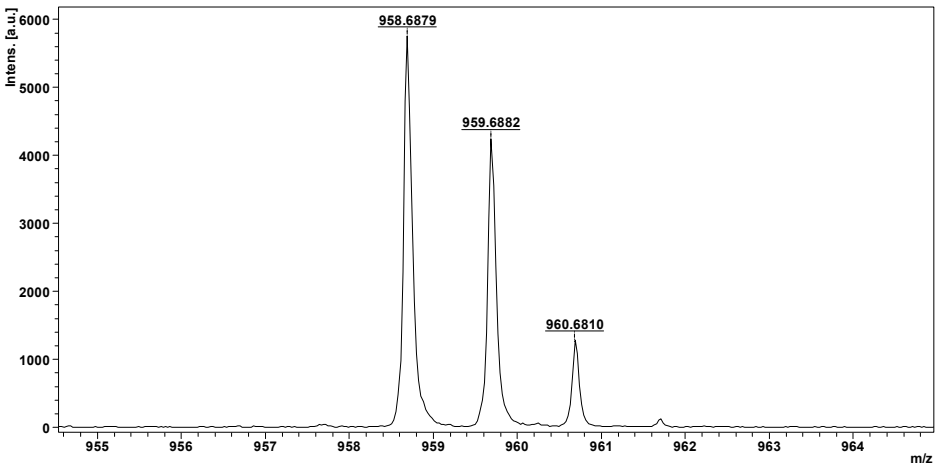


Fig. S41. ^{13}C NMR spectrum of compound **16** ($CDCl_3$, 75 MHz, rt).



Formula	Mass	Error (ppm)	DblEq	N rule	Electron Configuration
C 68 H 86 N 4	958.6852	2.7739	28.00	ok	odd

Fig. S42. HR mass spectrum (MOLDI-TOF) of compound **16.**

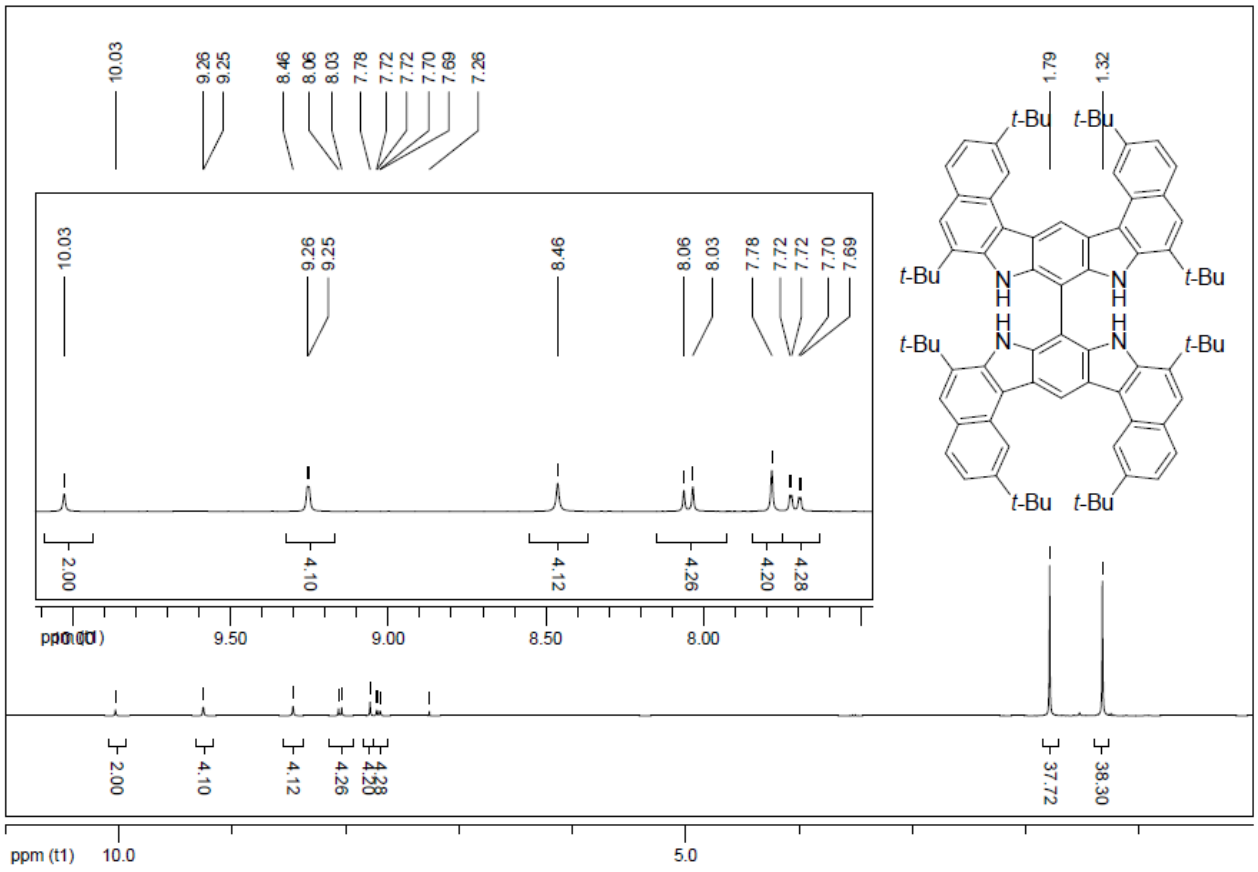


Fig. S43. ^{1}H NMR spectrum of compound **18** ($CDCl_3$, 300 MHz, rt).

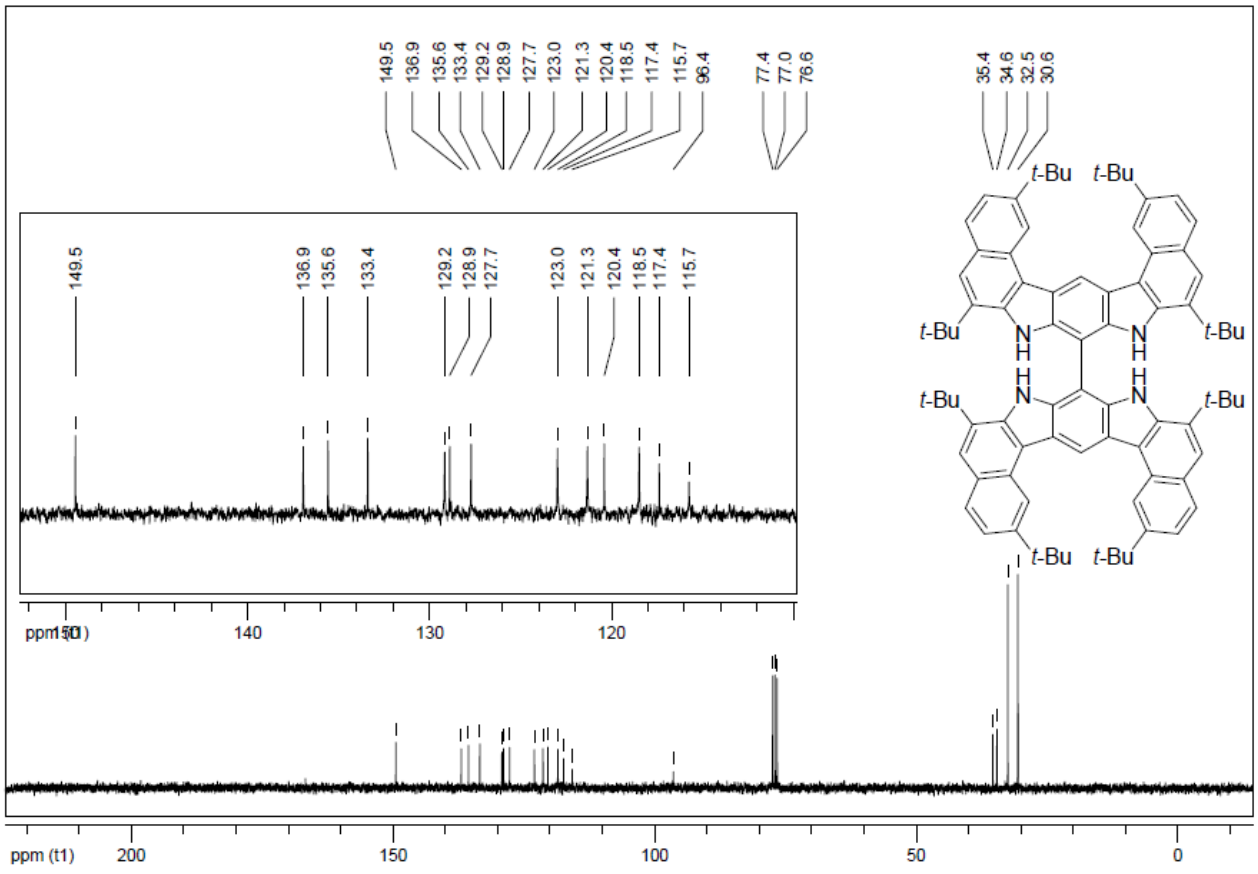
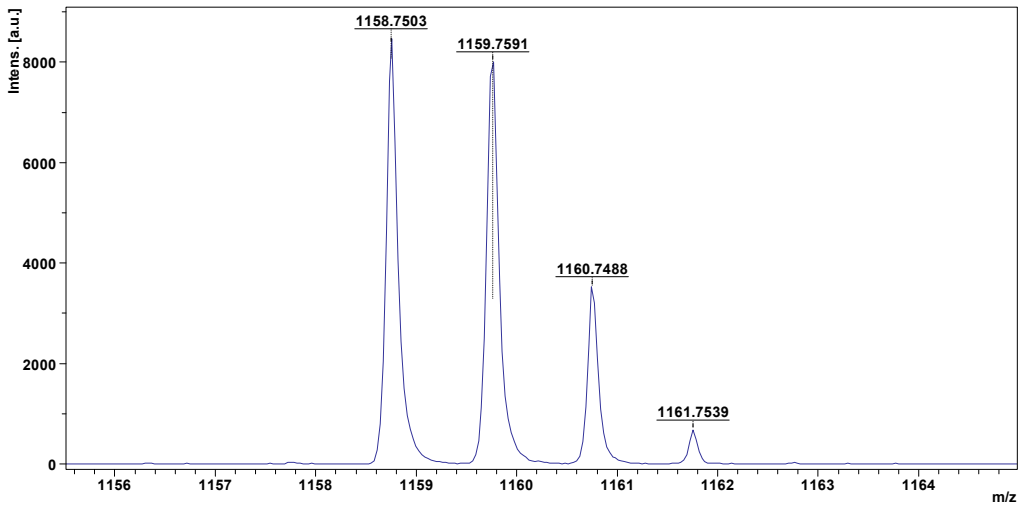


Fig. S44. ^{13}C NMR spectrum of compound **DBICZ-D** ($CDCl_3$, 75 MHz, rt).



Formula	Mass	Error (ppm)	DblEq	N rule	Electron Configuration
C 84 H 94 N 4	1,158.7473	2.5823	40.00	ok	odd

Fig. S45. HR mass spectrum (MOLDI-TOF) of compound **DBICZ-D.**

8. DFT calculation details

DFT calculations have been performed both at the B3LYP/6-31G*[1-5] level of theory and the UCAM-B3LYP[6] level of theory, as implemented in the Gaussian 09 program package.[7] NICS values at the UCAM-B3LYP/6-31G* level using the standard GIAO procedure (NMR pop=NCSall).[8] TD DFT calculations were conducted at the UCAM-B3LYP/6-31G* level for the singlet biradical of **1** and at the B3LYP/6-31G* level for the closed-shell of **2** and the data are summarized below.

Table S16. Selected TD-DFT (UCAM-B3LYP/6-31G*) calculated energies, oscillator strength and compositions of major electronic transitions of **1** (singlet biradical).

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
675.0	0.3050	H-1->L+0(+80%) H-1->L+0(+80%)
		H-2->L+0(+15%) H-2->L+0(+15%)
429.4	0.1208	164->167A(.579) 164->167B(-.57)
		165->167B(.256) 165->167A(-.255)
405.2	0.1553	164->167A(.652) 164->167B(.652)
273.7	1.0821	165->168B(.516) 165->168A(-.514)
		166->168B(.306) 166->168A(-.305)

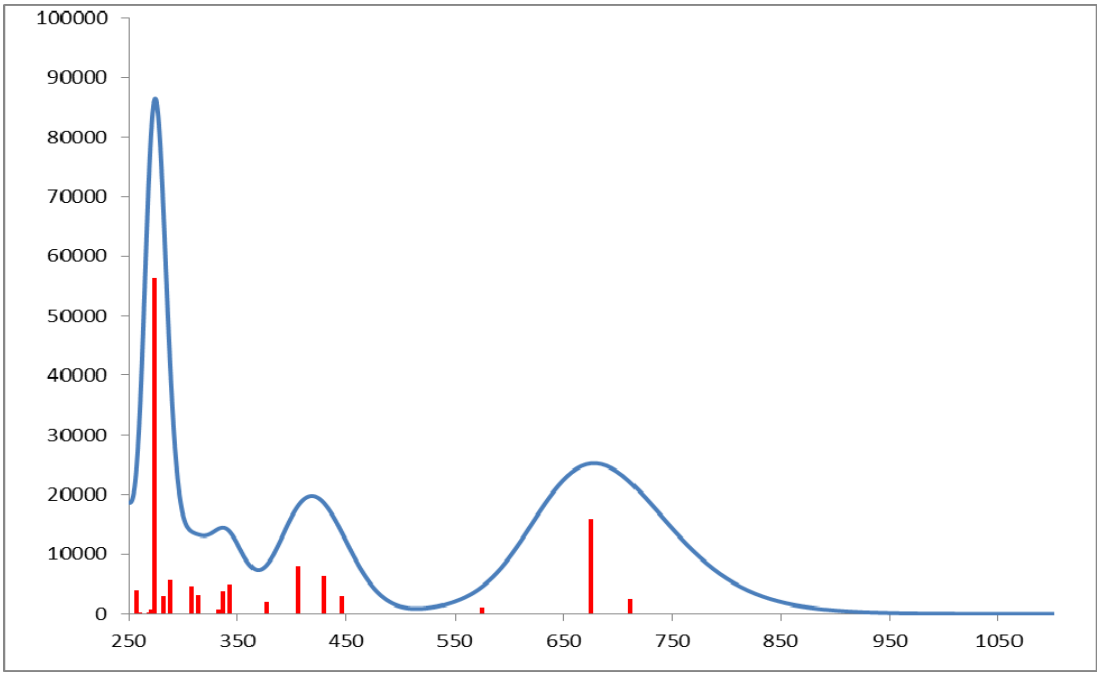


Fig. S46. Calculated (UCAM-B3LYP/6-31G*) absorption spectrum of **1** (singlet biradical).

Table S17. Selected TD-DFT (B3LYP/6-31G*) calculated energies, oscillator strength and compositions of major electronic transitions of **2** (closed-shell singlet).

Wavelength (nm)	Osc. Strength (*f*)	Major contributions
543.6	0.3358	H-1->L+0(+80%), H-2->L+0(+15%)
465.8	0.3247	H-2->L+0(+77%), H-1->L+0(14%)
429.5	0.1177	H-3->L+0(+81%)
304.3	0.6750	H-0->L+1(+83%)

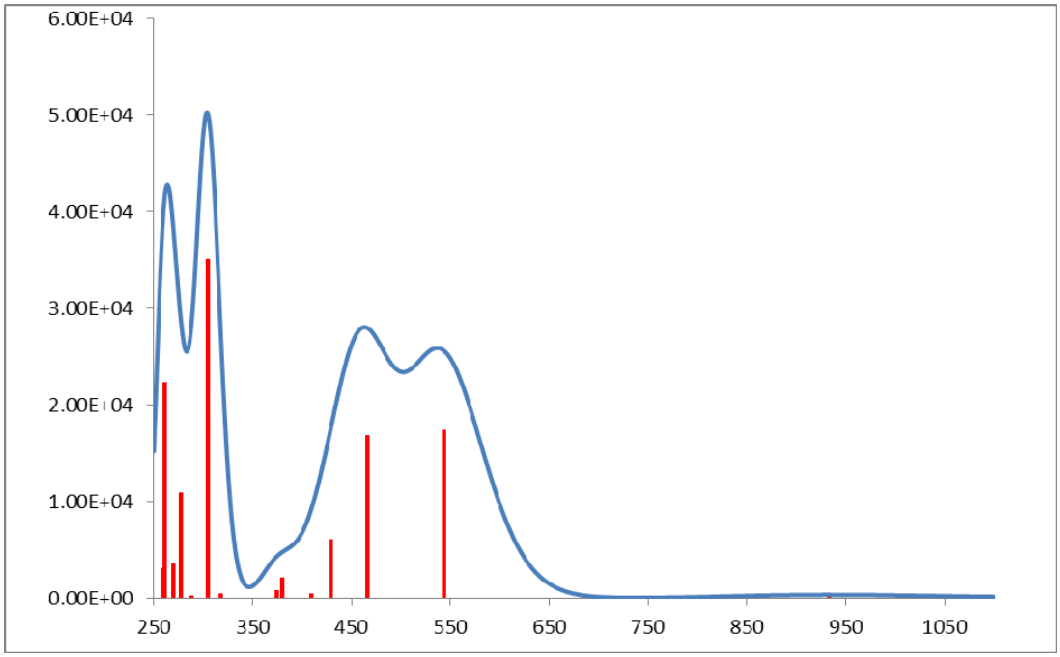


Fig. S47. Calculated (B3LYP/6-31G*) absorption spectrum of **2** (closed-shell singlet).

The energies and Cartesian coordinates of the optimized structures, and the calculated NICS data are shown below.

Compound **1**

Natural Orbital Coefficient
HOMO: 1.43409 LUMO: 0.56591
singlet biradical character y_0 = 0.269

Singlet Diradical Open Shell:
Sum of electronic and zero-point Energies= -1816.779809
Sum of electronic and thermal Energies= -1816.734171
Sum of electronic and thermal Enthalpies= -1816.733227
Sum of electronic and thermal Free Energies= -1816.857056

C	0.00062900	0.82937100	-0.00231800
C	-0.01215700	-2.08426400	0.00179600
C	1.18397800	0.05988200	0.01813100
C	-1.18954000	0.07005200	-0.01856100
C	-1.19080700	-1.35308400	-0.01709000
C	1.17274800	-1.36319000	0.01960800
H	-0.01677700	-3.17102100	0.00267700
C	2.57006300	-1.74600600	0.01366000
C	5.32568300	-1.75601800	-0.02110000
C	3.29587200	-0.51246300	0.00053300
C	3.22441000	-2.95897500	0.00826800
C	4.62631700	-2.97879400	-0.00700600
C	4.71519000	-0.50576000	-0.02032300
H	2.66040700	-3.88665100	0.01535700
H	6.40423400	-1.79429300	-0.03540600
C	-2.59149900	-1.72368000	-0.01117400
C	-5.34710400	-1.70909800	0.02205200
C	-3.25665700	-2.93076700	-0.00547700
C	-3.30633400	-0.48379300	0.00042300
C	-4.72546300	-0.46433400	0.02120600
C	-4.65872400	-2.93805300	0.00851000
H	-2.70091900	-3.86340900	-0.01170700
H	-6.42593600	-1.73767800	0.03584300
N	-2.46820400	0.58271000	0.00203800
N	2.46716800	0.56135500	-0.00242000
C	0.00631800	2.30100200	-0.00841500
C	0.01344000	5.13944800	-0.02313700
C	-0.88201300	3.02209200	-0.80919200
C	0.90272300	3.02541300	0.78744600
C	0.89573000	4.40933700	0.78210200
C	-0.87013600	4.41078500	-0.81957300
H	-1.58201700	2.48853100	-1.43990500
H	1.59981100	2.49289900	1.42224500
H	1.59913100	4.93115400	1.42381000
H	-1.57165500	4.92321100	-1.46692200
C	0.04502200	6.67077500	-0.00003000
C	-0.26565500	7.16484600	1.42449800
H	0.46083800	6.79109000	2.15153800
H	-1.25894500	6.83479300	1.74486900
H	-0.24218200	8.25959900	1.46112100
C	-0.98216100	7.28908600	-0.95551600
H	-2.00546900	7.00212300	-0.69394100
H	-0.79889600	6.99634200	-1.99420600
H	-0.92151500	8.38069300	-0.90392700
C	1.44337500	7.16122300	-0.41595100
H	2.22185600	6.78824300	0.25537500
H	1.48287000	8.25592700	-0.39769100
H	1.68855900	6.82836400	-1.42945500
C	-5.51279600	0.84665700	0.04489100
C	-5.17684500	1.67177500	-1.21203500
H	-4.11520600	1.92035200	-1.24328100
H	-5.75184300	2.60440400	-1.20846300

H	-5.43390000	1.12035200	-2.12280800
C	-5.13061100	1.65240600	1.30170800
H	-4.06689300	1.89433000	1.30431100
H	-5.36272600	1.08872700	2.21167900
H	-5.70126600	2.58733000	1.32984000
C	-7.02844300	0.61296300	0.06961200
H	-7.34419000	0.05682200	0.95826800
H	-7.37621600	0.07309600	-0.81721800
H	-7.54064900	1.57974400	0.08781300
C	-5.39758900	-4.28150700	0.01125400
C	-6.92245600	-4.12180100	0.02457800
H	-7.26971600	-3.59135800	0.91661900
H	-7.39291100	-5.10991500	0.02474400
H	-7.28438200	-3.58445400	-0.85746700
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H	-5.25904000	-4.54384200	2.17622900
H	-3.91503800	-5.27627700	1.29146800
H	-5.50426000	-6.05034000	1.27445900
C	-5.01226700	-5.07626900	-1.25040700
H	-3.93719300	-5.27036300	-1.29879000
H	-5.29522200	-4.53235600	-2.15712100
H	-5.52643900	-6.04344400	-1.25940600
C	5.35282000	-4.32893800	-0.01080300
C	5.51408300	0.79816600	-0.04425100
C	5.18541000	1.62611400	1.21272900
H	5.43790900	1.07249800	2.12344600
H	4.12590100	1.88358300	1.24417100
H	5.76825800	2.55385700	1.20908200
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H	7.37072400	0.00816300	0.81773900
H	7.54817000	1.51359600	-0.08685100
H	7.33866800	-0.00729400	-0.95777300
C	5.13899000	1.60723200	-1.30106300
H	5.36551400	1.04121100	-2.21098600
H	5.71829800	2.53680100	-1.32961100
H	4.07758200	1.85907200	-1.30339900
C	4.96055200	-5.12110100	1.25035200
H	3.88373400	-5.30519000	1.29898000
H	5.24891300	-4.58064800	2.15743300
H	5.46565100	-6.09304900	1.25832600
C	6.87907500	-4.18333500	-0.02454700
H	7.24624800	-3.65005700	0.85780100
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H	7.34043800	-5.17573200	-0.02570500
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H	3.86071400	-5.30900900	-1.29128500
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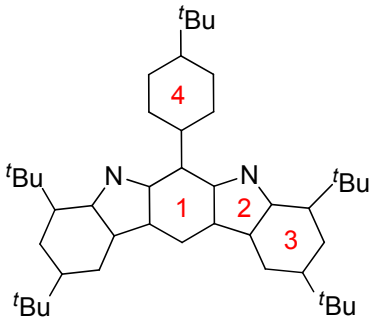
H	5.21112000	-4.58838800	-2.17596700



Bq dis-	NICS values (sigma zz)			
tance (Å)	ring 1	ring 2	ring 3	ring 4
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0.2000	40.920	62.509	19.651	-7.6091
0.3000	39.459	60.553	17.781	-8.6397
0.4000	37.417	57.670	15.386	-9.8486
0.5000	34.8447	53.8581	12.6562	-11.0643
0.6000	31.8446	49.2479	9.7901	-12.1353
0.7000	28.5600	44.0899	6.9700	-12.9519
0.8000	25.1524	38.6894	4.3438	-13.4536
0.9000	21.7762	33.3406	2.0140	-13.6267
1.0000	18.5585	28.2786	0.0371	-13.4938
1.1000	15.5896	23.6595	-1.5709	-13.1007
1.2000	12.9221	19.5633	-2.8250	-12.5050
1.3000	10.5765	16.0096	-3.7595	-11.7655
1.4000	8.5493	12.9773	-4.4193	-10.9369
1.5000	6.8216	10.4220	-4.8517	-10.0654
1.6000	5.3657	8.2889	-5.1024	-9.1880
1.7000	4.1503	6.5211	-5.2123	-8.3321
1.8000	3.1437	5.0643	-5.2162	-7.5171
1.9000	2.3155	3.8693	-5.1431	-6.7552
2.0000	1.6381	2.8925	-5.0163	-6.0530
2.1000	1.0865	2.0964	-4.8542	-5.4133
2.2000	0.6390	1.4486	-4.6710	-4.8358
2.3000	0.2767	0.9220	-4.4773	-4.3181
2.4000	-0.0162	0.4938	-4.2810	-3.8569
2.5000	-0.2531	0.1452	-4.0877	-3.4481

2.6000	-0.4451	-0.1391	-3.9012	-3.0873
2.7000	-0.6012	-0.3716	-3.7239	-2.7703
2.8000	-0.7285	-0.5624	-3.5571	-2.4930
2.9000	-0.8329	-0.7194	-3.4015	-2.2515
3.0000	-0.9189	-0.8491	-3.2570	-2.0423
3.1000	-0.9901	-0.9563	-3.1232	-1.8622
3.2000	-1.0493	-1.0453	-2.9996	-1.7082
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3.5000	-1.1746	-1.2306	-2.6820	-1.3777
3.6000	-1.2035	-1.2721	-2.5910	-1.3040
3.7000	-1.2275	-1.3059	-2.5063	-1.2455
3.8000	-1.2475	-1.3331	-2.4270	-1.2003
3.9000	-1.2638	-1.3547	-2.3526	-1.1668
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4.1000	-1.2873	-1.3835	-2.2161	-1.1292
4.2000	-1.2952	-1.3920	-2.1532	-1.1224
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4.8000	-1.3024	-1.3850	-1.8290	-1.1761
4.9000	-1.2985	-1.3769	-1.7819	-1.1919
5.0000	-1.2934	-1.3674	-1.7364	-1.2077

Singlet Closed Shell:

Sum of electronic and zero-point Energies= -1816.772416
Sum of electronic and thermal Energies= -1816.726964
Sum of electronic and thermal Enthalpies= -1816.726019
Sum of electronic and thermal Free Energies= -1816.850112

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C	1.18127100	0.06320600	0.02300700
C	-1.20966900	0.10765600	-0.01771000
C	-1.20621900	-1.34138300	-0.01747100
C	1.17085800	-1.39974400	0.02721600
H	-0.01271000	-3.17948800	-0.00985900
C	2.58348300	-1.76289900	0.01905700
C	5.32321300	-1.73228700	-0.02600900
C	3.28067300	-0.53558000	-0.00295700
C	3.25549600	-2.96620200	0.01839700
C	4.65789700	-2.96182600	-0.00207400
C	4.67679000	-0.48751600	-0.02965900
H	2.70555800	-3.90230200	0.03358800
H	6.40246600	-1.74033100	-0.04449400
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C	-5.30419900	-1.73386900	0.01920300
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C	-4.74076400	-0.49256800	0.01462100
C	-4.57317700	-2.98577400	0.00762900
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H	-6.38155100	-1.80186800	0.03431500
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C	-0.94155500	3.04947700	-0.77101000
C	0.90652900	3.03741800	0.75699100
C	0.90509900	4.42070400	0.75656000
C	-0.92122100	4.43712100	-0.77784300
H	-1.66735900	2.51885200	-1.37348000
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C	-0.20974300	7.17967500	1.45100900
H	0.54497700	6.80144100	2.14623700
H	-1.19024100	6.85367700	1.81220400
H	-0.17968000	8.27413300	1.48865600
C	-1.02410200	7.31582200	-0.89692400
H	-2.03718700	7.03285300	-0.59451800
H	-0.88523500	7.02706300	-1.94355300
H	-0.95576900	8.40681100	-0.84325500
C	1.42156000	7.17125600	-0.45943800
H	2.22531300	6.79167700	0.17753700
H	1.46800100	8.26556400	-0.43933000
H	1.62218100	6.84066500	-1.48341300
C	-5.56018900	0.79744600	0.03368100
C	-5.24663800	1.62530700	-1.22690900
H	-4.18962300	1.89132600	-1.26625400
H	-5.83728400	2.54813900	-1.22201000
H	-5.50067100	1.06677000	-2.13425300
C	-5.19798600	1.61789200	1.28662000
H	-4.13887900	1.87880700	1.29236600
H	-5.42400800	1.05491000	2.19863800
H	-5.78586200	2.54235900	1.30709000
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H	-7.36747500	-0.03783600	0.95203700
H	-7.40091200	-0.03081600	-0.82365200
H	-7.60743400	1.47522500	0.07452700
C	-5.31326100	-4.33281500	0.01441500
C	-6.83982000	-4.17979200	0.02642800
H	-7.19245600	-3.65043100	0.91709300
H	-7.30385200	-5.17093700	0.02873000
H	-7.20597500	-3.64791300	-0.85728300
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H	-5.17178500	-4.58686100	2.18040300

H	-3.83112000	-5.32294800	1.29441400
H	-5.42166000	-6.09690200	1.28577400
C	-4.92732700	-5.13198000	-1.24391600
H	-3.85208000	-5.32535300	-1.28798100
H	-5.20690800	-4.59042600	-2.15313700
H	-5.44224800	-6.09891200	-1.25203200
C	5.41040100	-4.29879300	-0.00018100
C	5.45043900	0.83452200	-0.06444800
C	5.11902300	1.65796600	1.19397800
H	5.39222100	1.11125000	2.10278500
H	4.05456900	1.89367100	1.23771800
H	5.68064500	2.59881200	1.18373300
C	6.96861700	0.61835300	-0.10301300
H	7.33135900	0.08608000	0.78232000
H	7.46962900	1.59089000	-0.13008900
H	7.28198200	0.06200800	-0.99230400
C	5.04935100	1.63322100	-1.31907200
H	5.27810300	1.06905800	-2.22952100
H	5.60917500	2.57448500	-1.35619800
H	3.98314200	1.86539600	-1.31382400
C	5.03928700	-5.09168100	1.26635300
H	3.96631000	-5.29658000	1.31981800
H	5.31933700	-4.53958200	2.16905500
H	5.56316400	-6.05373100	1.27927000
C	6.93304600	-4.12099300	-0.01960900
H	7.29082900	-3.57385700	0.85818400
H	7.27029300	-3.59066600	-0.91562700
H	7.41631500	-5.10300500	-0.01607000
C	5.00938500	-5.11134600	-1.24496800
H	3.93510100	-5.31479900	-1.27050900
H	5.53132500	-6.07451000	-1.25441900
H	5.26956000	-4.57426500	-2.16255100

Triplet:

Sum of electronic and zero-point Energies= -1816.771572
Sum of electronic and thermal Energies= -1816.725840
Sum of electronic and thermal Enthalpies= -1816.724896
Sum of electronic and thermal Free Energies= -1816.851293

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C	-0.01845000	-2.03152800	-0.00045000
C	1.19157200	0.13717100	0.01352800
C	-1.19938100	0.15311300	-0.02491600
C	-1.19097200	-1.29603500	-0.01818900
C	1.16379300	-1.31168900	0.01377200
H	-0.02569700	-3.11785800	0.00222900
C	2.56027600	-1.71098700	0.01130800
C	5.28385300	-1.80294600	-0.01971200
C	3.30039100	-0.49640900	0.00734500
C	3.17219800	-2.93971000	0.00006700
C	4.58014900	-3.00074500	-0.01731000

C	4.69580600	-0.51828800	-0.00274900
H	2.57960600	-3.84975600	0.00112900
H	6.36428200	-1.85025100	-0.03843500
C	-2.59268800	-1.67664000	-0.01355800
C	-5.31728800	-1.73170000	0.01869600
C	-3.22113100	-2.89694600	0.00431400
C	-3.31640000	-0.45223700	-0.01560500
C	-4.71195800	-0.45522300	-0.00526600
C	-4.62977900	-2.93888700	0.02249000
H	-2.64086100	-3.81488500	0.00798400
H	-6.39823700	-1.76429900	0.03801400
N	-2.45101700	0.64217100	-0.01577400
N	2.44967500	0.60945700	0.00232600
C	0.01117100	2.38667600	-0.01027200
C	0.02749200	5.23143000	-0.01392600
C	-0.95301700	3.11931800	-0.71047000
C	0.98820300	3.10957400	0.69025900
C	0.98703200	4.49324600	0.68870500
C	-0.93812100	4.50800700	-0.71395700
H	-1.72319600	2.59415800	-1.25952100
H	1.75143000	2.57519900	1.24003500
H	1.75768000	5.00920800	1.25316500
H	-1.70394200	5.02499100	-1.27981400
C	0.07047400	6.76237500	0.00997600
C	-0.05765300	7.25526600	1.46264300
H	0.75203600	6.87721700	2.09310900
H	-1.00482700	6.92888600	1.90360000
H	-0.02463300	8.34990100	1.49732000
C	-1.06348900	7.38975500	-0.80909400
H	-2.04791800	7.10419300	-0.42515800
H	-1.01075900	7.10194300	-1.86381900
H	-0.99273000	8.48102200	-0.76012600
C	1.41005800	7.24548900	-0.57458200
H	2.26273600	6.86408800	-0.00571100
H	1.45953000	8.33995300	-0.55810700
H	1.52606800	6.91469400	-1.61153900
C	-5.63152700	0.77423600	0.00533000
C	-4.90000600	2.11628100	-0.12508000
H	-4.19288700	2.28491800	0.68701100
H	-5.64423900	2.92057000	-0.11539200
H	-4.33886800	2.18187700	-1.06007100
C	-6.41347400	0.78906800	1.33341600
H	-5.73130400	0.87658200	2.18471400
H	-7.00957300	-0.11778500	1.47145200
H	-7.09589500	1.64558400	1.35638800
C	-6.62532600	0.67866600	-1.16931200
H	-7.26018200	-0.20978000	-1.11510000
H	-6.09534000	0.65561900	-2.12675700
H	-7.28312200	1.55418200	-1.16840400
C	-5.33938900	-4.29726500	0.04661300
C	-6.86630200	-4.16463300	0.06642600
H	-7.21697600	-3.62720400	0.95312500

H	-7.32074300	-5.16009700	0.08313100
H	-7.24162000	-3.64552600	-0.82109900
C	-4.91050000	-5.07448000	1.30459000
H	-5.18668600	-4.53059300	2.21341100
H	-3.83018400	-5.24350500	1.33187200
H	-5.40076600	-6.05368100	1.33134700
C	-4.94506700	-5.09984800	-1.20675500
H	-3.86580000	-5.26944300	-1.26023300
H	-5.24633800	-4.57427500	-2.11838600
H	-5.43550200	-6.07933600	-1.20039500
C	5.27097400	-4.36880500	-0.03383200
C	5.63202600	0.69852000	-0.02000900
C	4.91868200	2.05094900	0.10350300
H	4.35894300	2.12902300	1.03838400
H	4.21345600	2.22474800	-0.70915100
H	5.67355700	2.84518300	0.08919400
C	6.62490800	0.59566300	1.15477600
H	6.09513100	0.58518800	2.11255500
H	7.29474500	1.46198400	1.14880200
H	7.24740800	-0.30174600	1.10512900
C	6.41360700	0.69576200	-1.34840300
H	6.99781400	-0.21952400	-1.48156600
H	7.10710300	1.54318400	-1.37633400
H	5.73232600	0.78744900	-2.19996600
C	4.86508600	-5.15919100	1.22360300
H	3.78359300	-5.31383500	1.27734000
H	5.17296300	-4.63289700	2.13260900
H	5.34216900	-6.14525800	1.22278300
C	6.79960500	-4.25752800	-0.05361400
H	7.18174200	-3.73887500	0.83126700
H	7.15807300	-3.72986200	-0.94305400
H	7.24015500	-5.25930000	-0.06471700
C	4.83189700	-5.14671200	-1.28786400
H	3.74935300	-5.30083900	-1.31480300
H	5.30852700	-6.13275700	-1.30916200
H	5.11599700	-4.61158500	-2.19944500

Compound **2**

Singlet Closed Shell:

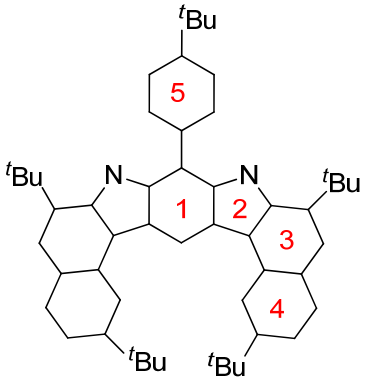
Sum of electronic and zero-point Energies= -2123.796098
Sum of electronic and thermal Energies= -2123.745320
Sum of electronic and thermal Enthalpies= -2123.744375
Sum of electronic and thermal Free Energies= -2123.879521

C	1.86331100	-0.00887900	0.04483800
C	-1.07552500	0.03660700	0.00002900
C	1.03044700	-1.20936600	0.01942700
C	1.17097300	1.16768500	0.03416100
C	-0.28235000	1.24676200	-0.00110700
C	-0.43784000	-1.15749400	0.03889200
H	-2.15571300	0.09662100	-0.04316700

C	3.33021100	-0.10316400	0.05979100
C	6.16180500	-0.26597800	0.11249200
C	3.98461700	-1.04064700	0.86220600
C	4.11668200	0.75054900	-0.72372100
C	5.49720800	0.66080300	-0.69958900
C	5.37120400	-1.10941200	0.89357800
H	3.40357900	-1.71279200	1.48103100
H	3.63294200	1.47830800	-1.36288200
H	6.06925800	1.33273000	-1.33179400
H	5.83232700	-1.84336300	1.54328200
C	7.69247300	-0.32325600	0.11202200
C	8.25548300	1.04340700	0.54154200
H	7.92136300	1.30413900	1.55071400
H	7.93901400	1.84437100	-0.13234100
H	9.35072400	1.01948100	0.54070000
C	8.18937300	-0.65649400	-1.30638000
H	7.80798800	-1.62800500	-1.63632300
H	9.28403900	-0.69583500	-1.32585900
H	7.86951900	0.09310600	-2.03564900
C	8.23645900	-1.38747900	1.07216500
H	7.89737400	-2.39224500	0.80115600
H	7.93804500	-1.19233300	2.10708600
H	9.33042700	-1.38760100	1.03816600
N	1.74101700	2.43658900	0.07012800
N	1.48555700	-2.42070000	-0.08212600
C	0.36960300	-3.27891500	-0.10940400
C	-0.83250200	-2.57334600	-0.01233200
C	-0.76147500	-5.34440800	-0.24214300
C	-2.07023600	-3.26144000	0.02052400
C	0.44854400	-4.69109200	-0.23558600
C	-2.00441800	-4.67723800	-0.11029800
C	-3.34120200	-2.65039200	0.19892200
H	-3.16927700	-6.49154800	-0.20553900
H	-0.79742800	-6.42283100	-0.34083700
C	-4.50627300	-3.37889600	0.23334700
H	-3.37401900	-1.57827900	0.33860300
C	-4.41805700	-4.78874100	0.06672300
H	-5.32412200	-5.38560500	0.07874000
C	-3.21547200	-5.41160900	-0.09449900
C	0.74262100	3.27655500	0.03918400
C	-0.57474700	2.59758700	-0.01418400
C	-0.29822000	5.41196900	0.01303900
C	-1.78555700	3.39550100	-0.07218200
C	0.86427400	4.72828800	0.06860800
C	-1.61322400	4.80029500	-0.06733700
C	-3.08427300	2.87906800	-0.14882400
H	-2.61541800	6.69214400	-0.14063300
H	-0.29256700	6.49583400	0.02620400
C	-4.21438200	3.69186100	-0.22987700
H	-3.21607000	1.80446500	-0.14756500
C	-4.01589700	5.07571500	-0.22602900
H	-4.86121100	5.74975800	-0.28765300

C	-2.74334600	5.61319100	-0.14346200
C	1.78625900	-5.42542500	-0.36546900
C	2.64783000	-5.16489300	0.88394600
H	2.13507900	-5.50497700	1.79006800
H	2.87496200	-4.10324900	0.98883600
H	3.59323300	-5.71330500	0.80486700
C	1.59228600	-6.94149500	-0.49753200
H	1.09439400	-7.36965400	0.37857100
H	2.57072300	-7.42302300	-0.58856300
H	1.01163900	-7.20478100	-1.38754000
C	2.53291800	-4.93021900	-1.61835600
H	1.94026100	-5.11169300	-2.52137600
H	3.48084400	-5.46981500	-1.72327300
H	2.74972600	-3.86303400	-1.55281200
C	2.23325800	5.40396800	0.15884100
C	3.08519800	5.02420600	-1.06678800
H	3.25551400	3.94808400	-1.10683600
H	4.05679200	5.52770200	-1.01252200
H	2.59480100	5.33687600	-1.99503400
C	2.95298800	4.95487600	1.44476100
H	3.11275600	3.87626200	1.45084800
H	2.37095000	5.22789100	2.33168600
H	3.92677700	5.45200300	1.51537100
C	2.10738700	6.93181700	0.19347400
H	1.53199900	7.27556700	1.05931900
H	1.63624500	7.32571400	-0.71316500
H	3.10555200	7.37440400	0.26456800
C	-5.61152600	3.06522400	-0.29755500
C	-6.71394900	4.11534800	-0.48331400
H	-6.75889400	4.81467300	0.35727300
H	-7.68604900	3.61665900	-0.54643100
H	-6.57696500	4.69164500	-1.40385400
C	-5.88398400	2.31594400	1.01848800
H	-5.85694000	3.00463700	1.86892200
H	-5.14352200	1.53295400	1.20076700
H	-6.87193900	1.84356900	0.99385300
C	-5.68718000	2.08880100	-1.48423900
H	-4.94173800	1.29254300	-1.41187200
H	-5.52122800	2.61294600	-2.43077300
H	-6.67411400	1.61578700	-1.52545200
C	-5.88686300	-2.75567000	0.45272900
C	-6.53252900	-3.36887800	1.70890700
H	-5.92105800	-3.17534100	2.59587300
H	-6.65758100	-4.45141000	1.61930200
H	-7.52344800	-2.93289300	1.87640300
C	-5.81455700	-1.24081500	0.64982100
H	-5.21252000	-0.97461600	1.52452500
H	-6.82000500	-0.83848900	0.80694800
H	-5.39346600	-0.73864900	-0.22631200
C	-6.77729700	-3.04051700	-0.77042500
H	-6.90280800	-4.11308900	-0.94329900
H	-6.34659100	-2.60431800	-1.67726800

H -7.77334400 -2.60850500 -0.62403400



Bq distance (Å)	NICS values (sigma zz) ring 1	ring 2	ring 3	ring 4	ring 5
0.0000	73.584	80.217	5.7496	-1.9025	-7.2898
0.1000	73.250	79.351	5.3338	-2.5048	-7.5017
0.2000	72.601	78.072	4.0539	-3.9906	-8.1694
0.3000	71.515	76.177	2.0726	-6.1678	-9.1792
0.4000	69.8338	73.4092	-0.3753	-8.7693	-10.3703
0.5000	67.4369	69.6051	-3.0275	-11.5051	-11.5697
0.6000	64.2916	64.7877	-5.6374	-14.1102	-12.6246
0.7000	60.4661	59.1632	-8.0062	-16.3799	-13.4243
0.8000	56.1112	53.0542	-10.0000	-18.1841	-13.9079
0.9000	51.4220	46.8098	-11.5506	-19.4670	-14.0620
1.0000	46.6037	40.7350	-12.6468	-20.2330	-13.9097
1.1000	41.8331	35.0522	-13.3187	-20.5293	-13.4976
1.2000	37.2516	29.8951	-13.6215	-20.4274	-12.8836
1.3000	32.9573	25.3218	-13.6220	-20.0081	-12.1272
1.4000	29.0080	21.3353	-13.3883	-19.3510	-11.2831
1.5000	25.4338	17.9042	-12.9830	-18.5279	-10.3977
1.6000	22.236	14.978	-12.4602	-17.5995	-9.5076
1.7000	19.404	12.499	-11.8641	-16.6151	-8.6401
1.8000	16.915	10.411	-11.2296	-15.6125	-7.8143
1.9000	14.740	8.6564	-10.5827	-14.6197	-7.0420
2.0000	12.850	7.1857	-9.9426	-13.6567	-6.3297
2.1000	11.211	5.9543	-9.3224	-12.7367	-5.6798

2.2000	9.7931	4.9230	-8.7309	-11.8679	-5.0919
2.3000	8.5660	4.0582	-8.1731	-11.0546	-4.5634
2.4000	7.5035	3.3311	-7.6517	-10.2983	-4.0911
2.5000	6.5817	2.7179	-7.1674	-9.5986	-3.6707
2.6000	5.7796	2.1984	-6.7198	-8.9535	-3.2980
2.7000	5.0792	1.7564	-6.3074	-8.3604	-2.9688
2.8000	4.4652	1.3783	-5.9283	-7.8159	-2.6791
2.9000	3.9246	1.0534	-5.5801	-7.3167	-2.4252
3.0000	3.4468	0.7727	-5.2607	-6.8593	-2.2037
3.1000	3.0225	0.5292	-4.9676	-6.4400	-2.0115
3.2000	2.6444	0.3172	-4.6984	-6.0556	-1.8459
3.3000	2.3061	0.1318	-4.4510	-5.7029	-1.7044
3.4000	2.0025	-0.0307	-4.2232	-5.3789	-1.5846
3.5000	1.7293	-0.1734	-4.0134	-5.0811	-1.4846
3.6000	1.4826	-0.2989	-3.8196	-4.8069	-1.4023
3.7000	1.2596	-0.4094	-3.6403	-4.5540	-1.3360
3.8000	1.0574	-0.5068	-3.4742	-4.3205	-1.2840
3.9000	0.8739	-0.5925	-3.3200	-4.1045	-1.2447
4.0000	0.7071	-0.6679	-3.1765	-3.9043	-1.2166
4.1000	0.5553	-0.7341	-3.0428	-3.7185	-1.1981
4.2000	0.4171	-0.7921	-2.9179	-3.5457	-1.1880
4.3000	0.2912	-0.8428	-2.8010	-3.3849	-1.1848
4.4000	0.1764	-0.8870	-2.6915	-3.2348	-1.1873
4.5000	0.0718	-0.9252	-2.5887	-3.0946	-1.1943
4.6000	-0.0236	-0.9582	-2.4920	-2.9634	-1.2048
4.7000	-0.1105	-0.9863	-2.4010	-2.8404	-1.2176
4.8000	-0.1896	-1.0102	-2.3151	-2.7250	-1.2319
4.9000	-0.2617	-1.0302	-2.2340	-2.6166	-1.2468
5.0000	-0.3272	-1.0467	-2.1573	-2.5145	-1.2617

Parent Compound **1**

Singlet Diradical Open Shell: $<S^2>= 0.9470$

Sum of electronic and zero-point Energies= -800.724034
Sum of electronic and thermal Energies= -800.710691
Sum of electronic and thermal Enthalpies= -800.709747
Sum of electronic and thermal Free Energies= -800.764206

C	0.00005000	-1.96747900	0.00016200
C	-0.00001600	0.91331900	-0.00002500
C	1.18513200	-1.23474300	0.00021300
C	-1.18512300	-1.23472500	-0.00008100
C	-1.18615900	0.18938700	-0.00015500
C	1.18615800	0.18936200	0.00011800
H	-0.00000500	1.99997200	-0.00002800
C	2.59197300	0.55255700	0.00021800
C	5.38270500	0.47232700	-0.00015900
C	3.29325900	-0.69571300	0.00022100

C	3.29431900	1.74471900	-0.00014400
C	4.69015200	1.69308600	-0.00027500
C	4.69737900	-0.73028000	0.00002900
H	2.78303400	2.70264200	-0.00033100
H	6.46766400	0.47731600	-0.00023700
C	-2.59203100	0.55256900	-0.00021300
C	-5.38272600	0.47227200	0.00012000
C	-3.29439500	1.74469500	0.00020000
C	-3.29325200	-0.69567900	-0.00026200
C	-4.69731600	-0.73033200	-0.00006300
C	-4.69024900	1.69302500	0.00029200
H	-2.78314000	2.70263500	0.00042200
H	-6.46768500	0.47719000	0.00014500
N	-2.46054400	-1.76780300	-0.00057300
N	2.46068000	-1.76781200	0.00040400
H	0.00004100	-3.05158600	0.00011900
H	-5.21167600	-1.68519000	-0.00023100
H	-5.25440900	2.62058200	0.00050500
H	5.25428900	2.62065600	-0.00048900
H	5.21177500	-1.68511900	0.00013000

Singlet Closed Shell:

Sum of electronic and zero-point Energies= -800.716521
Sum of electronic and thermal Energies= -800.703573
Sum of electronic and thermal Enthalpies= -800.702629
Sum of electronic and thermal Free Energies= -800.756279

C	-0.06376200	-1.99227200	0.00045900
C	0.02563900	0.92709400	-0.00053700
C	-1.21195600	-1.27902100	-0.00039100
C	1.17579800	-1.24252200	0.00058600
C	1.18075000	0.22807600	0.00071500
C	-1.20626000	0.18299900	-0.00029900
H	0.00765000	2.01369900	-0.00204400
C	-2.53224200	0.54247100	-0.00022900
C	-5.33610100	0.50572900	0.00001300
C	-3.28027300	-0.72976400	0.00002600
C	-3.24038400	1.78314300	-0.00025800
C	-4.59658700	1.75148500	-0.00012200
C	-4.71758800	-0.69817300	0.00002900
H	-2.70235500	2.72602400	-0.00028400
H	-6.42050000	0.55767800	0.00022500
C	2.60365000	0.56568000	0.00003800
C	5.37478700	0.43301100	-0.00023700
C	3.32738000	1.74290600	0.00075400
C	3.26919600	-0.67951100	-0.00052400
C	4.64981300	-0.76042700	-0.00074300
C	4.72397000	1.66348800	0.00047900
H	2.83370600	2.71019700	0.00141500
H	6.45962900	0.40126300	-0.00036100
N	2.36741500	-1.76527700	-0.00028700

N	-2.51501000	-1.79126200	0.00045100
H	-0.04667200	-3.07627900	0.00139400
H	5.14215500	-1.72682800	-0.00122300
H	5.30910700	2.57778700	0.00091500
H	-5.15923500	2.67982900	-0.00002400
H	-5.26528100	-1.63394100	0.00028900

Triplet:

Sum of electronic and zero-point Energies= -800.725118
Sum of electronic and thermal Energies= -800.712194
Sum of electronic and thermal Enthalpies= -800.711250
Sum of electronic and thermal Free Energies= -800.765790

C	0.00000200	-2.01229800	0.00022700
C	0.00000000	0.89917600	-0.00013400
C	-1.19404700	-1.27763700	0.00002900
C	1.19405000	-1.27763700	0.00012800
C	1.18332700	0.17518800	-0.00001700
C	-1.18332700	0.17518800	-0.00019300
H	0.00000100	1.98545900	-0.00012100
C	-2.59071800	0.54896000	-0.00020300
C	-5.36236800	0.50921100	0.00014700
C	-3.29366600	-0.68177000	-0.00003100
C	-3.27295600	1.74934700	-0.00043300
C	-4.67368400	1.71812300	-0.00023700
C	-4.67910500	-0.71007600	0.00020000
H	-2.74696200	2.69954800	-0.00073700
H	-6.44768200	0.51323700	0.00038600
C	2.59071700	0.54896000	0.00017600
C	5.36236600	0.50921300	-0.00013000
C	3.27295400	1.74934800	0.00054200
C	3.29366600	-0.68177000	0.00003200
C	4.67910500	-0.71007500	-0.00018400
C	4.67368200	1.71812400	0.00033300
H	2.74695900	2.69954900	0.00084800
H	6.44768000	0.51323800	-0.00041000
N	2.44169400	-1.78565100	-0.00074600
N	-2.44169200	-1.78565000	0.00049800
H	0.00000100	-3.09561700	0.00021800
H	5.20578400	-1.65803800	-0.00066200
H	5.22783100	2.65116500	0.00043900
H	-5.22783300	2.65116300	-0.00033100
H	-5.20578300	-1.65803900	0.00059200

Parent Compound **2**

Singlet Closed Shell:

Sum of electronic and zero-point Energies= -1107.740540
Sum of electronic and thermal Energies= -1107.722156
Sum of electronic and thermal Enthalpies= -1107.721212
Sum of electronic and thermal Free Energies= -1107.787722

C	-0.09082800	-3.01521400	0.00007600
C	0.01224400	-0.10542700	-0.00010400
C	1.15168900	-2.27675500	0.00004800
C	-1.23365000	-2.29832900	-0.00000200
C	-1.23665000	-0.83464000	-0.00006700
C	1.16975300	-0.80300500	-0.00006000
H	0.00483800	0.97640900	-0.00016200
N	-2.53547100	-2.81403500	-0.00004900
N	2.33944400	-2.80344900	0.00002200
C	3.24002200	-1.71834300	0.00005500
C	2.60052200	-0.48052700	-0.00000900
C	5.38715500	-0.69190300	0.00007800
C	3.35467900	0.71654900	-0.00001900
C	4.63762500	-1.83977500	0.00009700
C	4.77979200	0.59145300	0.00002500
C	2.79163600	2.01935500	-0.00005800
H	6.65201200	1.66432500	0.00003700
H	6.47185700	-0.74684700	0.00010200
C	3.58693500	3.13293700	-0.00006700
H	1.71432600	2.13318200	-0.00007000
C	4.99484900	3.00942900	-0.00004100
H	5.61407100	3.90076500	-0.00005900
C	5.57056500	1.76865000	0.00000700
C	-3.30246600	-1.76283800	-0.00009400
C	-2.56313200	-0.47747300	-0.00007500
C	-5.39903400	-0.59956200	0.00000200
C	-3.30286700	0.77189500	-0.00001800
C	-4.74254700	-1.77261400	-0.00006200
C	-4.71856100	0.69085800	0.00004000
C	-2.70400300	2.03777600	-0.00003500
H	-6.55484700	1.79795600	0.00017200
H	-6.48525500	-0.58070100	0.00001700
C	-3.46726700	3.19332300	0.00003800
H	-1.62496800	2.12303200	-0.00010900
C	-4.85790800	3.11065900	0.00012500
H	-5.45930800	4.01401300	0.00019400
C	-5.47084000	1.86843300	0.00011900
H	-0.08164100	-4.09906700	0.00010300
H	5.09213900	-2.82422700	0.00013600
H	3.13526200	4.12016000	-0.00009500
H	-2.97790900	4.16193600	0.00002200
H	-5.25467500	-2.72801100	-0.00009700

Triplet:

Sum of electronic and zero-point Energies= -1107.734935
Sum of electronic and thermal Energies= -1107.716529
Sum of electronic and thermal Enthalpies= -1107.715585
Sum of electronic and thermal Free Energies= -1107.782900

C	-0.00000900	-3.04445100	0.00043800
C	-0.00002200	-0.13397900	0.00003700
C	-1.19464700	-2.31352300	0.00038100

C	1.19460900	-2.31353300	0.00032200
C	1.19308800	-0.84807200	0.00031600
C	-1.19311200	-0.84806600	0.00017900
H	-0.00000300	0.94700700	-0.00044600
N	2.42909700	-2.82138400	0.00003200
N	-2.42911700	-2.82138800	0.00030000
C	-3.28080900	-1.71402600	0.00013400
C	-2.60140800	-0.48881900	0.00004900
C	-5.39297700	-0.61505700	-0.00023300
C	-3.32049200	0.73419800	-0.00008500
C	-4.68169600	-1.78764100	-0.00001300
C	-4.74863400	0.65090600	-0.00026100
C	-2.72434500	2.02052700	-0.00001700
H	-6.59255500	1.77019400	-0.00058800
H	-6.47897100	-0.63636500	-0.00037300
C	-3.49107200	3.15558700	-0.00017600
H	-1.64541300	2.10950500	0.00020900
C	-4.90055700	3.07249000	-0.00040000
H	-5.49509700	3.98029300	-0.00053300
C	-5.50885400	1.84670000	-0.00043400
C	3.28073400	-1.71402000	-0.00024600
C	2.60133800	-0.48880700	0.00007000
C	5.39293800	-0.61513800	-0.00085200
C	3.32048800	0.73420500	0.00018600
C	4.68162700	-1.78768100	-0.00069700
C	4.74861800	0.65086300	-0.00041900
C	2.72441500	2.02055700	0.00097100
H	6.59259600	1.77004800	-0.00100800
H	6.47893100	-0.63643200	-0.00127000
C	3.49120400	3.15559300	0.00092700
H	1.64549900	2.10964900	0.00185200
C	4.90066400	3.07243200	0.00010700
H	5.49526100	3.98019700	0.00003000
C	5.50890100	1.84659500	-0.00049700
H	-0.00007700	-4.12779200	0.00050900
H	-5.16826700	-2.75647500	0.00002100
H	-3.01153700	4.12953700	-0.00011300
H	3.01170100	4.12955900	0.00158000
H	5.16813400	-2.75654800	-0.00092500

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