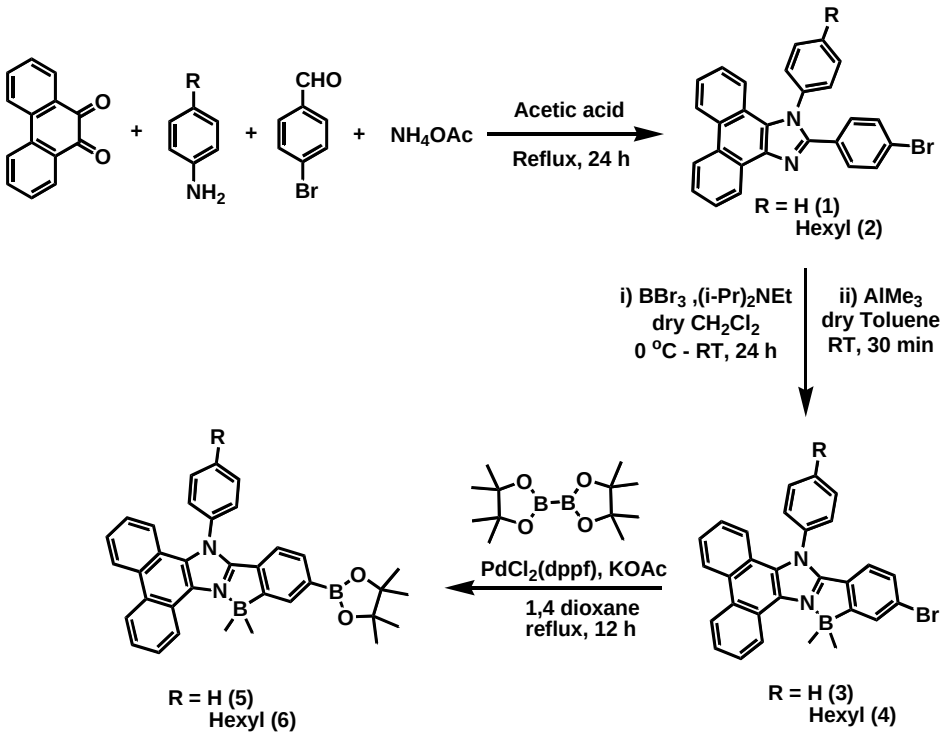
Supporting Information

for

Synthesis of π-extended B←N coordinated phenanthroimidazole dimers and their linear and nonlinear optical properties

Vanga Mukundam,[a] Shreenibasa Sa,[a] Anupa Kumari,[b] Anna Chandrasekar Murali,[a] Prakash Nayak,[a] Ritwick Das[b*] and Krishnan Venkatasubbaiah[a]*

[a]*School of Chemical Sciences,* [b]*School of Physical Sciences, National Institute of Science Education and Research (NISER), HBNI, Bhubaneswar-752050, Odisha (India).* **E-mail: krishv@niser.ac.in*



Scheme S1: Synthesis of compounds **1-6**

Experimental Section

General Information

All reagents and starting materials were purchased from Sigma-Aldrich, Alfa Aesar and Spectrochem chemical companies and used as received unless otherwise noted. THF and toluene were distilled from Na/benzophenone prior to use. Dichloromethane, N,N-Dimethylformamide and acetonitrile were distilled from CaH_2. 1,4-Dibromo-2,5-bis(hexyloxy)benzene, 2,7-dibromo-9,9-dihexyl-9H-fluorene, 2,7-dibromo-9-hexyl-9H-carbazole, were prepared by following literature reported methods.[1-3] All 400 MHz ^{1}H, 100 MHz ^{13}C and 128 MHz ^{11}B NMR spectra were recorded on a Bruker ARX 400 spectrometer operating at 400 MHz. All ^{1}H and ^{13}C NMR spectra were referenced internally to solvent signals. ^{11}B NMR spectra were referenced externally to $BF_3 \cdot Et_2O$ in $CDCl_3$ ($\delta = 0$). ESI mass spectra were recorded using a Bruker microTOF-QII mass spectrometer. MALDI was recorded on Applied Biosystems Q10 4800 MALDI TOF/TOF analyzer using 4000 series explorer software for acquisition and GPS explorer software, version 3.6 for analysis. The absorbance spectra were recorded with a JASCO V-730 UV-Visible spectrometer. The fluorescence spectra were recorded using Edinburgh FS5 spectrofluorometer. Fluorescence quantum yields of **7-11** in various solvents were measured by using quinine sulfate as reference and fluorescence quantum yields of their solid powders were measured by integrating sphere technique using Edinburgh FS5 spectrofluorometer.

Single-crystal X-ray diffraction data were collected on a Bruker APEX-II diffractometer (or) Rigaku Oxford X-ray diffractometer. Mo-Kα radiation (0.71073 Å) or Cu-Kα radiation (1.54184 Å). SADABS absorption corrections were applied. The structures were solved and refined with SHELX suite of programs. All non-hydrogen atoms were refined with anisotropic displacement coefficients. The H atoms were placed at calculated positions and were refined as riding atoms. In compound **7**, electron density resulting from one disordered solvent molecule was removed using OLEX solvent mask. Crystallographic data for compounds **7-10** has been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC- 1945661-1945664. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44) 1223-336-033; email: deposit@ccdc.cam.ac.uk). DFT calculations were performed with the Gaussian09 program.[4] The structures were optimized using 6-31G(d) (B3LYP) as the basis set. Frequency calculations confirmed the optimized structures to be local minimum structures. Excitation data were determined using TD-DFT (B3LYP) calculations.

Synthesis of compound 1

A mixture of 9,10-phenanthrenequinone (3.68 g, 17.67 mmol), aniline (1.93 mL, 21.20 mmol), 4-bromobenzaldehyde (3.27 g, 17.67 mmol), ammonium acetate (6.81 g, 88.34 mmol), and acetic acid (175 mL) was refluxed for 24 h under nitrogen. After cooling to room temperature, the reaction mixture was then poured into water and the solid was filtered. The solid product was washed with water, methanol and dried under vacuum. The resultant solid was

recrystallized from CH_2Cl_2/*n*-hexane mixture to obtain the pure product. Yield: 6.36 g, (80%). mp: 250 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.87 (d, *J* = 8 Hz, 1H), 8.77 (d, *J* = 8 Hz, 1H), 8.70 (d, *J* = 16 Hz, 1H), 7.76 (t, *J* = 8 Hz, 1H), 7.68 – 7.60 (m, 4H), 7.53 – 7.41 (m, 7H), 7.27 (t, *J* = 8 Hz, 1H), 7.17 (d, *J* = 8 Hz, 1H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$): δ = 149.82, 138.66, 137.55, 131.55, 130.91, 130.41, 130.10, 129.58, 129.47, 129.13, 128.43, 128.41, 127.47, 127.23, 126.44, 125.85, 125.16, 124.25, 123.47, 123.26, 123.04, 122.81, 120.95 ppm. HR-MS (ESI): calcd. for $C_{27}H_{18}Br_1N_2$ ([M + H]$^+$): 449.0648, found : 449.0649.

Synthesis of compound 2

A mixture of 9,10-phenanthrenequinone (3.00 g, 14.41 mmol), 4-hexylaniline (3.69 mL, 18.73 mmol), 4-bromobenzaldehyde (2.66 g, 14.41 mmol), ammonium acetate (5.55 g, 72.05 mmol), and acetic acid (150 mL) was refluxed for 24 h under nitrogen. The reaction mixture was poured into water and extracted with dichloromethane (2 x 100 mL). The combined organic layers were washed with aqueous $NaHCO_3$ and then with brine solution, dried over Na_2SO_4 and concentrated. The resultant residue was purified by silica gel column chromatography using *n*-hexane/dichloromethane mixture as eluent. Yield: 5.75 g, (75%). mp: 141 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.87 (d, *J* = 8 Hz, 1H), 8.76 (d, *J* = 8 Hz, 1H), 8.70 (d, *J* = 8 Hz, 1H), 7.75 (t, *J* = 8 Hz, 1H), 7.66 (t, *J* = 8 Hz, 1H), 7.53 – 7.37 (m, 9H), 7.29 – 7.21 (m, 2H), 2.81 (t, *J* = 8 Hz, 2H), 1.78 – 1.74 (m, 2H), 1.41 (s, 6H), 0.97 (t, *J* = 6.5 Hz, 3H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$): δ = 149.84, 145.20, 137.47, 136.07, 131.48, 130.87, 130.33, 129.68, 129.43, 128.78, 128.48, 128.40, 127.41, 127.27, 126.36, 125.77, 125.08, 124.19, 123.36, 123.24, 123.14, 122.78, 121.00, 35.77, 31.80, 31.20, 28.87, 22.79, 14.24 ppm. HR-MS (ESI): calcd. for $C_{33}H_{30}Br_1N_2$ ([M + H]$^+$): 533.1587, found : 533.1579.

Synthesis of compound 3

To a stirred solution of compound **1** (4.50 g, 10.01 mmol), and N,N-diisopropylethylamine (*i*-Pr_2NEt (1.74 mL, 10.01 mmol) in 150 mL of dichloromethane at 0 °C was added BBr_3 (1.0 M in dichloromethane, 30.03 mL, 30.03 mmol) under nitrogen. After being stirred at room temperature for 24 h, saturated K_2CO_3 aqueous solution was added to the reaction mixture and extracted with CH_2Cl_2. The combined organic layers were washed with water, dried over $MgSO_4$ and concentrated under vacuum to afford the crude product **3a**. Under nitrogen atmosphere $AlMe_3$ (2.0 M in toluene, 10.01 mL, 20.02 mmol) was added to the crude product **3a** at room temperature in CH_2Cl_2 and toluene (80 mL : 80 mL). After being stirred at this temperature for 0.5 h, the reaction was quenched by adding water and extracted with CH_2Cl_2. The combined organic layers were washed with water, brine, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography using *n*-hexane/dichloromethane mixture as eluent. Yield: 2.70 g, (55%). mp: 253 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.31 (d, *J* = 8 Hz, 1H), 8.72 (d, *J* = 8 Hz, 2H), 7.88 (t, *J* = 8 Hz, 3H), 7.80 (t, *J* = 8 Hz, 2H), 7.74 – 7.69 (m, 3H), 7.55 – 7.51 (m, 1H), 7.31 (t, *J* = 8 Hz, 1H), 7.23 (d, *J* = 8 Hz, 1H), 7.14 (d, *J* = 8 Hz, 1H), 6.31 (d, *J* = 8 Hz, 1H), 0.55 (s, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$): δ = 176.27, 152.66, 136.63, 132.35, 131.52, 131.19, 130.99, 129.32, 129.06, 129.00, 128.35, 127.97, 127.55, 127.02, 126.80, 126.11, 126.03, 125.78, 125.54, 124.15, 123.41, 123.38, 122.35, 122.19, 120.54, 7.07 ppm. ^{11}B NMR (128 MHz, $CDCl_3$): δ = 0.90 (s) ppm. HR-MS (ESI): calcd. for $C_{29}H_{23}B_1Br_1N_2$ ([M + H]$^+$): 489.1137, found : 489.1138.

Synthesis of compound 4

Compound **4** was prepared following a procedure similar to that used for compound **3**. The quantities involved are as follows: Compound **2** (5.80 g, 10.87 mmol), N,N-diisopropylethylamine (*i*-Pr_2NEt) (1.89 mL, 10.87 mmol), BBr_3 (1.0 M in dichloromethane, 32.61 mL, 32.61 mmol) and $AlMe_3$ (2.0 M in toluene, 10.87 mL, 21.74 mmol). Yield: 3.74 g, (60%). mp: 171 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.29 (d, *J* = 8.0 Hz, 1H), 8.70 (t, *J* = 8.0 Hz, 2H), 7.87 (t, *J* = 8 Hz, 2H), 7.73 (t, *J* = 8 Hz, 1H), 7.55 – 7.48 (m, 5H), 7.31 – 7.24 (m, 2H), 7.14 (d, *J* = 8 Hz, 1H), 6.33 (d, *J* = 8 Hz, 1H), 2.92 (t, *J* = 8 Hz, 2H), 1.88 – 1.84(m, 2H), 1.48 (s, 6H), 1.03 (s, 3H), 0.54 (s, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$): δ = 176.26, 152.76, 146.78, 133.98, 132.30, 131.03, 130.93, 129.28, 129.12, 128.98, 127.96, 127.50, 126.94, 126.72, 126.02, 125.95, 125.88, 125.53, 124.07, 123.46, 123.36, 122.41, 122.28, 120.59, 35.85, 31.75, 31.14, 28.92, 22.76, 14.25, 7.07 ppm. ^{11}B NMR (128 MHz, $CDCl_3$): δ = 1.17 (s) ppm. HR-MS (ESI): calcd. for $C_{35}H_{35}B_1Br_1N_2$ ($[M + H]^+$): 573.2077, found : 573.2074.

Synthesis of compound 5

Degassed 1,4-dioxane was added to a mixture of compound **3** (4.29 g, 8.77 mmol), potassium acetate (2.58 g, 26.31 mmol), bis(pinacolato)diboron (2.67 g, 10.52 mmol), Pd(dppf)Cl_2 (192 mg, 0.263 mmol, 3 mol%) under nitrogen atmosphere in a two necked round bottom flask fitted with refluxing condenser . After being stirred at 100 °C temperature for 12 h, the reaction mixture was poured into water, extracted with CH_2Cl_2. The combined organic layers were washed with brine solution, dried over Na_2SO_4 and concentrated. The residue was purified by silica gel column chromatography using *n*-hexane/ethyl acetate mixture as eluent. Yield: 4.00 g, (85%). mp: >300 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.31 (d, *J* = 8 Hz, 1H), 8.77 – 8.73 (m, 2H), 8.15 (d, *J* = 4.2 Hz, 1H), 7.88 – 7.71 (m, 7H), 7.55 (t, *J* = 8 Hz, 1H), 7.47 – 7.44 (m, 1H), 7.32 – 7.24 (m, 2H), 6.42 (d, *J* = 8 Hz, 1H), 1.37 (s, 12H), 0.49 (s, 6H) ppm. ^{13}C NMR (101 MHz, $CDCl_3$): δ = 172.05, 153.42, 136.90, 135.51, 131.48, 131.34, 131.22, 131.05, 130.31, 129.59, 129.34, 129.11, 128.98, 128.50, 127.50, 126.94, 126.73, 126.00, 125.76, 124.14, 123.60, 123.32, 122.33, 120.65, 120.10, 83.78, 24.99, 7.17 ppm. ^{11}B NMR (128 MHz, $CDCl_3$): δ = 32.75 (Boronate, s), 0.75 (BMe_2, s) ppm. HR-MS (ESI): calcd. for $C_{35}H_{35}B_2N_2O_2$ ($[M + H]^+$): 537.2891, found : 537.2915.

Synthesis of compound 6

Compound **6** was prepared following a procedure similar to that used for compound **5**. The quantities involved are as follows: Compound **4** (3.02 g, 5.27 mmol), potassium acetate (1.55 g, 15.81 mmol), bis(pinacolato)diboron (1.60 g, 6.32 mmol), Pd(dppf)Cl_2 (116 mg, 0.158 mmol, 3 mol%). Yield: 2.94 g, (90%). mp: 237 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.29 (d, *J* = 4 Hz, 1H), 8.75 (t, *J* = 8 Hz, 2H), 8.13 (d, *J* = 4 Hz, 1H), 7.84 (t, *J* = 8 Hz, 1H), 7.72 (t, *J* = 8 Hz, 1H), 7.62 – 7.53 (m, 5H), 7.46 – 7.43 (m, 1H), 7.31 – 7.29 (m, 2H), 6.42 (d, *J* = 4 Hz, 1H), 2.90 (t, *J* = 8 Hz, 2H), 1.84 – 1.79 (m, 2H), 1.48 – 1.43 (m, 6H), 1.36 (s, 12H), 1.00 (s, 3H), 0.48 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): δ = 171.95, 153.52, 146.61, 135.45, 134.24, 131.46, 131.13, 130.89, 130.20, 129.69, 129.25, 129.13, 128.93, 128.09, 127.43, 126.85, 126.63, 125.90, 125.71, 124.03, 123.63, 123.29, 122.38, 120.67, 120.15, 83.73, 35.86, 31.75, 31.33, 28.94, 24.98, 22.75, 14.23, 7.22. ^{11}B NMR (128 MHz, $CDCl_3$): δ = 38.56(Boronate, s), 3 (BMe_2, s) ppm. HR-MS (ESI): calcd. for $C_{41}H_{47}B_2N_2O_2$ ($[M + H]^+$): 621.3832, found : 621.3827.

NLO Measurements:

The NLO measurements were carried out using single-beam Z-scan experiment[5] for all the dimers in solution. For this purpose, CH_2Cl_2 was used as a solvent and the concentration for Phe-dimer and all its derivatives solution were kept at 10 μM. The Z-scan experimental arrangement is shown in Figure S1, which consists of Yb-doped fiber laser source (Model: Cazadero,M/S Calmar Inc., USA) as pump which emits Fourier-transform limited (FTL) ultrashort pulses ($\Delta\tau \approx 370$fs) at an operating wavelength of λ= 1030 nm. The pump laser is frequency-doubled for carrying out two-photon absorption measurements. In order to achieve it, the pump beam is optimally focused (using a convex lens L_1 of 75 mm focal length) to a waist w_0 = 28 μm at the center of a 4 mm long LiB_3O_6 (LBO) crystal (with crystal cut $\theta = 90^0$, $\varphi = 11.3^0$) whose entry and exit faces are anti-reflection (AR) coated at 1030 nm as well as 515 nm wavelength. A zero-order half-wave plate was employed just before the lens L_1 in order to obtain an appropriate polarization for carrying out type-I (e+e→o) phase-matching.[6] This generates transform-limited green ultrashort ($\Delta\tau \approx 300$ fs) pulses at 1 kHz repetition rate (RR) and average energy of 3 μJ. The frequency doubling arrangement is marked (as (a)) in the Figure S1.

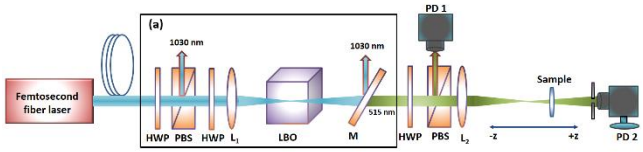


Figure S1: Schematic of Z-scan experimental setup. Inset 1(a) represents experimental setup of second harmonic generation (SHG) of the pump beam. HWP: half wave plate, PBS: polarizing beam splitter, L1: lens (75mm), L2: lens (100mm), PD1: reference photodetector, PD2: signal photodetector.

The nonlinear (NLO) coefficients, namely, nonlinear refractive index (n_2) and nonlinear absorption (β) were estimated using closed-aperture (CA) and open-aperture (OA) single-beam Z-scan technique. All the measurements were carried out at 515 nm wavelength and at 1 kHz repetition rate (RR). In order to perform the experiment, the frequency-doubled beam was split into two beams using a polarizing beam splitter (PBS1). The reflected beam was detected by a semiconductor photodiode sensor PD1 (model: PD300-3W-V1, M/S Ophir Inc., USA) and it served as a reference beam for ascertaining unwanted fluctuations. The transmitted beam was focused at z = 0 by a lens L_1 (f = 100 mm) and a 1 mm thick quartz cell with dimer solution moved along the *z*-axis through z = 0. The open-aperture (OA) transmitted beam was measured by photodiode sensor PD2 (model: PD300-3W-V1, M/S Ophir Inc., USA). For closed-aperture (CA) Z-scan measurements, the transmitted power was measured through a partially closed aperture with linear transmittance of 0.1 by photodetector (PD2). Before the measurements on phenanthroimidazole dimers, the Z-scan set-up was precisely calibrated using standard 3-Methyl Indole (3MI) at similar green laser fluence.

In order to obtain the value of nonlinear absorption coefficient (β), the measured open-aperture (OA) normalized transmittance is fitted with an analytical expression is given by M. Sheikh Bahae *et al*.[5],

$$T_{OA}(z, S = 1) = 1 - \frac{\beta I_0 L_{eff}}{2^{\frac{3}{2}}(1 + x^2)}$$

where $x = z/z_0$, z_0 being the Rayleigh length, I_0 is the on-axis peak irradiance at focus ($z = 0$), L_{eff} is the effective sample length which is given by $L_{eff} = (1\text{-}e^{\alpha L})/\alpha$ (L is cuvette thickness and α is linear absorption coefficient).

The measured data for closed aperture (CA) normalized transmittance has been fitted with the analytical expression mentioned below:[7]

$$T_{CA}(z, \Delta\varphi_0) = 1 - \frac{4\Delta\varphi_0 x}{(x^2 + 9)(x^2 + 1)} - \frac{2(x^2 + 3)\Delta\Psi_0}{(x^2 + 9)(x^2 + 1)}$$

where T_{CA} represents the normalized transmittance, $x = z/z_0$, $\Delta\varphi_0$ is the on-axis phase-shift at focus. It is related to nonlinear refractive index through $\Delta\varphi_0 = kn_2 I_0 L_{eff}$, $k = 2\text{p}/\lambda$, $\lambda = 515$ nm, $\Delta\Psi_0 = \beta I_0 L_{eff}/2$ are the respective phase changes due to nonlinear absorption. It is worthwhile to point out that the two-photon absorption (TPA) or nonlinear absorption (NLA) has been accounted for in the expression defining T_{CA}. In fact, the asymmetry in the CA normalised transmission is a signature of NLA being present in the trace.

References:

1. B. Pal, W.-C. Yen, J.-S. Yang, W.-F. Su, *Macromolecules* 2007, **40**, 8189.
2. N. A. Rice, A. Adronov, *Macromolecules* 2013, **46**, 10, 3850.
3. B. N. Norris, S. Zhang, C. M. Campbell, J.T. Auletta, P. Calvo-Marzal, G. R. Hutchison, T. Y. Meyer, *Macromolecules* 2013, **46**, 1384.
4. Gaussian 09 (Rev. C.02), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, _. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
5. M. S. Bahae, A. A. Said, T. H. Wei, D. J. Hagan, E. W. V. Stryland, *IEEE Journal of Quantum Electron.*,1990, **26**, 760.

6. M. K. Shukla, S. Kumar, R. Das, *Appl. Phys. B*, 2016, **122**, 114.
7. M. Yin, H. Li, S. H. Tang, W. Ji, *Appl. Phys. B*, 2000, **70**, 587.

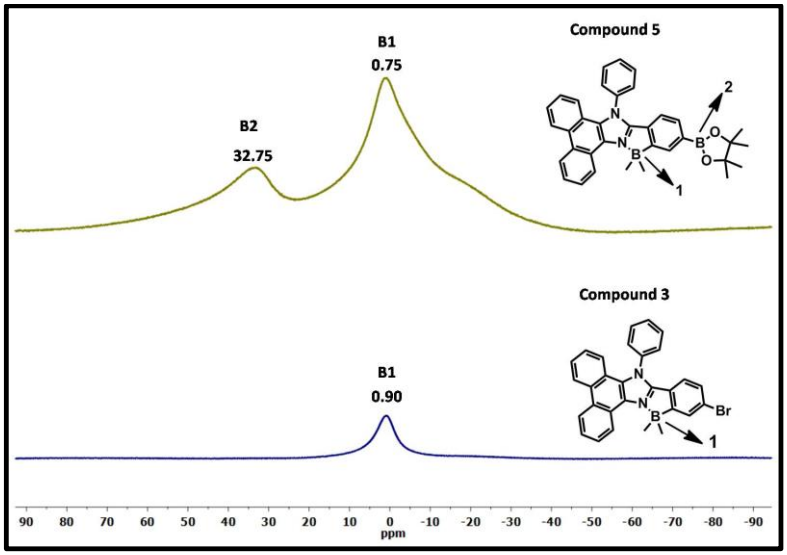
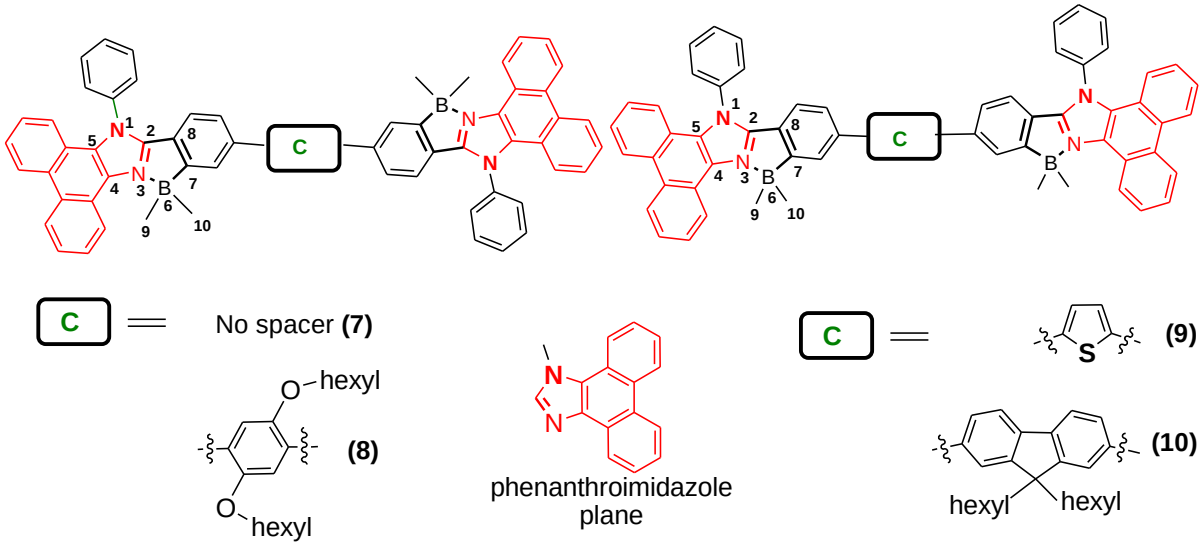


Figure S2: ^{11}B NMR of compounds **3** and **5**.

Table S1: Comparison of selected bond lengths [Å] and bond angles [deg] (X-ray and DFT) for compounds **7- 10**.



Compound	7		8		9		10	
	X-ray	DFT	X-ray	DFT	X-ray	DFT	X-ray	DFT
B6-C9	1.604(4)	1.630	1.623(6)	1.629	1.620(5)	1.630	1.604(6)	1.630
B6-C10	1,616(4)	1.630	1.605(6)	1.629	1.632(5)	1.630	1.610(5)	1.629
B6-C7	1.622(3)	1.623	1.621(5)	1.626	1.617(5)	1.623	1.606(5)	1.623
B6-N3	1.656(3)	1.671	1.661(5)	1.680	1.645(4)	1.671	1.653(4)	1.672
N3-C4	1.388(3)	1.385	1.382(4)	1.385	1.389(3)	1.395	1.384(4)	1.385
C4-C5	1.365(3)	1.391	1.371(4)	1.391	1.376(4)	1.397	1.368(4)	1.391
N1-C5	1.404(2)	1.404	1.403(4)	1.405	1.410(4)	1.415	1.402(4)	1.404
N3-C2	1.332(3)	1.340	1.340(4)	1.340	1.329(4)	1.352	1.325(4)	1.339
N1-C2	1.350(3)	1.364	1.348(4)	1.364	1.353(4)	1.373	1.356(4)	1.364
C2-C8	1.449(3)	1.447	1.448(4)	1.447	1.449(4)	1.443	1.451(4)	1.447
C7-C8	1.397(3)	1.414	1.402(4)	1.413	1.396(4)	1.422	1.409(4)	1.414
C9-B6-C10	116.7(2)	115.4	115.6(3)	115.3	115.3(3)	115.4	114.9(3)	115.5
C9-B6-C7	111.1(2)	111.6	111.8(3)	111.5	111.8(3)	111.4	112.6(3)	111.3
C10-B6-C7	111.1(2)	111.4	112.4(3)	111.4	111.6(3)	111.5	110.8(3)	111.5
C9-B6-N3	112.3(2)	110.4	110.0(3)	110.7	109.5(3)	110.6	111.0(3)	110.4
C10-B6-N3	108.5(2)	110.7	110.0(3)	110.6	111.4(3)	110.6	110.8(3)	110.7
C7-B6-N3	94.9(2)	95.4	95.1(3)	95.2	95.5(3)	95.4	114.9(3)	95.4

Table S2: Crystal data and structure refinement parameters for compounds **7**, **8, 9** & **10**.

Compound	**7**	**8**	**9**	**10**
Empirical formula	$C_{70}H_{68}B_2N_4$	$C_{78}H_{74}B_2Cl_6N_4O_2$	$C_{62}H_{46}B_2N_4S$	$C_{83}H_{76}B_2N_4$
Formula weight	986.90	1333.73	900.71	1151.09
Temperature/K	100.00	296.15	296.15	296.15
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	C2/c	*C*2/c	*P*-1	*P*-1
a/Å	16.7657(16)	24.990(2)	10.0256(8)	15.4087(5)
b/Å	17.7131(16)	18.4811(17)	11.0728(11)	16.2830(6)
c/Å	38.891(3)	17.3011(17)	23.605(2)	16.8471(8)
α/°	90	90	82.719(5)	103.453(4)
β/°	95.378(7)	108.166(6)	81.300(5)	115.561(4)
γ/°	90	90	78.268(6)	105.550(3)
Volume/Å^3	11498.7(18)	7592.2(12)	2523.7(4)	3365.7(3)
Z	8	4	2	2
ρ_{calcd}/g cm^{-3}	1.140	1.167	1.185	1.136
μ/mm^{-1}	0.065	0.272	0.108	0.492
F (000)	4208.0	2792.0	944.0	1224.0
2θ range for data collection/°	3.352 to 56.956	2.792 to 50.874	1.754 to 50.812	8.688 to 136.476
Index ranges	$-22 \le h \le 22$, $-23 \le k \le 23$, $-52 \le l \le 0$	$-30 \le h \le 30$, $-22 \le k \le 22$, $-20 \le l \le 20$	$-12 \le h \le 11$, $-13 \le k \le 13$, $-28 \le l \le 28$	$-18 \le h \le 18$, $-19 \le k \le 16$, $-20 \le l \le 17$
Reflns. collected	28794	46270	24254	33325
Independent reflns	14456 [R_{int} = 0.0593, R_{sigma} = 0.0809]	7001 [R_{int} = 0.1419, R_{sigma} = 0.0947]	9227 [R_{int} = 0.0722, R_{sigma} = 0.1251]	12279 [R_{int} = 0.0367, R_{sigma} = 0.0428]
Data/restraints/ parameters	14456/0/691	7001/55/456	9227/0/626	12279/102/976
GOF on F^2	1.107	0.933	0.896	1.031
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0731, wR_2 = 0.2060	R_1 = 0.0764, wR_2 = 0.1972	R_1 = 0.0614, wR_2 = 0.1345	R_1 = 0.0830, wR_2 = 0.2417
R indices (all data)	R_1 = 0.1209, wR_2 =0.2287	R_1 = 0.1665, wR_2 = 0.2331	R_1 = 0.1535, wR_2 = 0.1577	R_1 = 0.1181, wR_2 = 0.2715
Largest diff. peak /hole [e Å^{-3}]	0.96/-0.61	0.35/-0.34	0.23/-0.28	0.42/-0.39

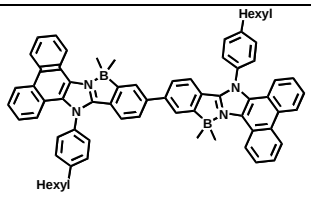
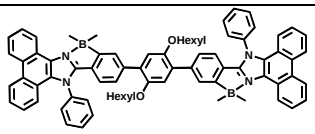
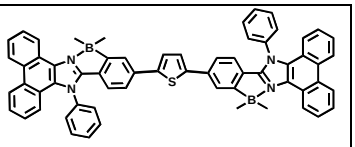
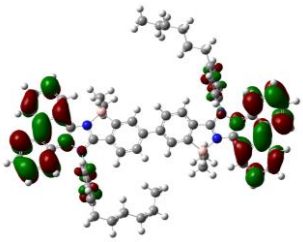
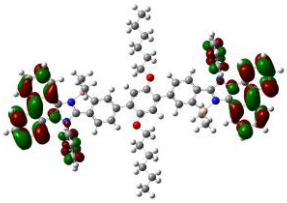
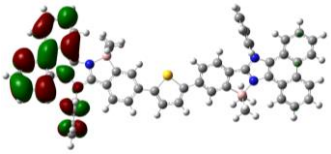
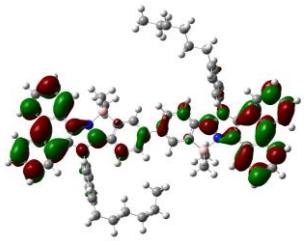
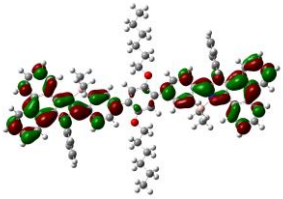
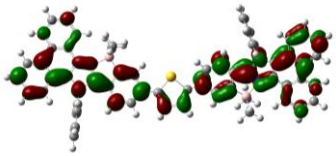
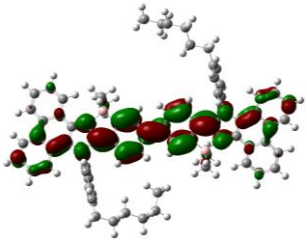
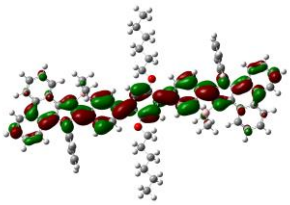
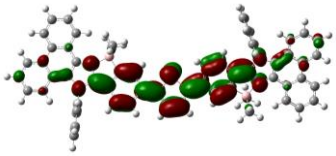
Table S3. Calculated electronic transitions for compound **7-11** from TD-DFT (B3LYP) calculations

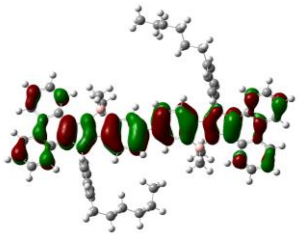
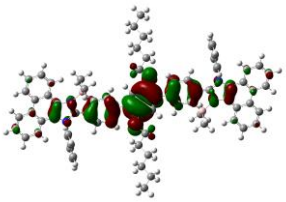
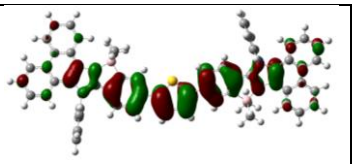
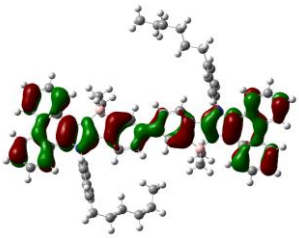
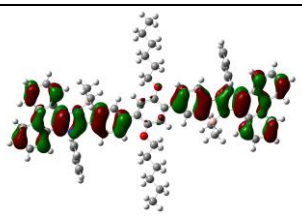
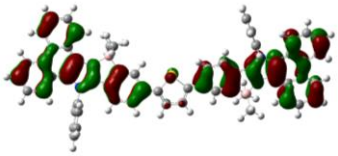
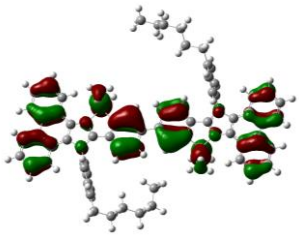
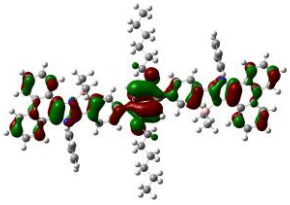
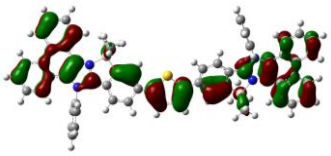
Compound	Transition	MO contributions	Energy gap eV (nm)	Oscillator strength/f
7	$S_0 \rightarrow S_1$	HOMO→LUMO	3.19 (387)	1.7772
	$S_0 \rightarrow S_2$	HOMO-1→LUMO	3.61 (342)	0.0006
		HOMO-1→LUMO+2		
		HOMO→LUMO+1		
		HOMO→LUMO+3		
	$S_0 \rightarrow S_3$	HOMO-1→LUMO+1	3.67 (337)	0.0245
		HOMO-1→LUMO+3		
		HOMO→LUMO+2		
8	$S_0 \rightarrow S_1$	HOMO→LUMO	3.05 (405)	1.4967
	$S_0 \rightarrow S_2$	HOMO→LUMO+1	3.40 (364)	0.0000
	$S_0 \rightarrow S_3$	HOMO-2→LUMO	3.54 (349)	0.0354
		HOMO-2→LUMO+2		
		HOMO-1→LUMO+1		
		HOMO-1→LUMO+3		
		HOMO→LUMO+2		
9	$S_0 \rightarrow S_1$	HOMO→LUMO	2.73 (454)	2.2820
	$S_0 \rightarrow S_2$	HOMO-1→LUMO	3.30 (331)	0.0035
		HOMO→LUMO+1		
	$S_0 \rightarrow S_3$	HOMO-1→LUMO	3.40 (363)	0.0587

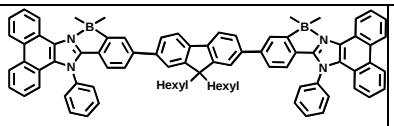
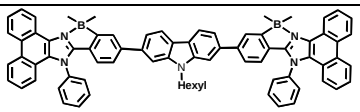
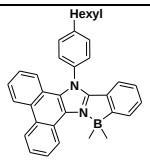
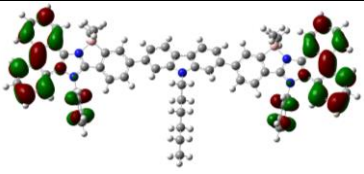
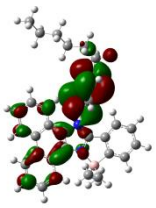
		HOMO→LUMO+1 HOMO→LUMO+2 HOMO→LUMO+3		
10	$S_0 \rightarrow S_1$ $S_0 \rightarrow S_2$ $S_0 \rightarrow S_3$	HOMO-1→LUMO+1 HOMO→LUMO HOMO-1→LUMO HOMO→LUMO+1 HOMO-2→LUMO+1 HOMO-1→LUMO HOMO→LUMO+1	3.12 (397) 3.48 (355) 3.57 (344)	2.6668 0.0109 0.0005
11	$S_0 \rightarrow S_1$ $S_0 \rightarrow S_2$ $S_0 \rightarrow S_3$	HOMO-2→LUMO+1 HOMO→LUMO HOMO-1→LUMO HOMO-2→LUMO HOMO→LUMO+1	3.14 (394) 3.33 (371) 3.48 (356)	2.6432 0.0116 0.0272
Monomer	$S_0 \rightarrow S_1$ $S_0 \rightarrow S_2$ $S_0 \rightarrow S_3$	HOMO-1→LUMO HOMO→LUMO HOMO→LUMO+1 HOMO-2→LUMO HOMO→LUMO HOMO→LUMO+1 HOMO→LUMO+2 HOMO→LUMO HOMO→LUMO+1	3.69 (335) 3.84 (322) 3.91 (316)	0.2258 0.1941 0.0557

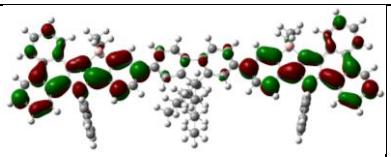
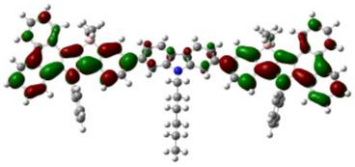
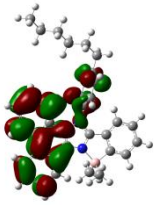
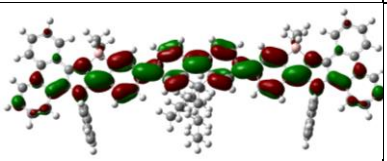
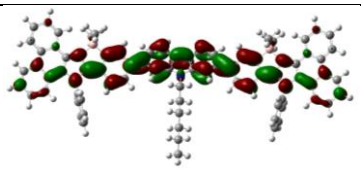
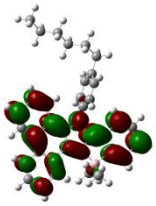
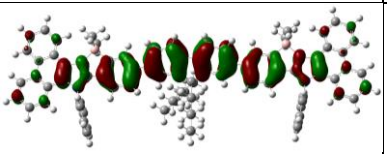
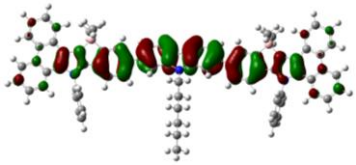
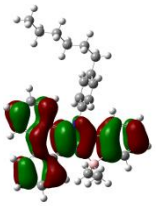
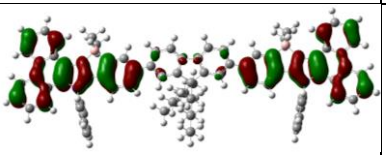
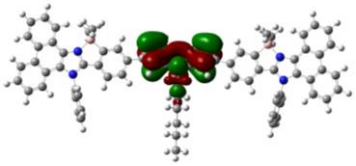
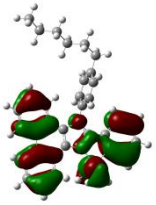
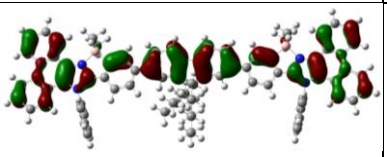
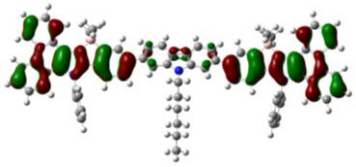
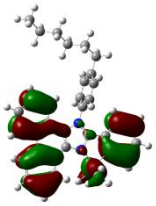
		HOMO→LUMO+2 HOMO→LUMO+3		

Table S4. Computed orbitals for compounds **7**-**11**

Compound	 **7**	 **8**	 **9**
LUMO+2	 -0.9248 eV	 -0.9248 eV	 -1.0064 eV
LUMO+1	 -0.9792 eV	 -1.088 eV	 -1.1968 eV
LUMO	 -1.4416 eV	 -1.3328 eV	 -1.768 eV

HOMO	 -5.0592 eV	 -4.8416 eV	 -4.896 eV
HOMO-1	 -5.44 eV	 -5.304 eV	 -5.412 eV
HOMO-2	 -5.984 eV	 -5.3584 eV	 -5.8208 eV

Compound	 **10**	 **11**	 **Monomer**
LUMO+2	 -1.0064 eV	 -0.9792 eV	 -0.864 eV

LUMO+1	 -1.224 eV	 -1.1968 eV	 -0.972 eV
LUMO	 -1.496 eV	 -1.4416 eV	 -1.161 eV
HOMO	 -5.032 eV	 -5.0048 eV	 -5.319 eV
HOMO-1	 -5.358 eV	 -5.1952 eV	 -5.967 eV
HOMO-2	 -5.6848 eV	 -5.3312 eV	 -6.048 eV

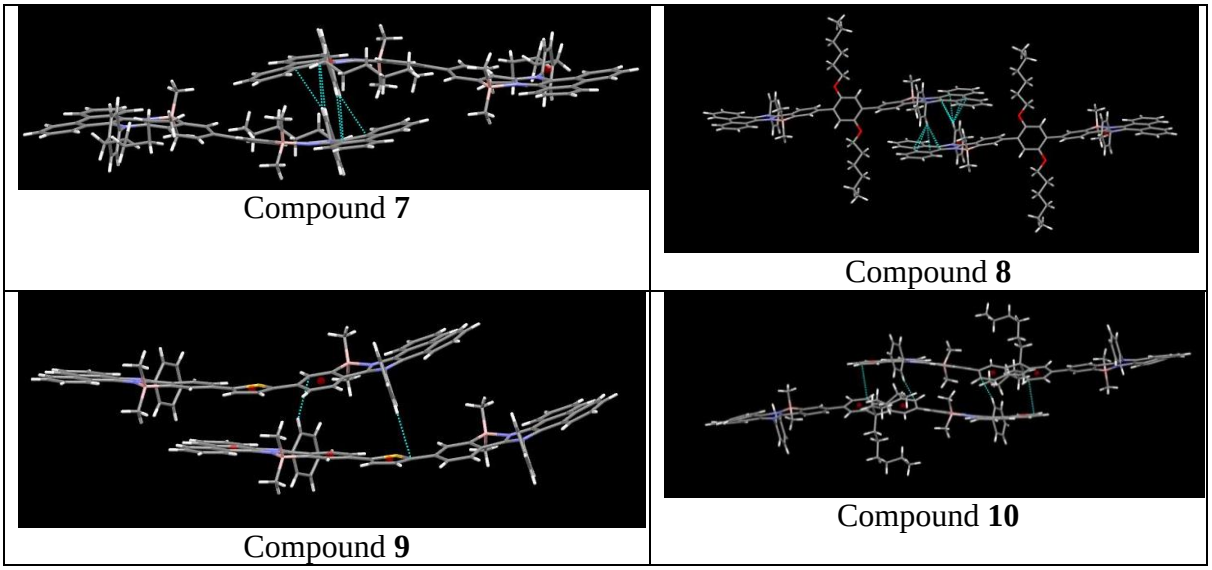


Figure S3. X-ray crystal packing of compounds **7**-**10**

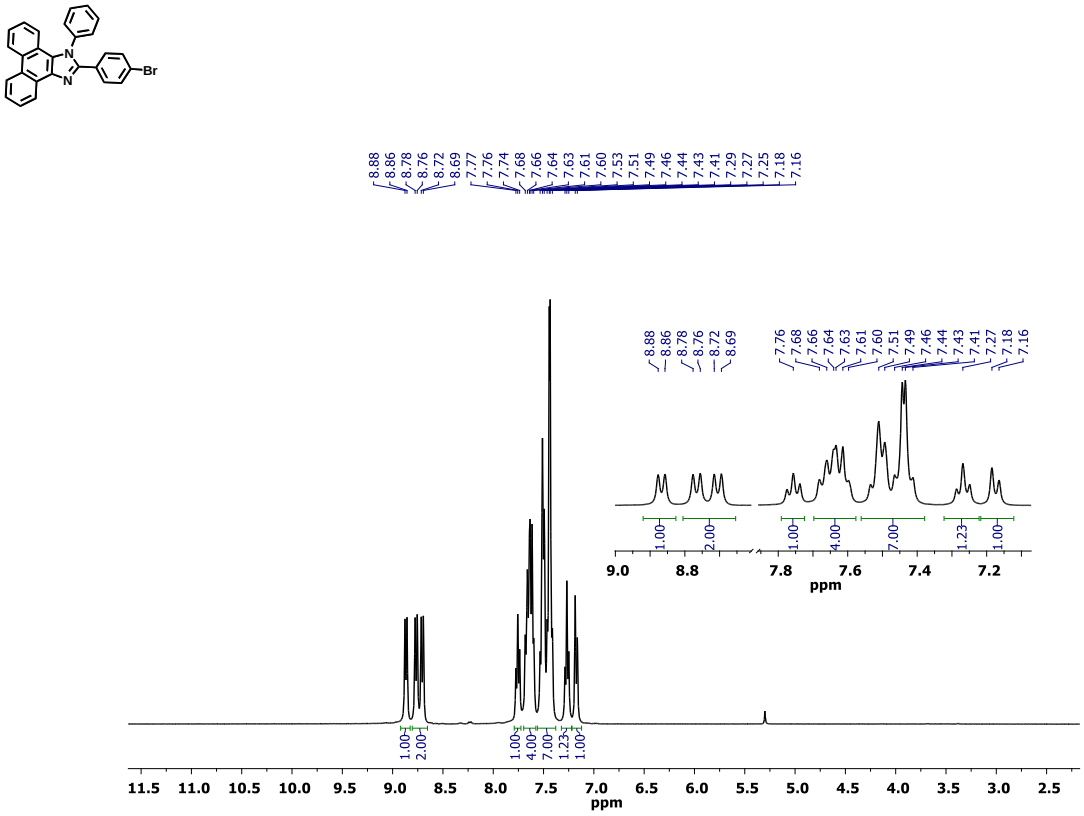
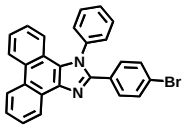


Figure S4. ^{1}H NMR spectrum of compound **1**



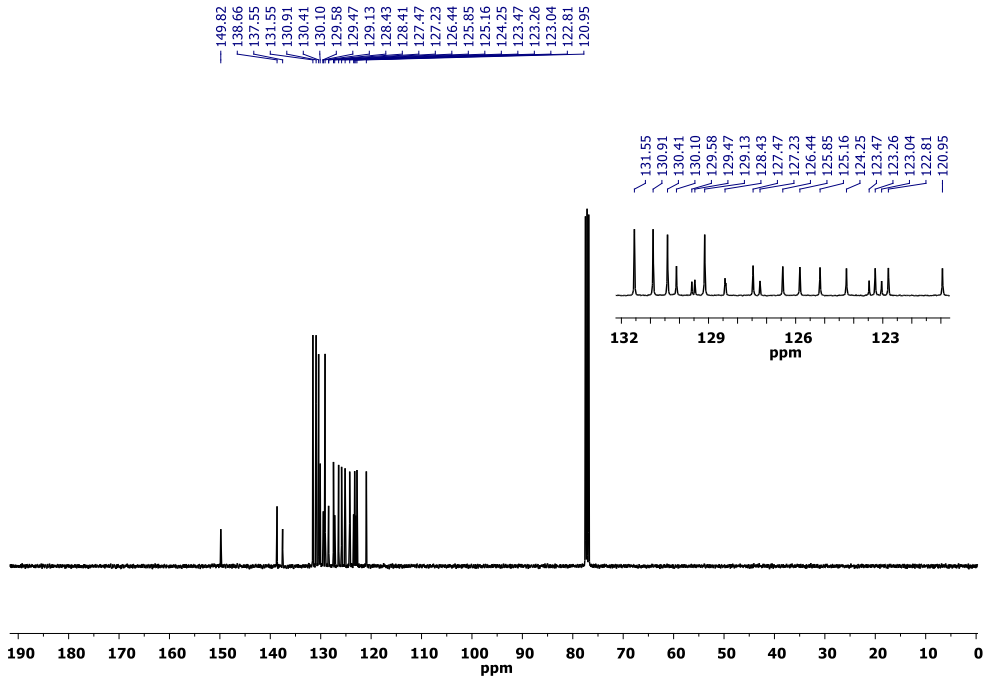
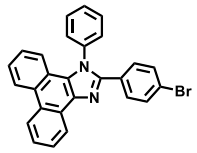


Figure S5. ^{13}C NMR spectrum of compound **1**



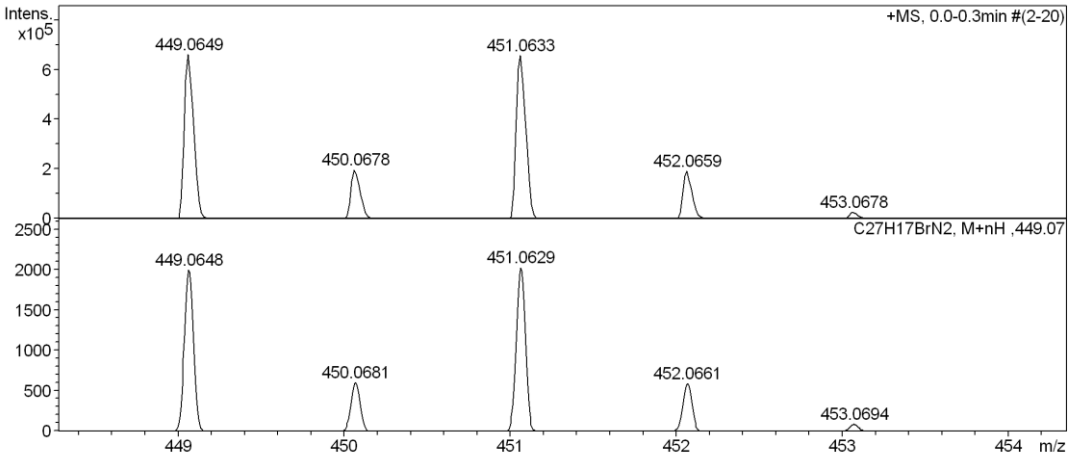


Figure S6. HRMS of compound **1**

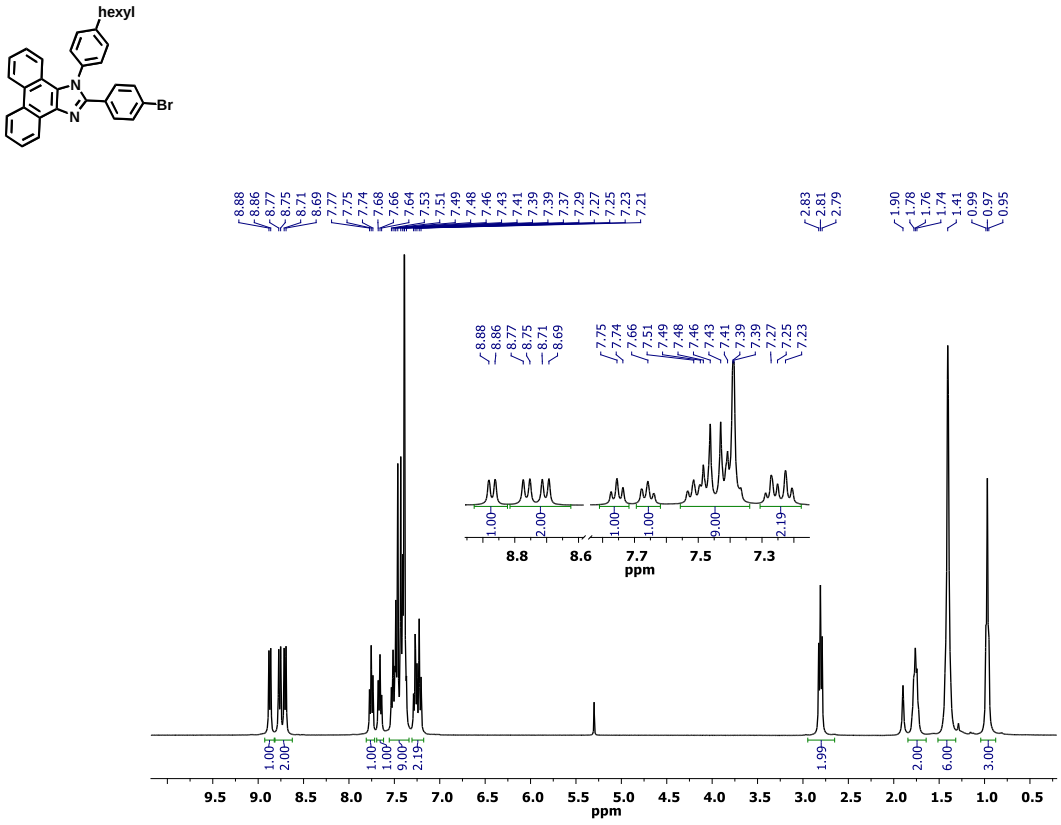


Figure S7.[1]H NMR spectrum of compound **2**

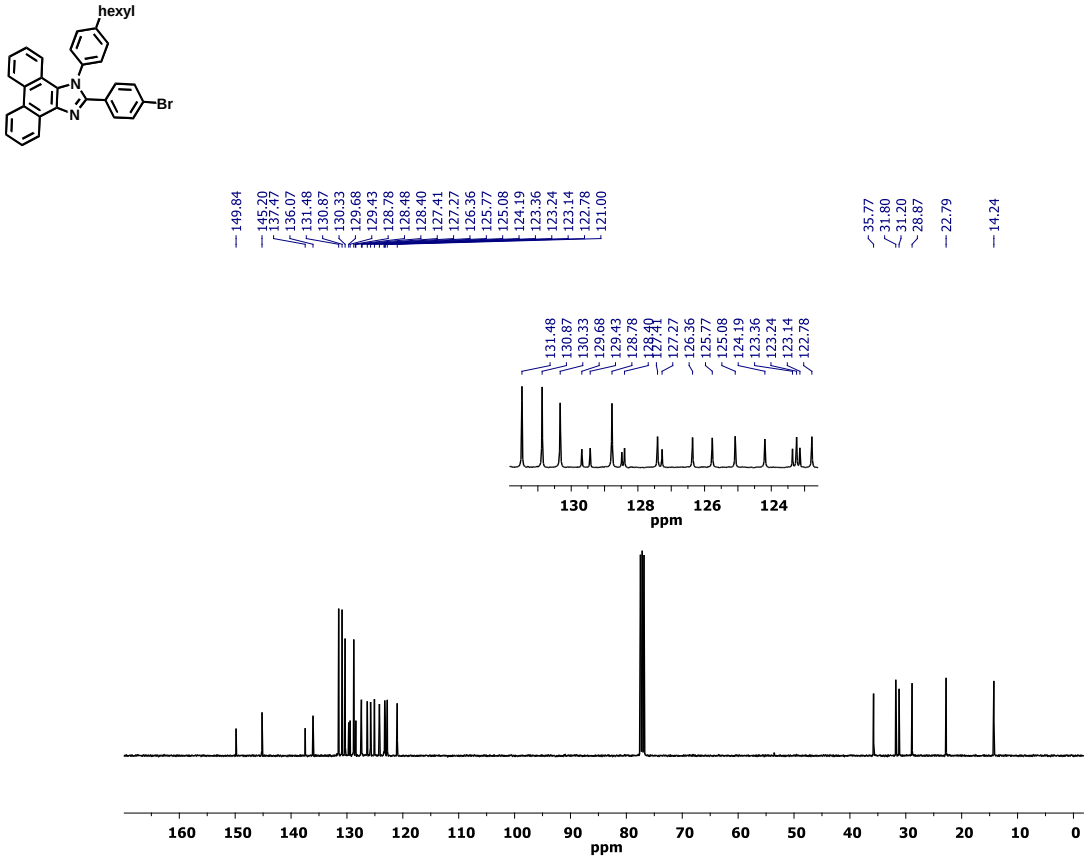


Figure S8.[13]C NMR spectrum of compound **2**

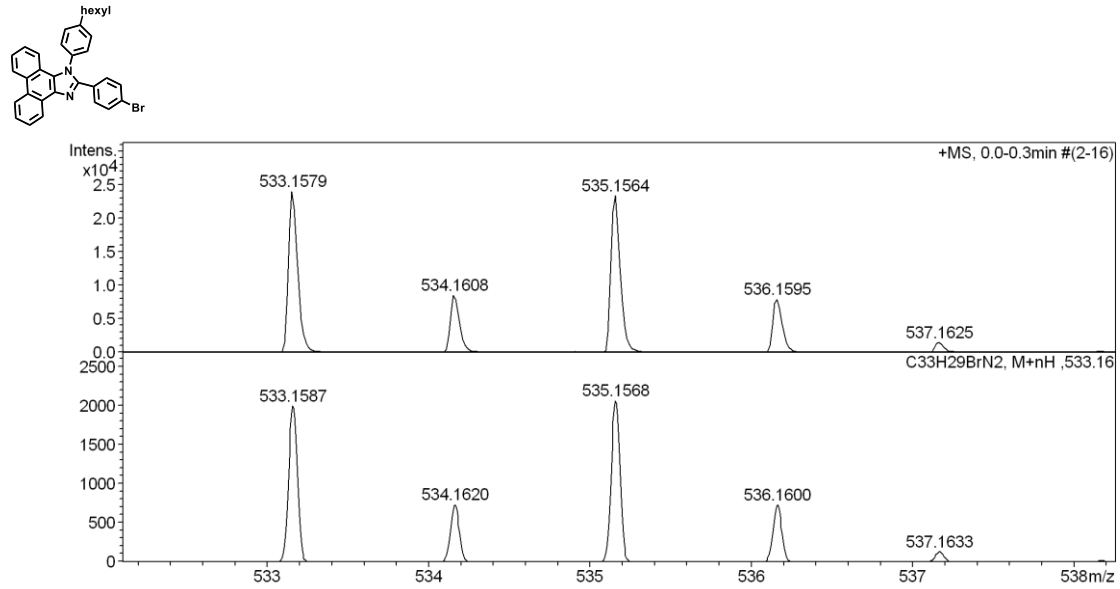


Figure S9. HRMS of compound **2**

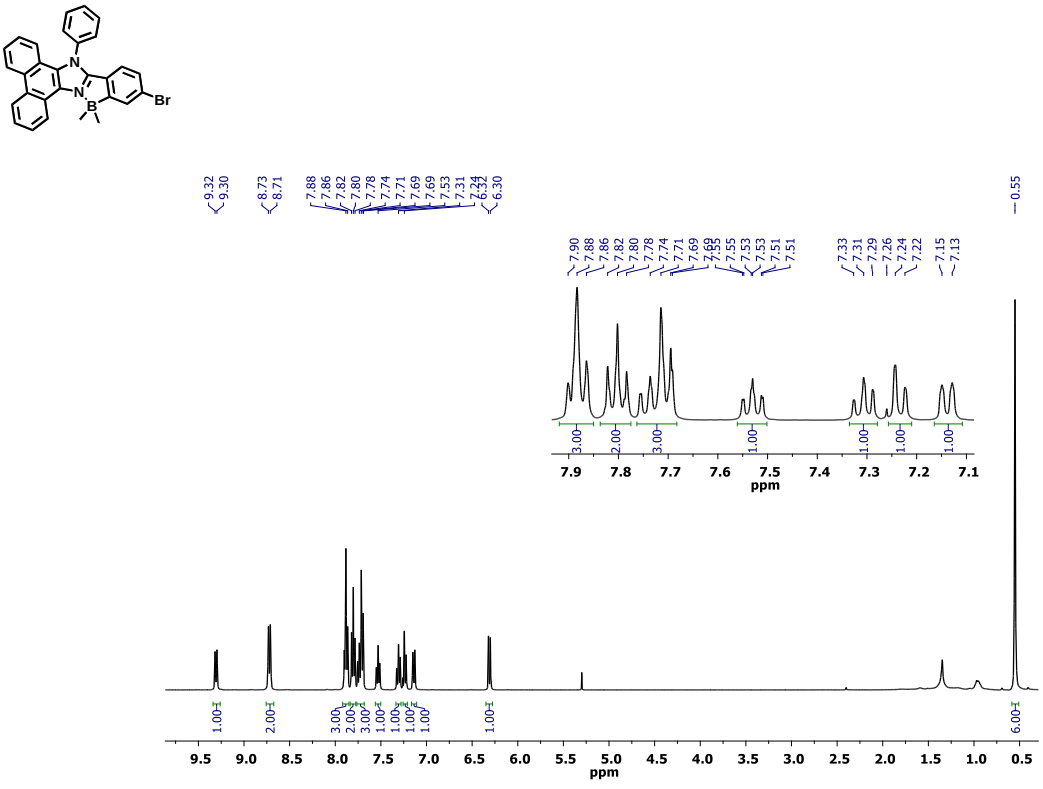


Figure S10. ^{1}H NMR spectrum of compound **3**

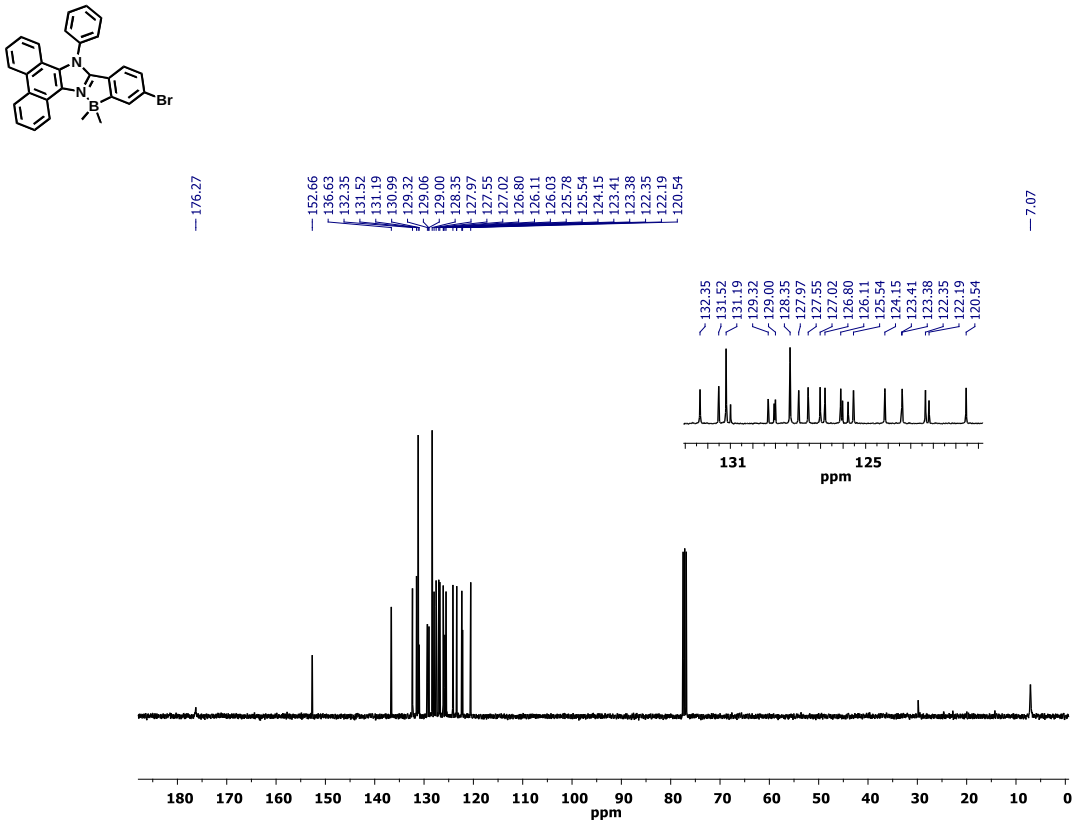


Figure S11. ^{13}C NMR spectrum of compound **3**

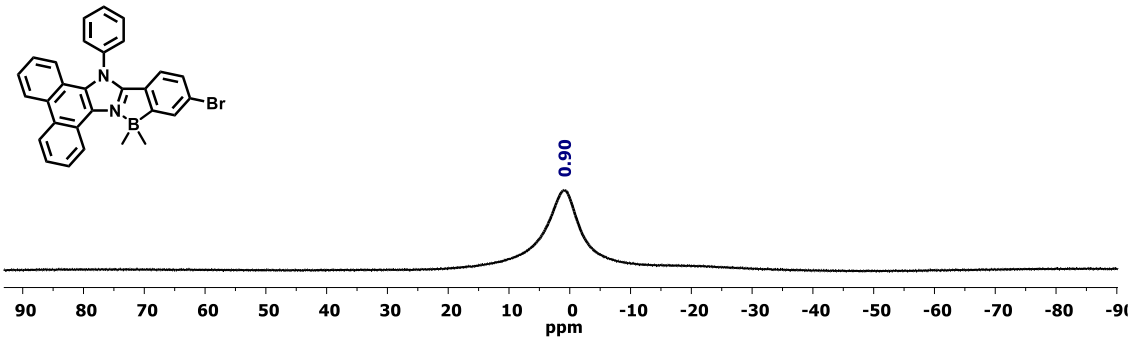


Figure S12. ^{11}B NMR spectrum of compound **3**

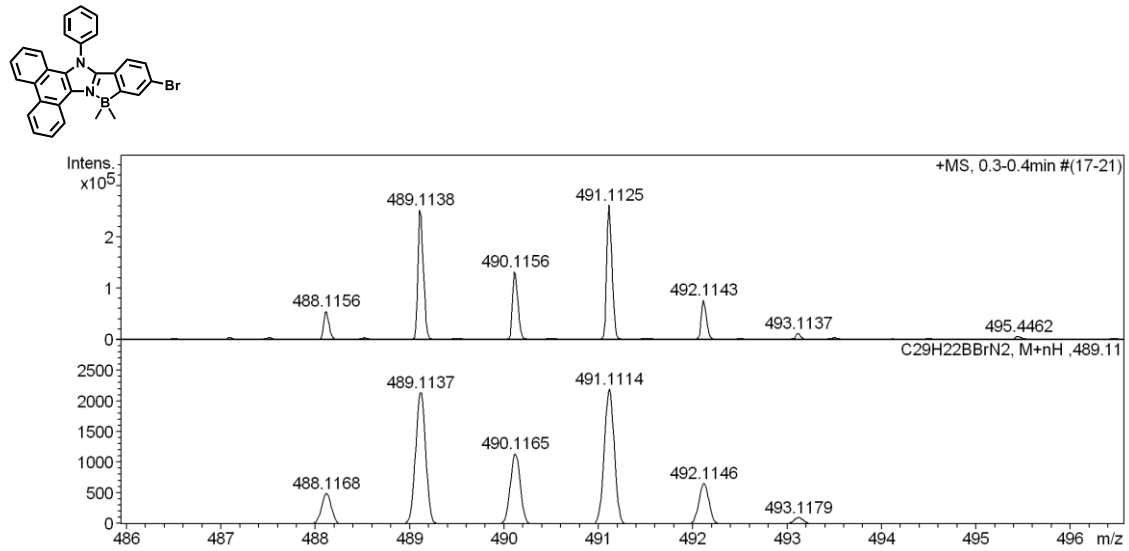


Figure S13. HRMS of compound **3**

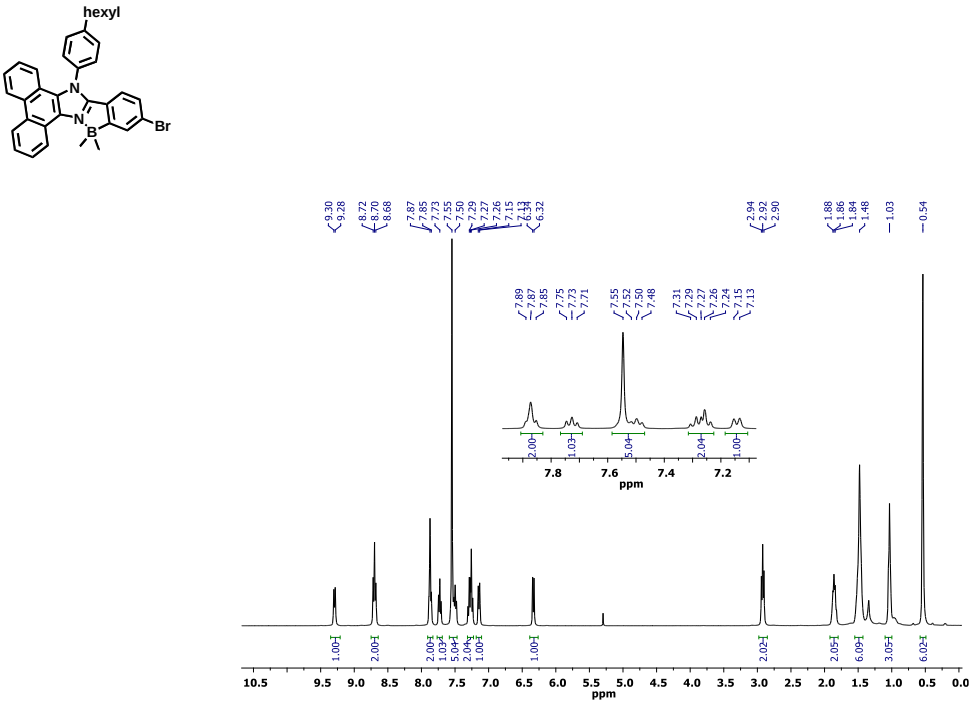


Figure S14. ^{1}H NMR spectrum of compound **4**

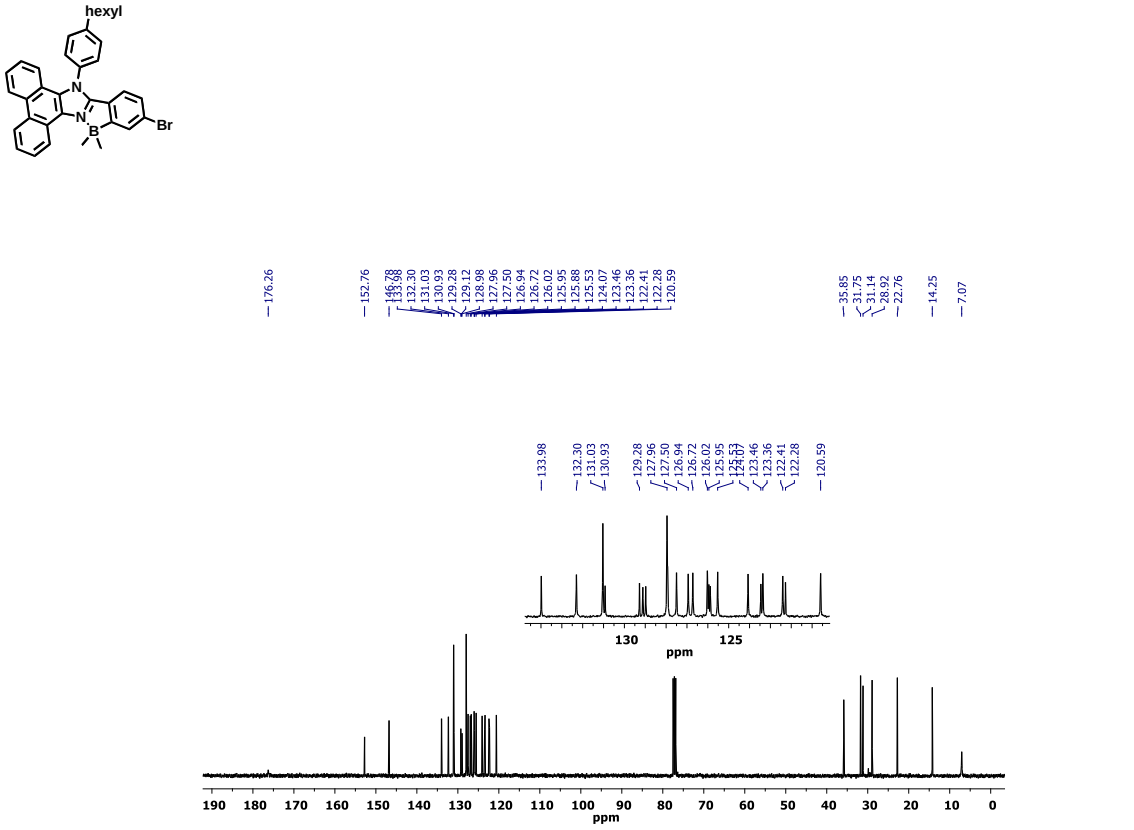


Figure S15. ^{13}C NMR spectrum of compound **4**

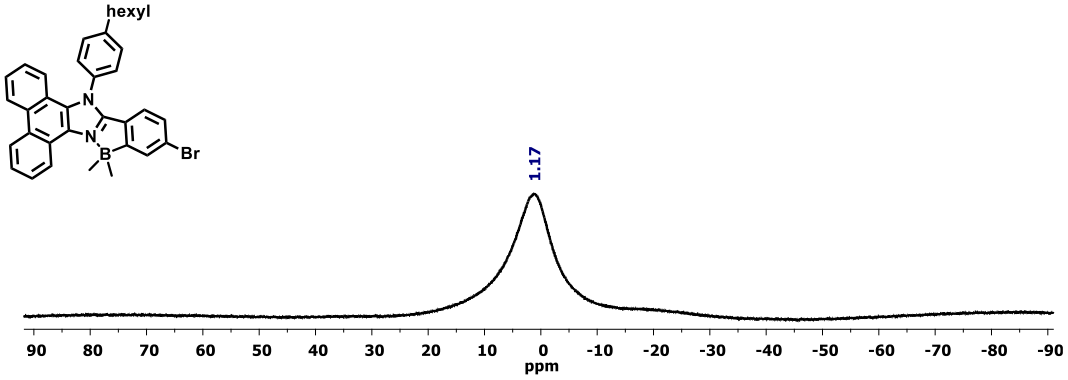
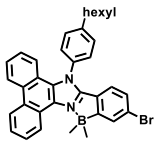


Figure S16. ^{11}B NMR spectrum of compound **4**



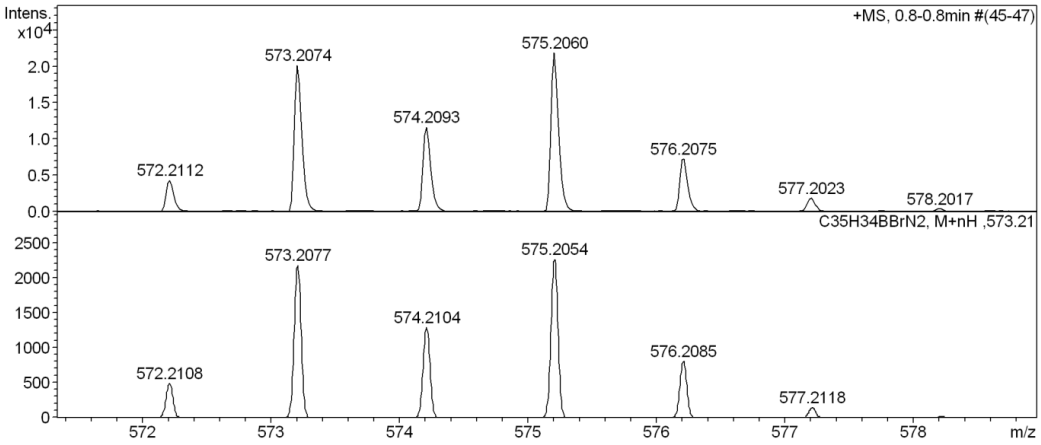
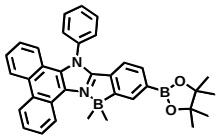


Figure S17. HRMS of compound **4**



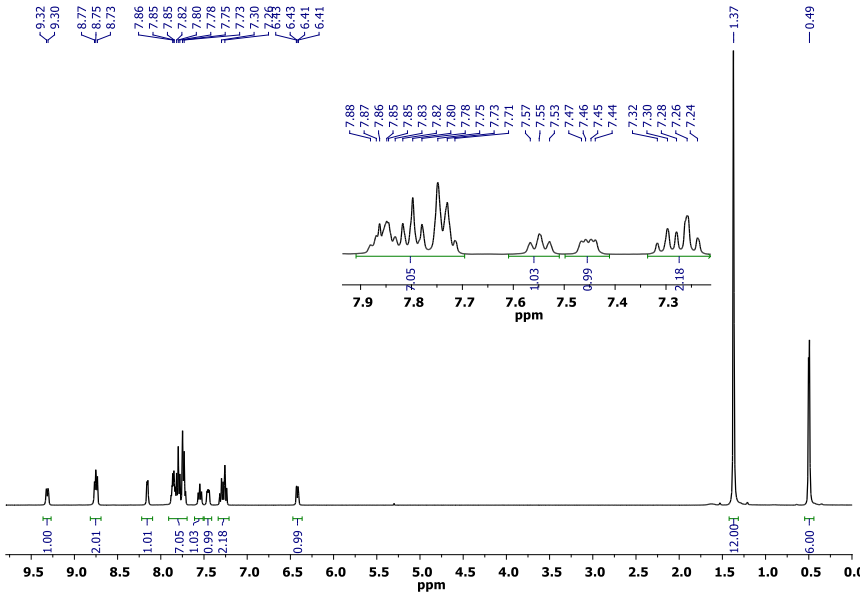
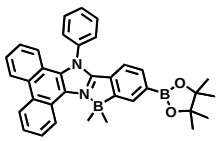


Figure S18. ^{1}H NMR spectrum of compound **5**



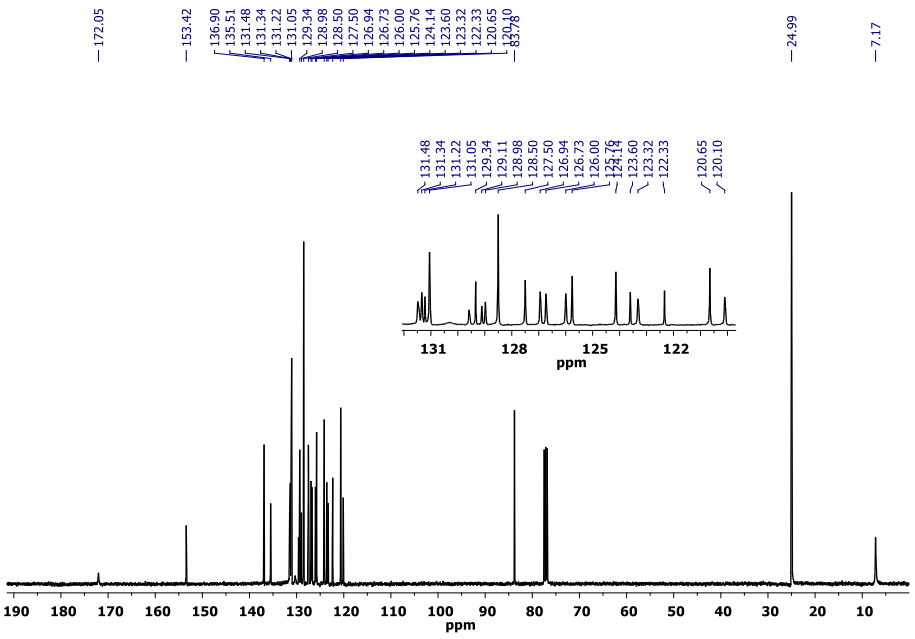


Figure S19. ^{13}C NMR spectrum of compound **5**

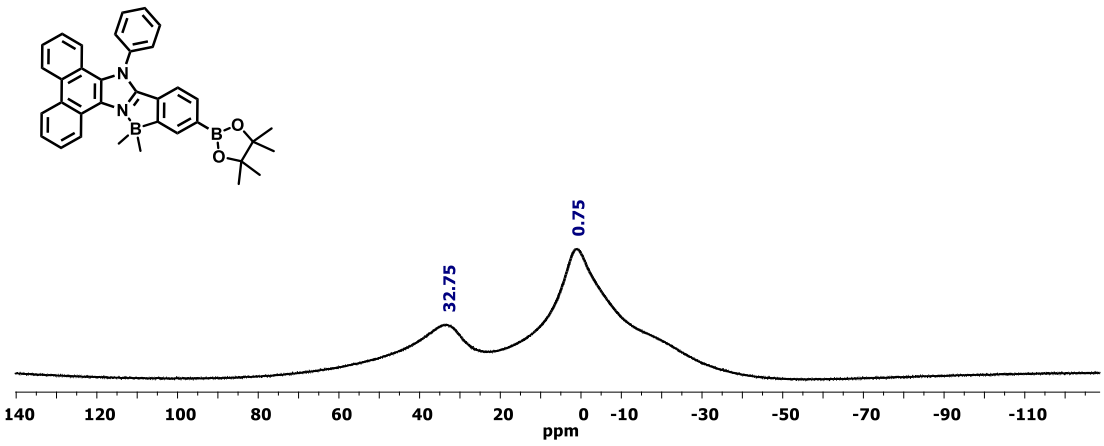


Figure S20. ^{11}B NMR spectrum of compound **5**

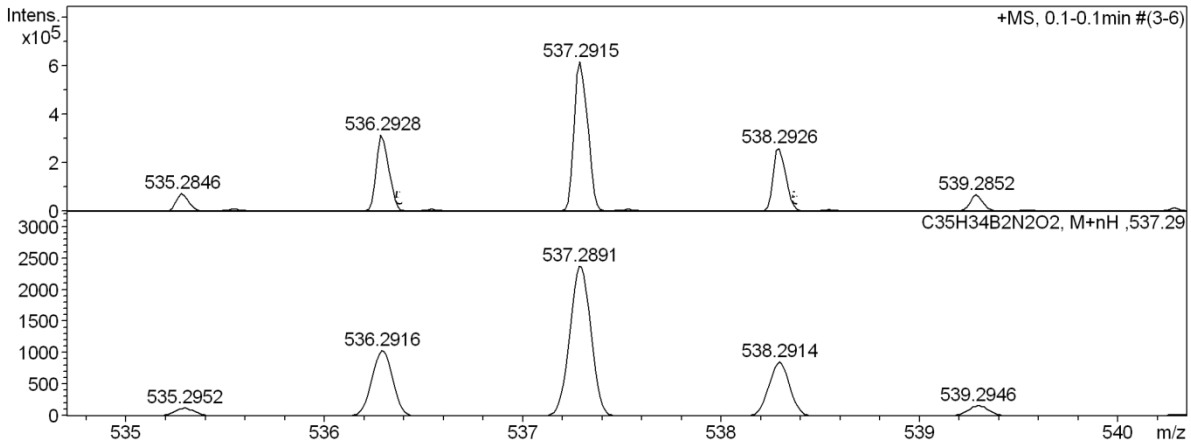


Figure S21. HRMS of compound **5**

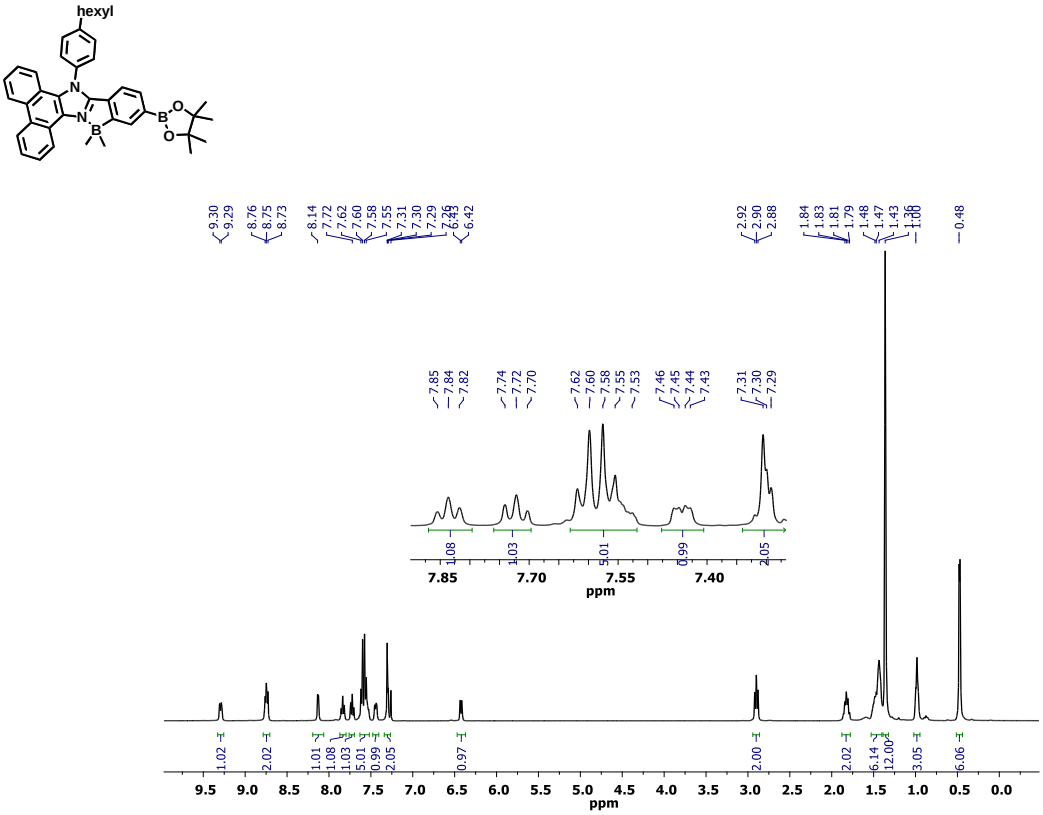
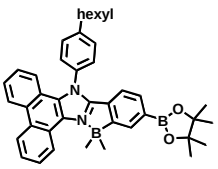


Figure S22. ^{1}H NMR spectrum of compound **6**



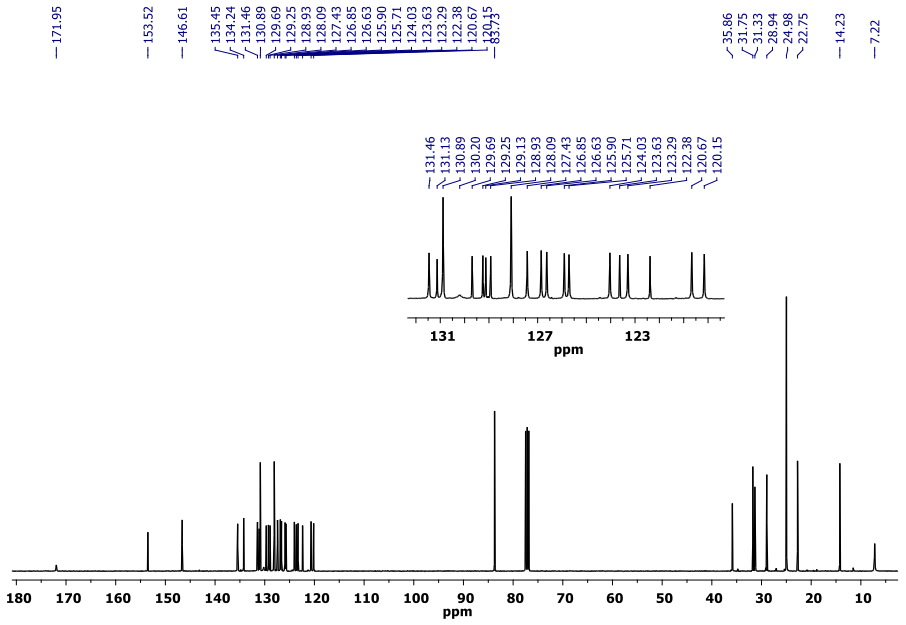


Figure S23. ^{13}C NMR spectrum of compound **6**

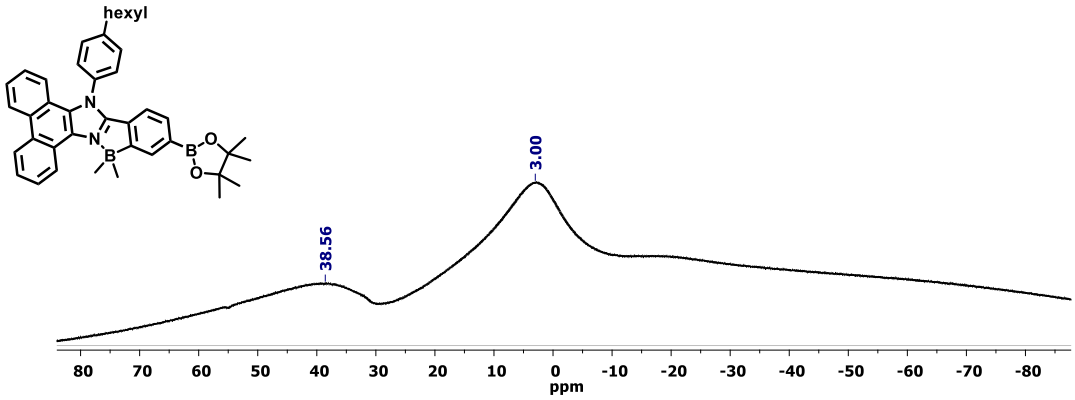
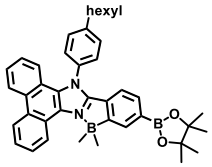


Figure S24. ^{11}B NMR spectrum of compound **6**



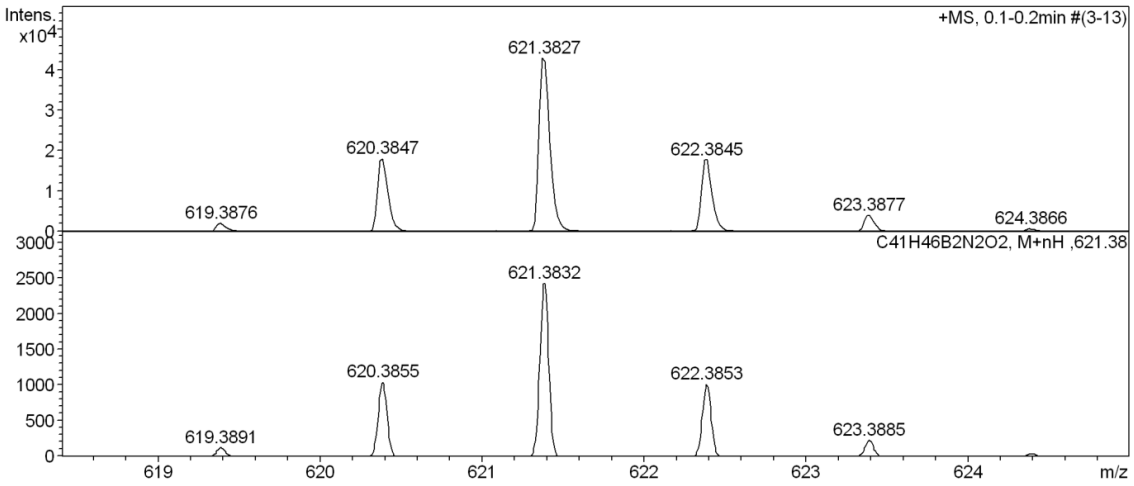


Figure S25. HRMS of compound **6**

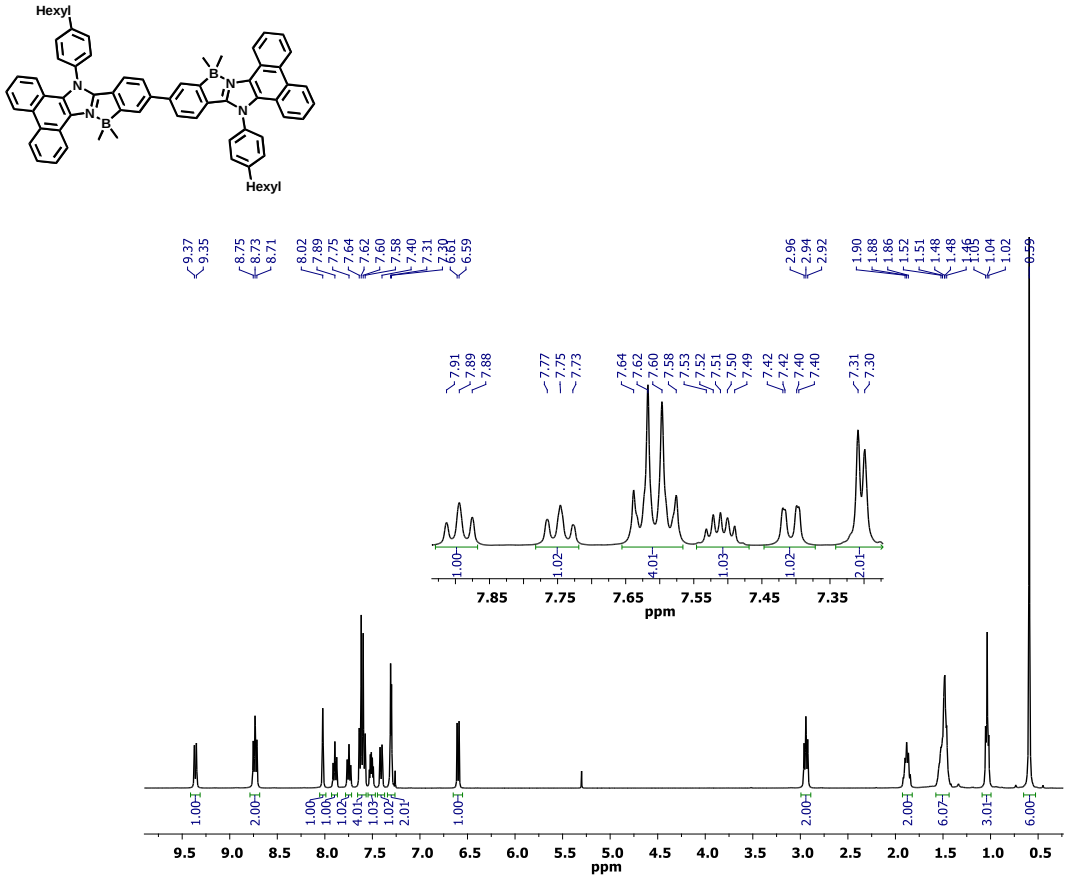


Figure S26. ^{1}H NMR spectrum of compound **7**

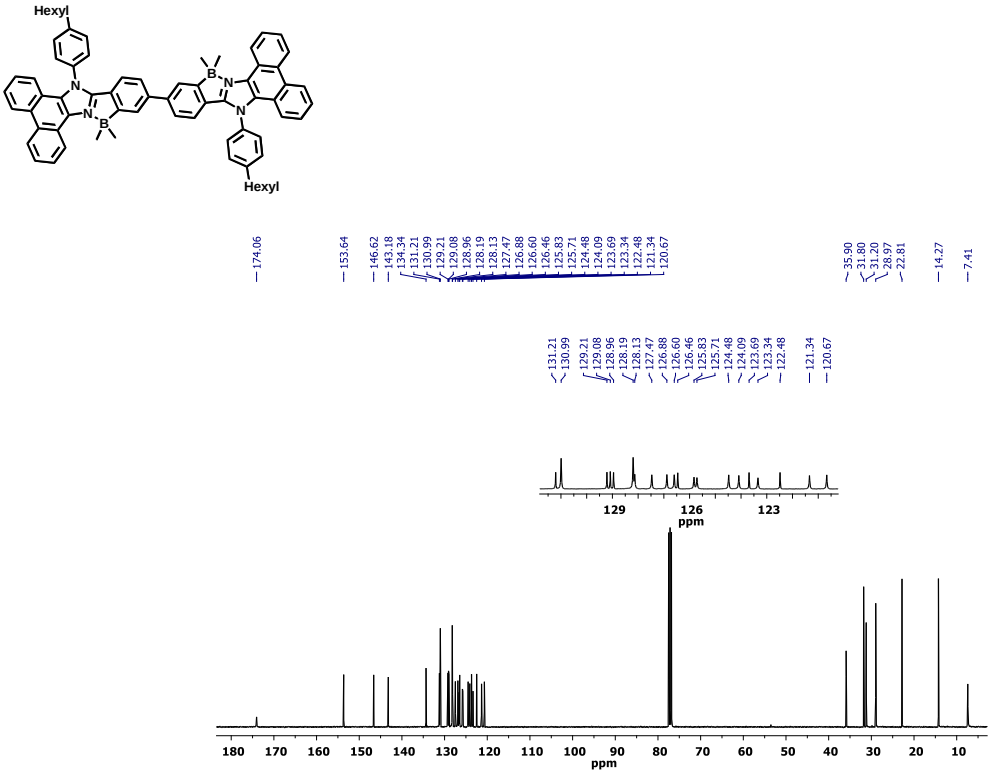


Figure S27. ^{13}C NMR spectrum of compound **7**

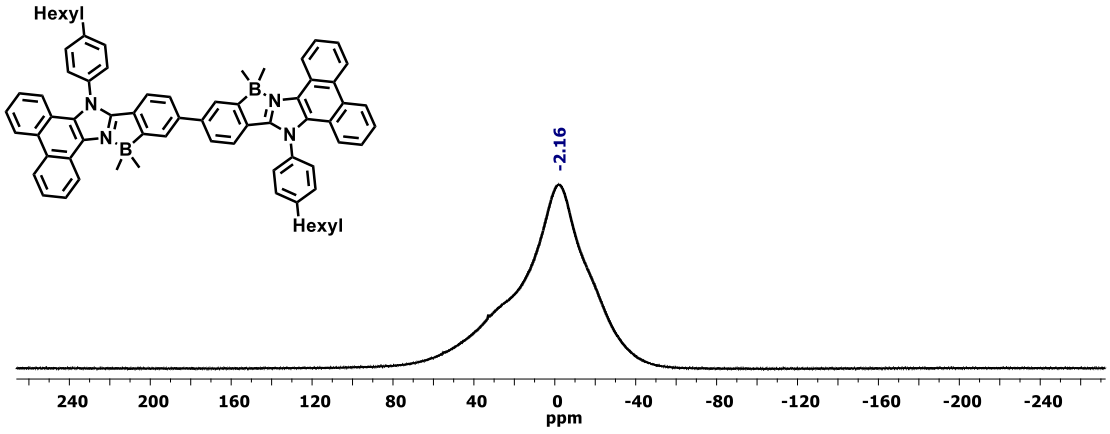


Figure S28. ^{11}B NMR spectrum of compound **7**

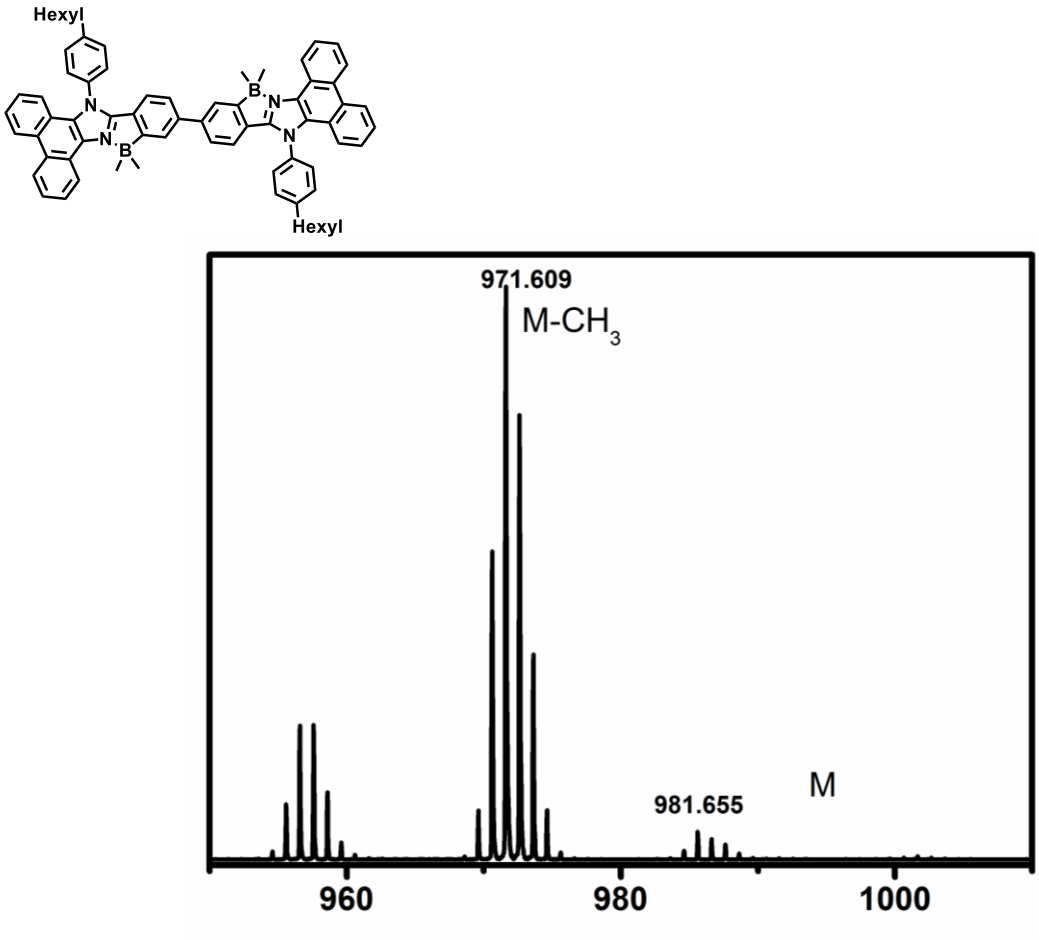


Figure S29. MALDI mass of compound **7**

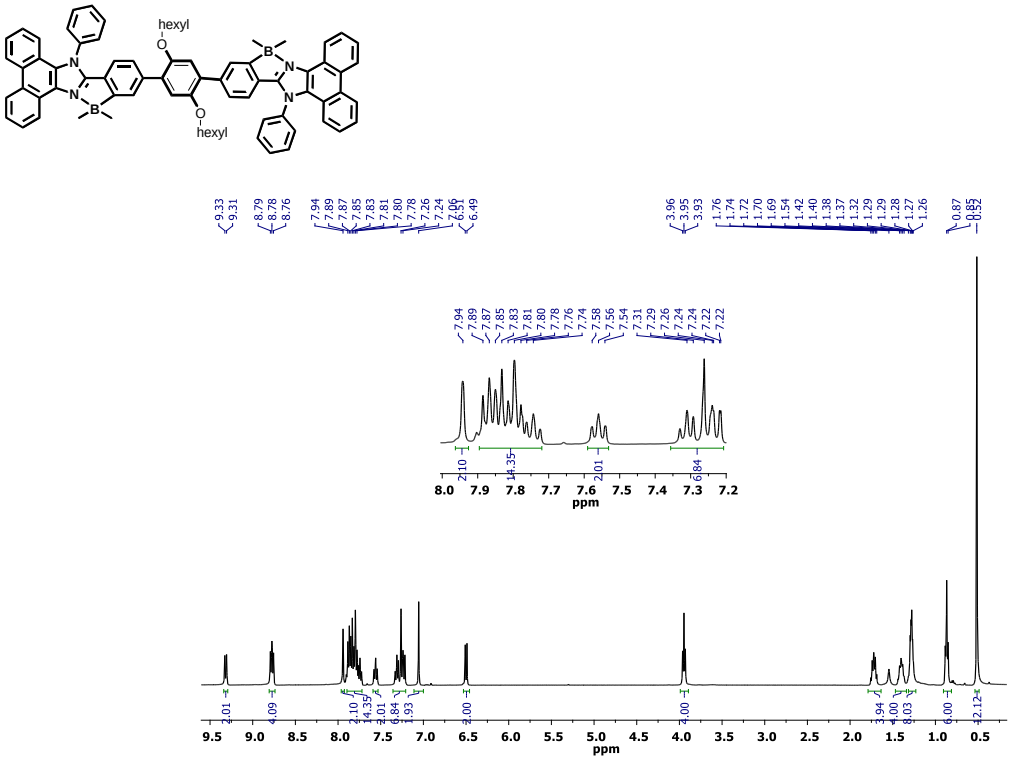


Figure S30. ^{1}H NMR spectrum of compound **8**

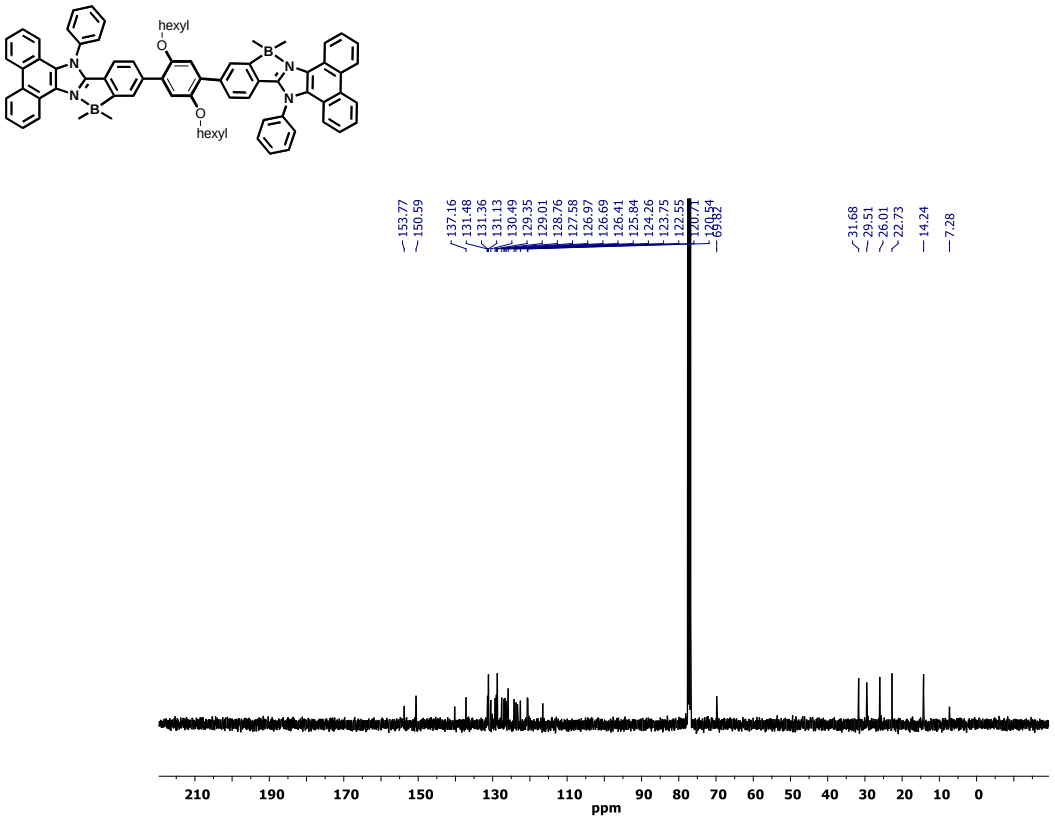


Figure S31. ^{13}C NMR spectrum of compound **8**

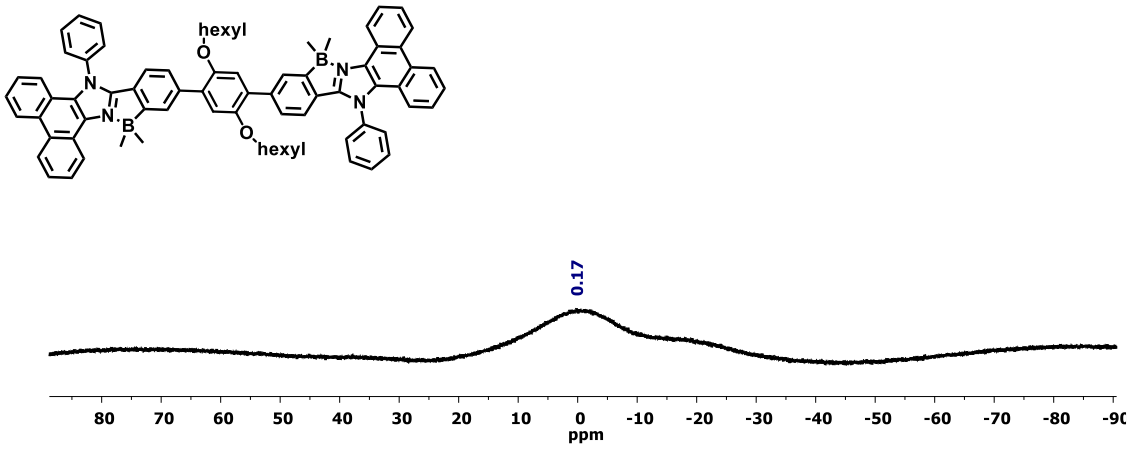


Figure S32. ^{11}B NMR spectrum of compound **8**

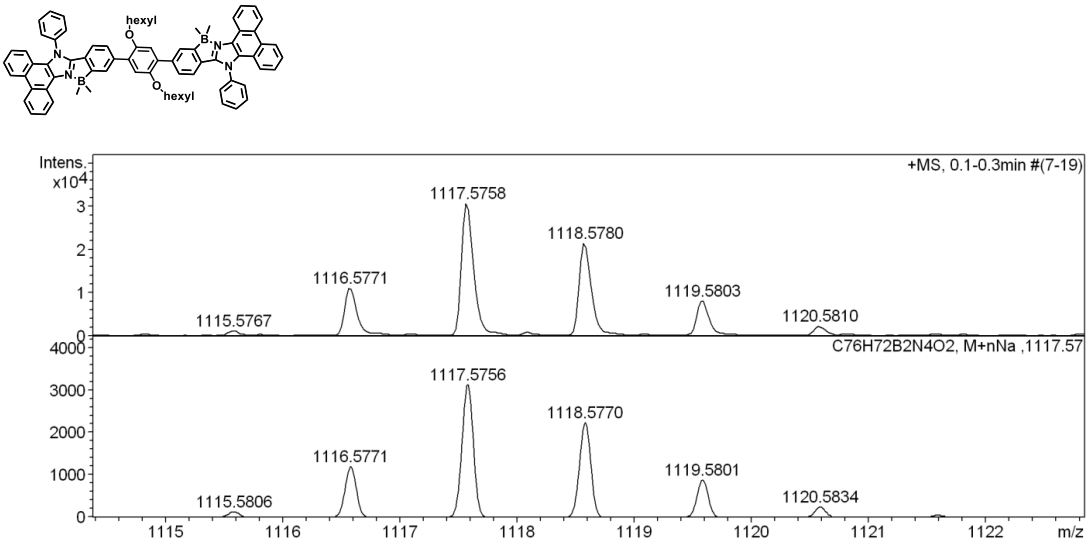


Figure S33. HRMS of compound **8**

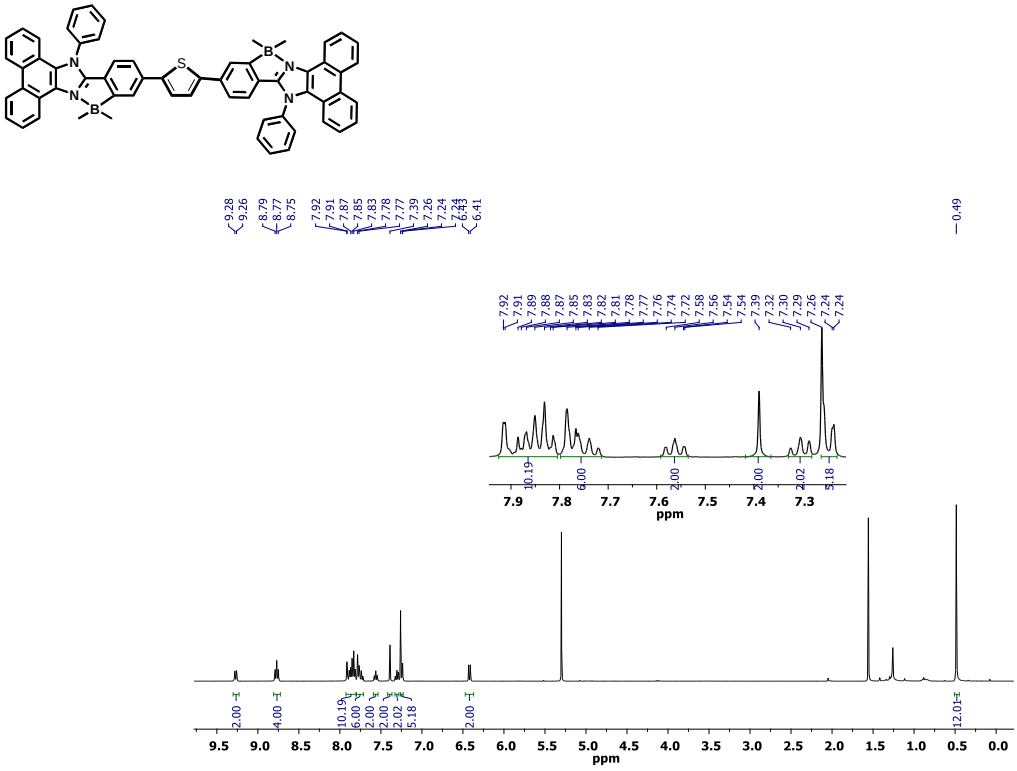


Figure S34. ^{1}H NMR spectrum of compound **9**

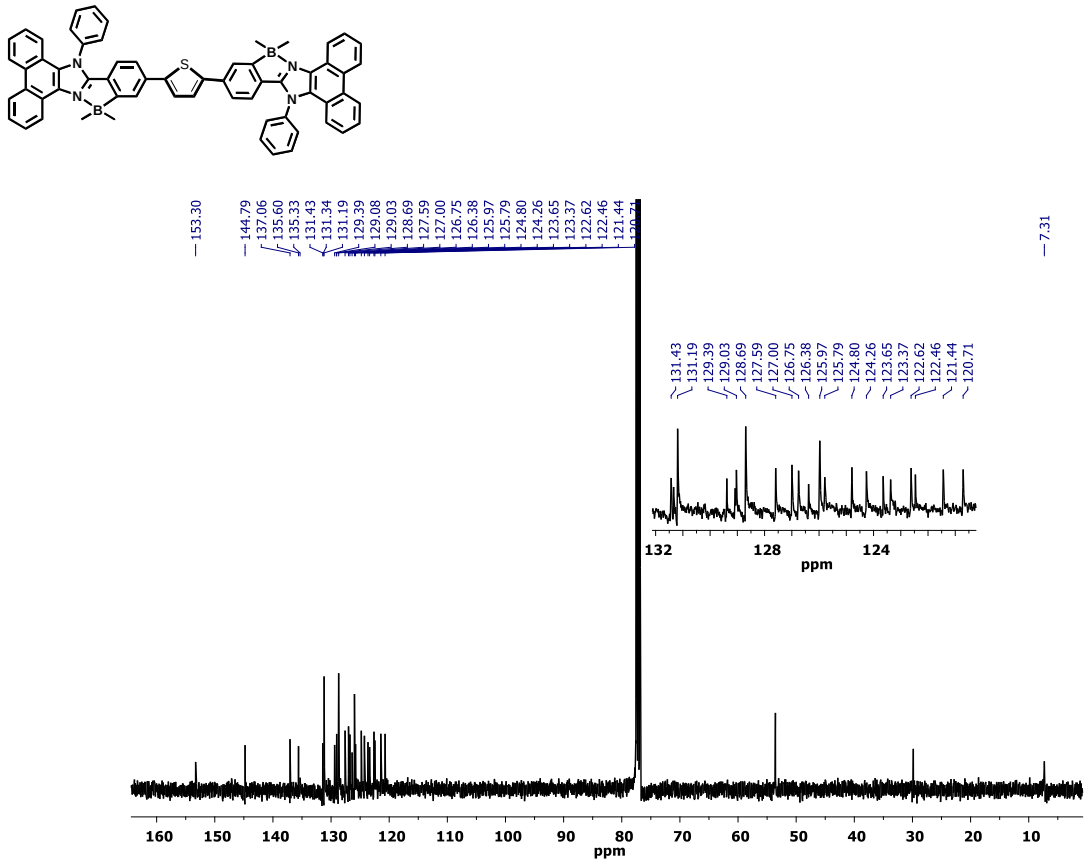


Figure S35. ^{13}C NMR spectrum of compound **9**

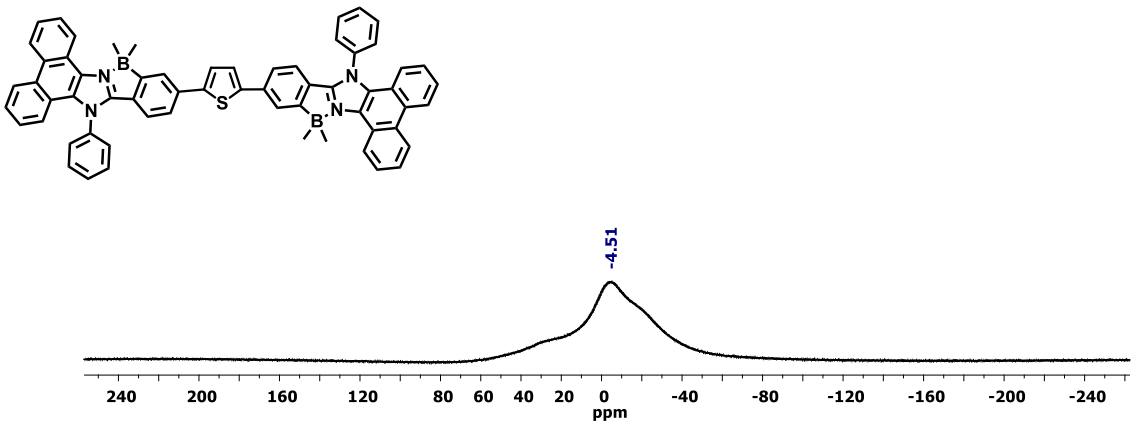
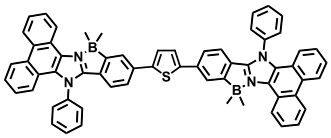


Figure S36. ^{11}B NMR spectrum of compound **9**



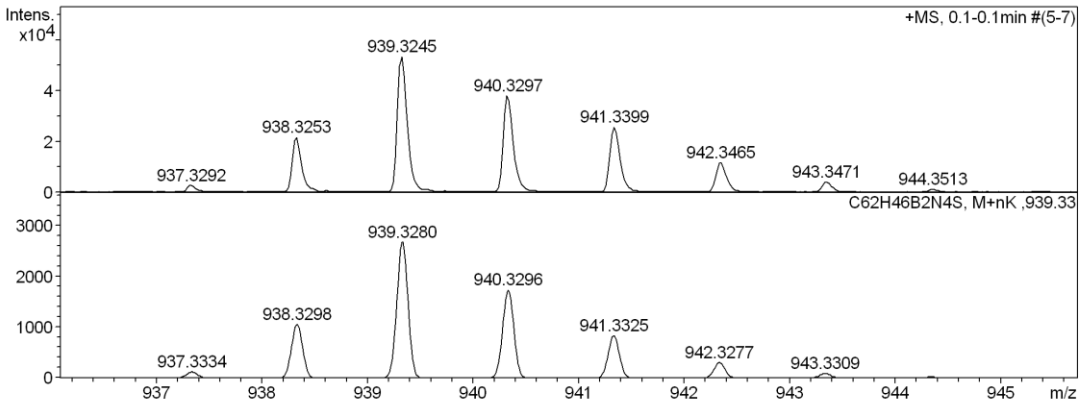
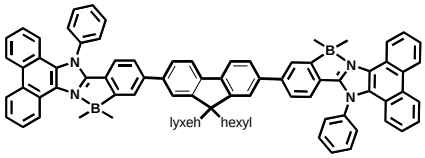


Figure S37. HRMS of compound **9**



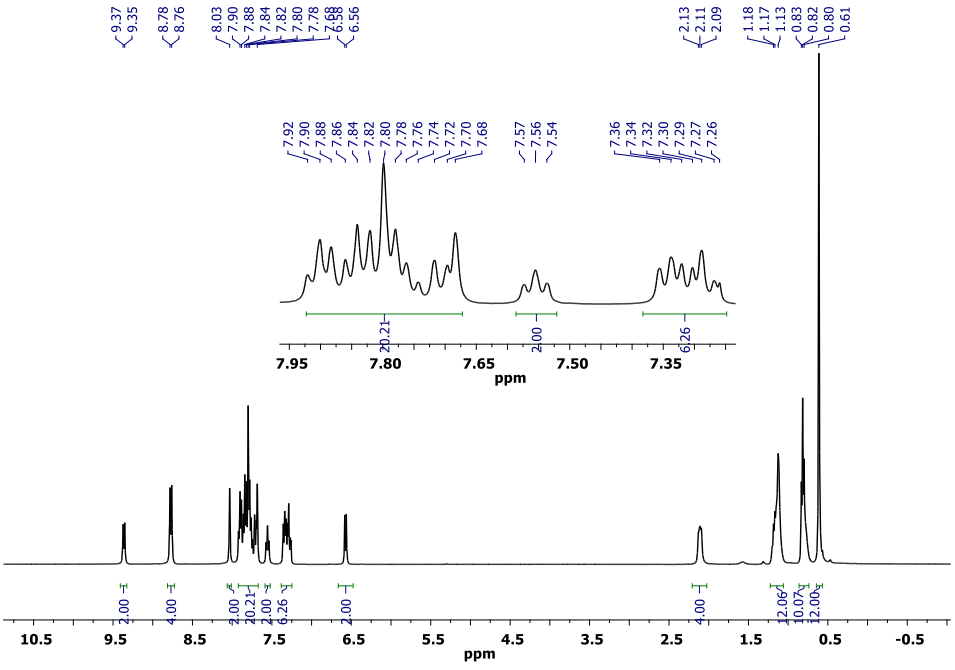


Figure S38.[1]H NMR spectrum of compound **10**

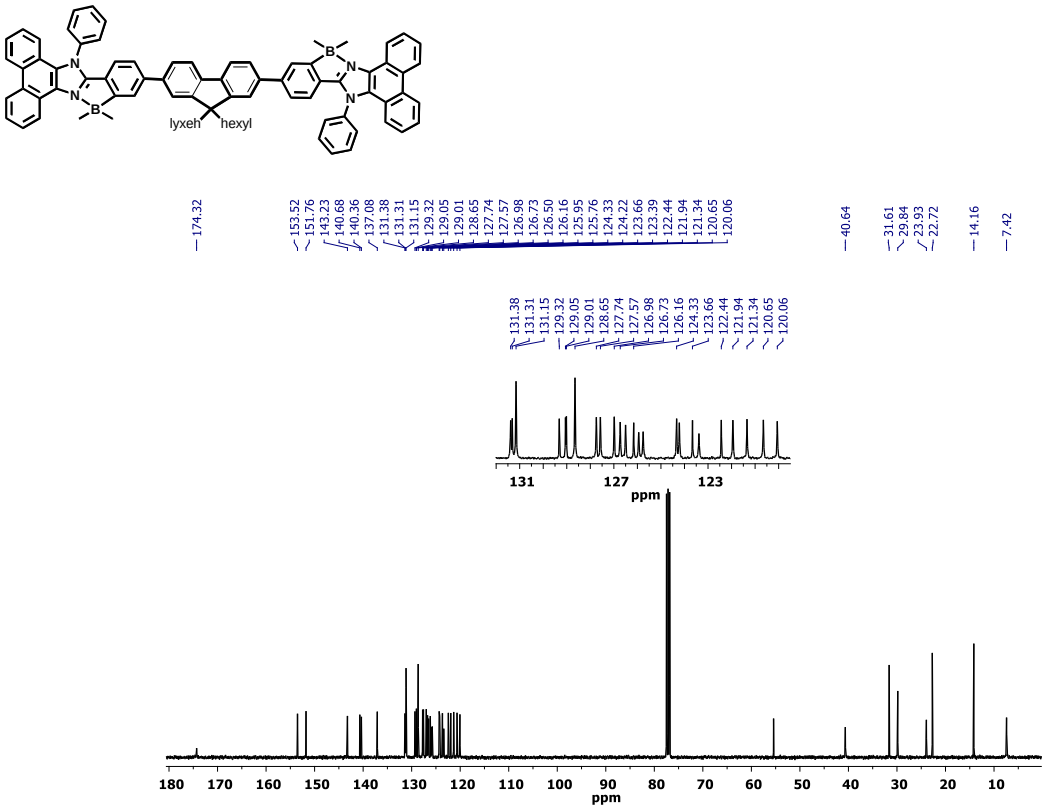


Figure S39. ^{13}C NMR spectrum of compound **10**

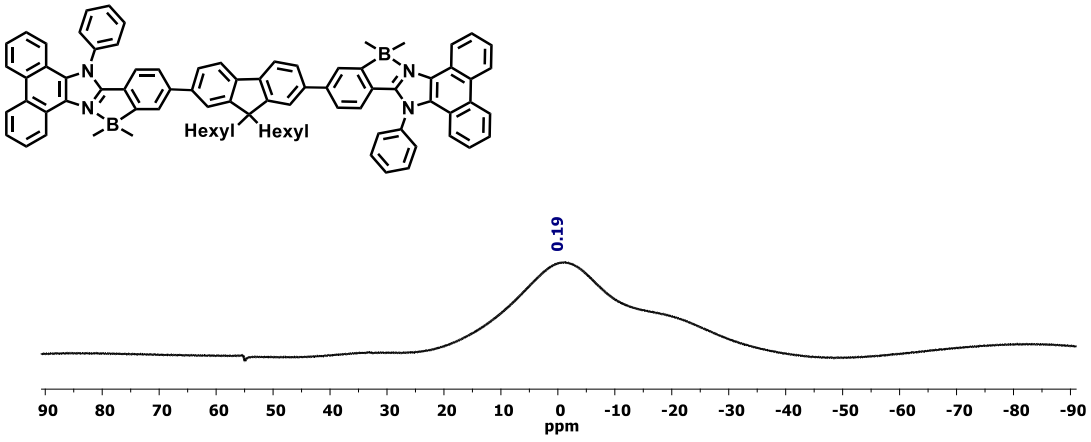


Figure S40. ^{11}B NMR spectrum of compound **10**

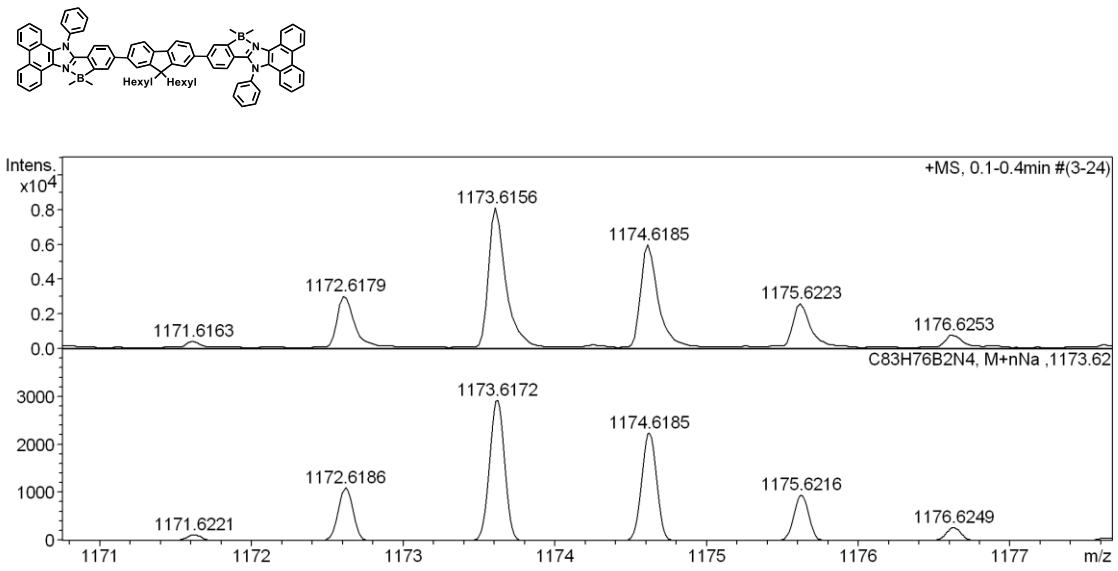


Figure S41. HRMS of compound **10**

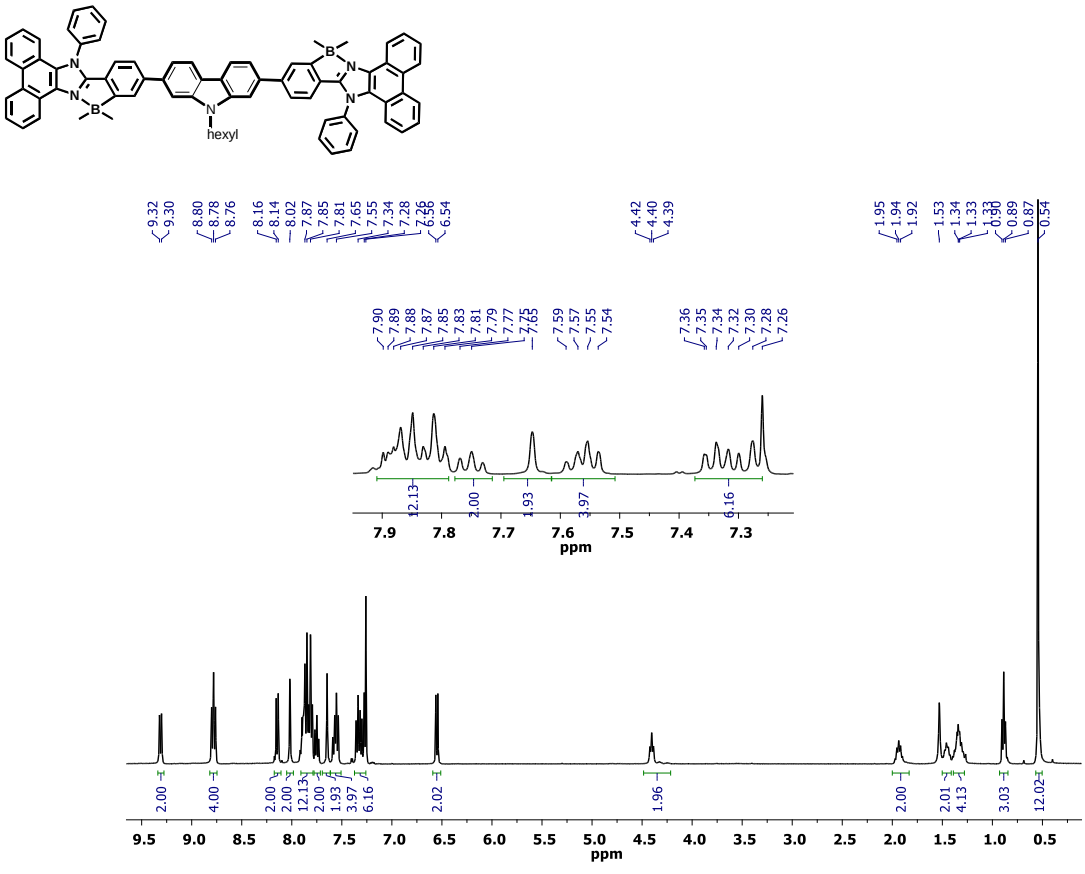


Figure S42.[1]H NMR spectrum of compound **11**

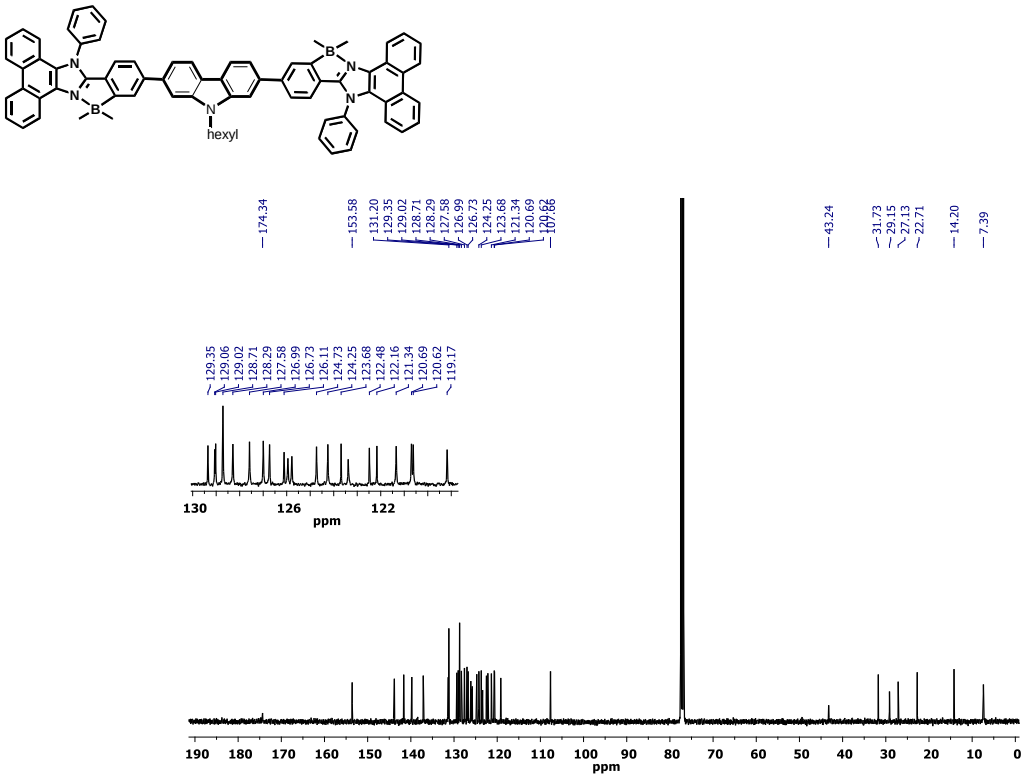


Figure S43. ^{13}C NMR spectrum of compound **11**

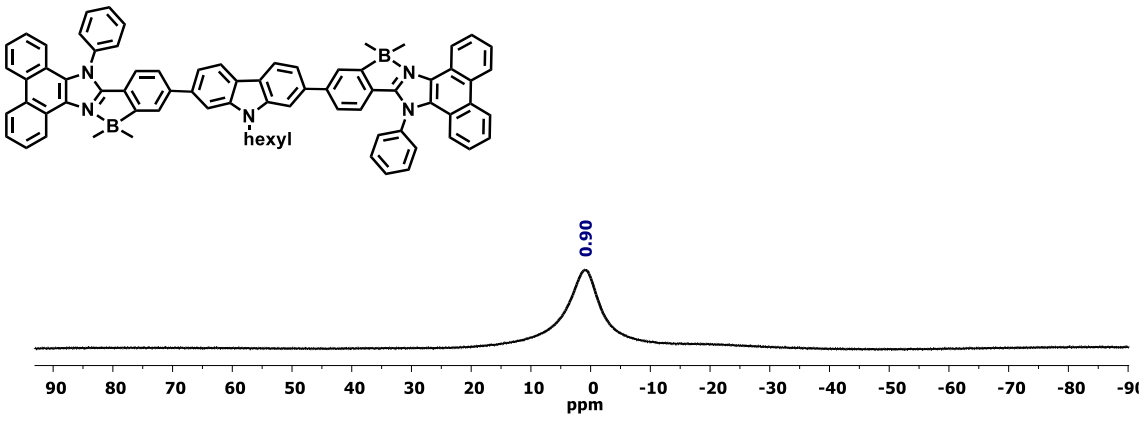
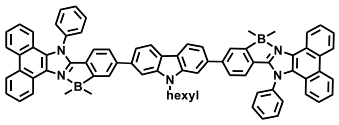


Figure S44. ^{11}B NMR spectrum of compound **11**



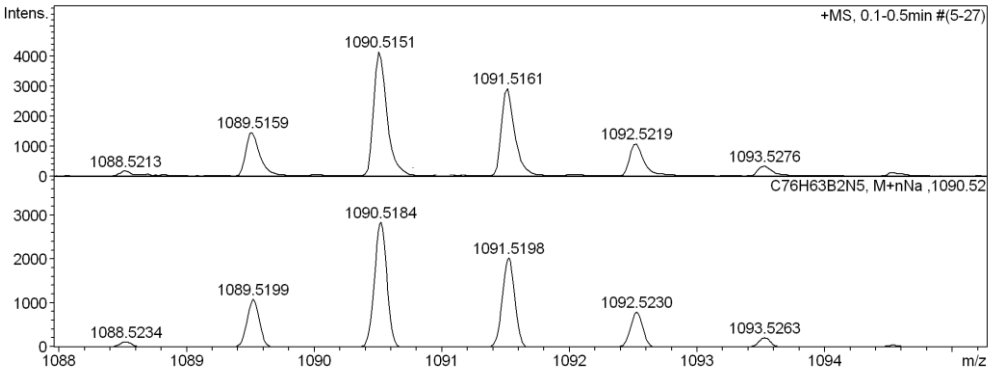


Figure S45. HRMS of compound **11**

Optimized x,y,z coordinates for compounds **7-11,** calculated on Gaussian 03 at the B3LYP//6-31g(d) level

Compound **7**

7	0	6.141106	-0.470907	0.059162
7	0	5.287303	1.512395	0.596767
7	0	-6.029918	0.143680	0.000196
7	0	-5.179850	-1.795728	0.684154
6	0	6.156729	-1.865382	-0.286285
6	0	3.587195	-0.068920	0.218000
6	0	8.637942	0.175965	0.165409
6	0	-6.041821	1.518884	-0.415881
6	0	8.909631	2.601616	0.792755
6	0	0.796795	-0.135234	0.244142
6	0	2.882269	1.113317	0.544057
6	0	7.494697	2.777102	0.874064
6	0	4.999467	0.244563	0.271810
6	0	6.140128	-4.594334	-0.956345
6	0	-7.389159	-3.035751	1.043224
6	0	6.961274	4.036978	1.216580
1	0	5.888866	4.150980	1.273518
6	0	-8.527275	-0.494329	0.137323
6	0	2.932083	-1.269913	-0.090019

1	0	3.480191	-2.170002	-0.346455
6	0	6.112149	-2.250686	-1.626245
1	0	6.083358	-1.492490	-2.402815
6	0	6.667146	1.633652	0.595984
6	0	-3.476827	-0.245298	0.204531
6	0	-6.559724	-1.916096	0.685996
6	0	7.222707	0.401914	0.261608
6	0	6.185296	-4.180204	0.384356
1	0	6.217649	-4.926214	1.174704
6	0	-7.112864	-0.711793	0.260480
6	0	-5.995130	4.210790	-1.216014
6	0	6.190737	-2.829613	0.724159
1	0	6.225177	-2.516903	1.763317
6	0	-8.803615	-2.865969	0.943677
6	0	1.489600	1.050107	0.555214
1	0	0.919783	1.933774	0.833228
6	0	9.482978	1.299876	0.437849
6	0	1.543348	-1.289355	-0.077098
1	0	1.023023	-2.202967	-0.347833
6	0	-1.382026	-1.337300	0.635800
1	0	-0.814460	-2.198364	0.981086
6	0	-4.889626	-0.554730	0.269990
6	0	-2.819017	0.929961	-0.186262
1	0	-3.364338	1.809035	-0.511746
6	0	-1.430429	0.949354	-0.166462
1	0	-0.907105	1.840346	-0.499343
6	0	6.105500	-3.607487	-1.951070
1	0	6.072800	-3.903780	-2.996315
6	0	-2.774685	-1.400272	0.621906
6	0	-10.480700	0.858928	-0.399690
1	0	-10.903307	1.799175	-0.742900
6	0	-11.319394	-0.210217	-0.052409
1	0	-12.398514	-0.105866	-0.122442
6	0	-9.617727	-3.967420	1.296100
1	0	-10.696496	-3.884433	1.235687
6	0	-9.109005	0.717071	-0.305888
1	0	-8.474976	1.549363	-0.579006
6	0	-9.374427	-1.594102	0.489847
6	0	-6.090673	3.863177	0.140261
1	0	-6.146313	4.647634	0.891126
6	0	6.117231	-6.068562	-1.303960
1	0	6.915153	-6.578264	-0.747880
1	0	6.350654	-6.195495	-2.368693
6	0	4.776959	-6.771496	-0.991987
1	0	4.915420	-7.850889	-1.143355
1	0	4.540472	-6.640009	0.073304
6	0	7.788590	5.112955	1.476874
1	0	7.358625	6.075435	1.739298
6	0	-10.770539	-1.403992	0.379832
1	0	-11.444275	-2.211883	0.639113
6	0	-0.686449	-0.178476	0.242054
6	0	10.879719	1.103007	0.349878
1	0	11.551832	1.928969	0.549520
6	0	-9.078668	-5.167941	1.722265
1	0	-9.737961	-5.990964	1.984212
6	0	-7.686660	-5.320517	1.815524

1	0	-7.258504	-6.261176	2.150131
6	0	10.594999	-1.214029	-0.251900
1	0	11.019798	-2.178248	-0.517014
6	0	-6.109781	2.530547	0.544771
1	0	-6.178836	2.268530	1.596122
6	0	9.180967	4.954956	1.400469
1	0	9.838954	5.795475	1.603496
6	0	-3.676235	-2.977181	2.607986
1	0	-3.857593	-2.106168	3.252669
1	0	-2.661737	-3.331607	2.840491
1	0	-4.360093	-3.769604	2.939814
5	0	3.871105	2.363800	0.852177
6	0	9.721989	3.726601	1.066128
1	0	10.801016	3.640036	1.016450
5	0	-3.766325	-2.622768	1.019508
6	0	3.703597	3.541062	-0.263553
1	0	4.379724	4.396352	-0.133850
1	0	2.683202	3.946649	-0.205847
1	0	3.838510	3.178970	-1.292218
6	0	-6.857631	-4.267034	1.479732
1	0	-5.785379	-4.376115	1.549116
6	0	-5.914210	5.662625	-1.634237
1	0	-6.621849	6.256524	-1.040196
1	0	-6.224071	5.763825	-2.682091
6	0	3.762240	2.848005	2.404391
1	0	3.947333	2.035693	3.120608
1	0	2.741026	3.207019	2.596911
1	0	4.432067	3.674500	2.676006
6	0	-5.953764	1.838438	-1.771431
1	0	-5.900939	1.042949	-2.508436
6	0	3.594444	-6.288831	-1.840752
1	0	3.834914	-6.424384	-2.906483
1	0	3.456336	-5.210281	-1.692896
6	0	11.431410	-0.120126	0.014193
1	0	12.510916	-0.228602	-0.042299
6	0	9.222784	-1.066308	-0.176910
1	0	8.590996	-1.918683	-0.385152
6	0	-3.585021	-3.889195	0.008327
1	0	-4.246274	-4.741285	0.214505
1	0	-2.557828	-4.272258	0.095456
1	0	-3.729023	-3.619492	-1.047125
6	0	-5.930899	3.177565	-2.161115
1	0	-5.859512	3.423111	-3.217768
6	0	2.290035	-7.032529	-1.519764
1	0	2.037121	-6.878629	-0.460031
1	0	2.461936	-8.112259	-1.637030
6	0	1.088688	-6.625228	-2.389178
1	0	1.343563	-6.773159	-3.448681
1	0	0.257989	-7.311907	-2.178974
6	0	-4.498674	6.252984	-1.461669
1	0	-4.188808	6.120444	-0.417456
1	0	-3.790156	5.670151	-2.066969
6	0	0.605706	-5.185567	-2.174984
1	0	-0.280222	-4.972833	-2.783317
1	0	1.372359	-4.450105	-2.444581
1	0	0.332196	-5.014406	-1.126068

6	0	-1.097322	9.122520	-0.231116
1	0	-0.732638	9.177587	0.800747
1	0	-1.143311	10.145680	-0.624317
1	0	-0.349849	8.575848	-0.818873
6	0	-2.466687	8.438797	-0.304663
1	0	-3.185998	8.990392	0.318224
6	0	-4.416796	7.733744	-1.856251
1	0	-5.118325	8.313125	-1.237343
1	0	-4.765154	7.843448	-2.893223
6	0	-3.010716	8.346107	-1.737533
1	0	-3.031404	9.355885	-2.171389
1	0	-2.390404	7.434869	0.133102
1	0	-2.308804	7.766198	-2.355188

Compound **8**

8	0	1.215536	2.453027	-0.463572
6	0	13.510236	0.585521	0.794475
1	0	14.579830	0.717088	0.932024
6	0	13.037670	-0.489253	0.063362
1	0	13.760070	-1.179210	-0.356130
6	0	11.657318	-0.708433	-0.146219
6	0	10.742680	0.230938	0.431118
6	0	9.345867	-0.015566	0.204950
7	0	8.210372	0.700583	0.619909
6	0	7.116850	0.041359	0.138081
6	0	5.688427	0.261836	0.217233
6	0	4.955828	1.284381	0.838677
1	0	5.443539	2.087223	1.381050
6	0	3.569898	1.254336	0.756446
1	0	2.988527	2.035123	1.232186
6	0	2.902707	0.217447	0.069961
6	0	1.418792	0.141885	0.035810
6	0	0.591812	1.256425	-0.222424
6	0	0.795006	-1.096769	0.252548
1	0	1.431498	-1.943645	0.476602
6	0	3.670069	-0.787963	-0.546964
1	0	3.155677	-1.571355	-1.099418
6	0	5.063416	-0.790800	-0.490242
5	0	6.129878	-1.835154	-1.128015
7	0	7.486713	-1.045513	-0.553379
6	0	8.870425	-1.100107	-0.526088
6	0	11.247417	1.323757	1.175129
1	0	10.563729	2.037445	1.613729
6	0	12.606477	1.499945	1.354995
1	0	12.968666	2.347168	1.930750
6	0	8.138357	1.902455	1.403393
6	0	8.136057	3.143874	0.763277
1	0	8.203510	3.188259	-0.319254
6	0	8.044998	4.308094	1.526796
1	0	8.041728	5.275533	1.033208
6	0	7.954897	4.229023	2.918499
1	0	7.882637	5.137297	3.509934
6	0	7.954436	2.983224	3.550424

1	0	7.880794	2.919266	4.632112
6	0	8.044950	1.814223	2.794174
1	0	8.042955	0.838367	3.269676
6	0	1.381424	4.732207	-1.136216
1	0	2.077997	4.418913	-1.924300
1	0	1.986597	4.925333	-0.240810
6	0	0.643233	6.008949	-1.558364
1	0	0.019185	5.797506	-2.439185
1	0	-0.049985	6.313758	-0.760604
6	0	1.588058	7.174174	-1.879313
1	0	2.278133	6.871071	-2.680605
1	0	2.216561	7.385610	-1.001340
6	0	11.168675	-1.851493	-0.923095
6	0	12.050614	-2.789355	-1.508863
1	0	13.121408	-2.672453	-1.390800
6	0	11.588956	-3.868115	-2.241267
1	0	12.298702	-4.566610	-2.676038
6	0	10.210103	-4.057930	-2.421305
1	0	9.842512	-4.903638	-2.995547
6	0	9.316490	-3.162390	-1.865126
1	0	8.254031	-3.300678	-2.000318
6	0	9.768697	-2.056186	-1.116198
6	0	6.095097	-1.805680	-2.757608
1	0	6.251714	-0.799911	-3.171240
1	0	5.103280	-2.133286	-3.100676
1	0	6.821290	-2.469632	-3.245166
6	0	0.430071	3.579027	-0.844105
1	0	-0.267223	3.845948	-0.035673
1	0	-0.168297	3.335762	-1.734607
6	0	5.996149	-3.312670	-0.451377
1	0	6.084568	-3.292617	0.643737
1	0	6.718451	-4.053891	-0.818042
1	0	4.999933	-3.719372	-0.677639
6	0	0.857394	8.456096	-2.298836
1	0	0.225029	8.242403	-3.172229
1	0	0.172107	8.761856	-1.495560
6	0	1.807261	9.612282	-2.627816
1	0	2.481722	9.348506	-3.451831
1	0	2.429542	9.873318	-1.762731
1	0	1.255632	10.511727	-2.924172
8	0	-1.215536	-2.452917	0.463591
6	0	-13.510202	-0.585723	-0.794401
1	0	-14.579793	-0.717324	-0.931940
6	0	-13.037657	0.489134	-0.063395
1	0	-13.760072	1.179120	0.356024
6	0	-11.657310	0.708360	0.146167
6	0	-10.742653	-0.231052	-0.431072
6	0	-9.345844	0.015502	-0.204926
7	0	-8.210334	-0.700666	-0.619810
6	0	-7.116826	-0.041370	-0.138048
6	0	-5.688398	-0.261821	-0.217182
6	0	-4.955779	-1.284409	-0.838531
1	0	-5.443472	-2.087312	-1.380827
6	0	-3.569849	-1.254325	-0.756304
1	0	-2.988459	-2.035147	-1.231965
6	0	-2.902682	-0.217358	-0.069914

6	0	-1.418771	-0.141779	-0.035761
6	0	-0.591794	-1.256318	0.222469
6	0	-0.794987	1.096874	-0.252508
1	0	-1.431480	1.943748	-0.476570
6	0	-3.670064	0.788089	0.546926
1	0	-3.155687	1.571540	1.099310
6	0	-5.063411	0.790893	0.490198
5	0	-6.129896	1.835284	1.127871
7	0	-7.486713	1.045561	0.553308
6	0	-8.870427	1.100125	0.526005
6	0	-11.247368	-1.323956	-1.174974
1	0	-10.563666	-2.037675	-1.613501
6	0	-12.606424	-1.500187	-1.354826
1	0	-12.968596	-2.347475	-1.930496
6	0	-8.138291	-1.902616	-1.403171
6	0	-8.135963	-3.143969	-0.762927
1	0	-8.203420	-3.188244	0.319608
6	0	-8.044871	-4.308265	-1.526326
1	0	-8.041580	-5.275654	-1.032638
6	0	-7.954764	-4.229335	-2.918037
1	0	-7.882477	-5.137668	-3.509378
6	0	-7.954330	-2.983602	-3.550090
1	0	-7.880682	-2.919753	-4.631783
6	0	-8.044877	-1.814524	-2.793960
1	0	-8.042902	-0.838717	-3.269563
6	0	-1.381478	-4.732108	1.136181
1	0	-2.078042	-4.418815	1.924272
1	0	-1.986656	-4.925197	0.240771
6	0	-0.643318	-6.008878	1.558299
1	0	-0.019262	-5.797470	2.439123
1	0	0.049890	-6.313687	0.760530
6	0	-1.588173	-7.174085	1.879226
1	0	-2.278237	-6.870981	2.680527
1	0	-2.216684	-7.385485	1.001250
6	0	-11.168692	1.851509	0.922928
6	0	-12.050650	2.789414	1.508596
1	0	-13.121441	2.672480	1.390542
6	0	-11.589015	3.868259	2.240890
1	0	-12.298775	4.566785	2.675587
6	0	-10.210166	4.058119	2.420912
1	0	-9.842592	4.903894	2.995066
6	0	-9.316533	3.162538	1.864828
1	0	-8.254078	3.300861	2.000008
6	0	-9.768718	2.056248	1.116014
6	0	-6.095115	1.805966	2.757466
1	0	-6.251709	0.800233	3.171194
1	0	-5.103306	2.133627	3.100504
1	0	-6.821324	2.469948	3.244960
6	0	-0.430096	-3.578944	0.844097
1	0	0.267191	-3.845864	0.035660
1	0	0.168277	-3.335715	1.734606
6	0	-5.996200	3.312740	0.451093
1	0	-6.084616	3.292581	-0.644020
1	0	-6.718521	4.053978	0.817686
1	0	-4.999995	3.719487	0.677319
6	0	-0.857540	-8.456035	2.298719

1	0	-0.225165	-8.242378	3.172112
1	0	-0.172266	-8.761797	1.495432
6	0	-1.807436	-9.612203	2.627679
1	0	-2.481886	-9.348425	3.451704
1	0	-2.429729	-9.873204	1.762592
1	0	-1.255830	-10.511669	2.924014

Compound 9

7	0	-8.097383	-0.927714	0.200963
16	0	-0.090053	-0.233297	0.129977
6	0	5.058530	-1.467173	-0.200754
5	0	6.396031	-2.322464	-0.554457
6	0	9.964935	-1.535356	-0.612280
7	0	-6.953570	0.921078	-0.320181
6	0	-8.239665	3.659968	-0.984645
1	0	-7.162143	3.617301	-1.017831
6	0	-13.297083	0.184382	0.110110
1	0	-14.380744	0.229747	0.140954
6	0	-12.631176	-1.021263	0.391624
1	0	-13.196954	-1.913082	0.640631
6	0	-11.246916	-1.072230	0.350885
1	0	-10.750453	-2.006457	0.569092
6	0	-10.480212	0.076142	0.028644
6	0	-9.045173	0.097353	-0.030197
6	0	-6.849079	-0.384757	0.014571
6	0	-5.497329	-0.884135	0.095756
6	0	-4.624196	0.194171	-0.216307
6	0	-3.251087	-0.056612	-0.205678
1	0	-2.564173	0.745545	-0.459349
6	0	-2.732224	-1.333483	0.106644
6	0	-1.296352	-1.598093	0.108620
6	0	1.290143	-1.424120	0.119791
6	0	2.678548	-0.972415	0.128601
6	0	3.721839	-1.865501	-0.214640
1	0	3.474648	-2.879305	-0.513609
7	0	7.464887	-1.056244	-0.278426
6	0	8.820840	-0.725893	-0.293604
6	0	11.253643	-0.915822	-0.536869
6	0	11.384059	0.495151	-0.151910
6	0	12.647837	1.129531	-0.076028
1	0	13.544294	0.567915	-0.304934
6	0	12.782348	2.462007	0.283905
1	0	13.768339	2.912561	0.330411
6	0	-8.326617	-2.303101	0.565449
6	0	-8.453883	-3.272281	-0.437361
1	0	-8.394926	-2.975504	-1.478509
6	0	-8.654028	-4.609725	-0.079639
1	0	-8.752680	-5.363877	-0.852913
6	0	-8.723342	-4.973221	1.271309
1	0	-8.877502	-6.011443	1.545775
6	0	-8.591057	-3.998307	2.268364
1	0	-8.640654	-4.278694	3.314955
6	0	-8.390393	-2.658898	1.918427

1	0	-8.282848	-1.893068	2.678367
5	0	-5.421431	1.572748	-0.544652
6	0	-5.014019	-2.164174	0.415907
1	0	-5.682836	-2.979832	0.664918
6	0	-3.640105	-2.376949	0.423737
1	0	-3.258172	-3.354348	0.695922
6	0	6.636990	-3.524994	0.519067
1	0	6.681795	-3.162095	1.555781
1	0	7.545919	-4.115379	0.339859
1	0	5.791752	-4.227579	0.462586
6	0	6.778433	0.048544	0.091367
6	0	5.346614	-0.120935	0.159511
6	0	4.334105	0.791899	0.495916
1	0	4.557504	1.816159	0.770228
6	0	3.012195	0.358747	0.479680
1	0	2.225239	1.052367	0.755444
7	0	7.644098	1.090893	0.317815
6	0	8.954517	0.614863	0.076023
6	0	10.223598	1.282564	0.160513
6	0	11.640967	3.224840	0.586377
1	0	11.739501	4.268224	0.867585
6	0	10.384583	2.643326	0.525088
1	0	9.517915	3.243808	0.759802
6	0	9.857384	-2.893391	-0.987382
1	0	8.878153	-3.343094	-1.040367
6	0	10.985067	-3.641848	-1.283892
1	0	10.883956	-4.683425	-1.570033
6	0	12.257501	-3.046251	-1.212263
1	0	13.144634	-3.627228	-1.442901
6	0	12.382721	-1.714079	-0.847075
1	0	13.376306	-1.286759	-0.801669
6	0	7.224831	2.405400	0.734934
6	0	7.120359	2.696632	2.100700
1	0	7.371056	1.934972	2.830491
6	0	6.692779	3.966476	2.502384
1	0	6.609598	4.196240	3.559103
6	0	6.369205	4.934966	1.543583
1	0	6.035473	5.918238	1.857814
6	0	6.471980	4.634145	0.179449
1	0	6.217430	5.381541	-0.564167
6	0	6.899388	3.366703	-0.229971
1	0	6.981000	3.117777	-1.282063
6	0	0.791708	-2.707595	0.102025
1	0	1.432832	-3.580212	0.108378
6	0	-0.628898	-2.802832	0.093514
1	0	-1.145313	-3.754357	0.060932
6	0	-5.115684	2.719955	0.571925
1	0	-5.664853	3.658258	0.414922
1	0	-4.045490	2.973288	0.538544
1	0	-5.332731	2.381210	1.594940
6	0	-8.311441	1.241527	-0.353488
6	0	-8.958266	2.489694	-0.652187
6	0	-8.899945	4.845303	-1.265274
1	0	-8.332462	5.734494	-1.518798
6	0	-10.305319	4.889724	-1.219996
1	0	-10.828315	5.815138	-1.438668

6	0	-11.027701	3.750776	-0.896385
1	0	-12.107803	3.819046	-0.871568
6	0	-10.389027	2.520088	-0.603433
6	0	-11.151771	1.312524	-0.262523
6	0	-12.566836	1.319373	-0.208806
1	0	-13.106841	2.232962	-0.421364
6	0	6.425971	-2.768344	-2.121536
1	0	5.579702	-3.444055	-2.316964
1	0	7.334091	-3.310506	-2.418040
1	0	6.317135	-1.914288	-2.804932
6	0	-5.211304	2.032878	-2.093904
1	0	-5.495427	1.248200	-2.809416
1	0	-4.144763	2.246272	-2.260271
1	0	-5.759511	2.943298	-2.372572

Compound 10

6	0	15.227003	1.310646	-0.338360
6	0	14.927963	-0.028078	-0.160778
6	0	13.600643	-0.489132	-0.008727
6	0	12.553361	0.487345	-0.043201
6	0	12.881048	1.851667	-0.226056
6	0	14.193959	2.258608	-0.371432
6	0	13.295695	-1.910829	0.178865
6	0	11.947041	-2.352645	0.338570
6	0	10.913395	-1.352462	0.305868
6	0	11.214314	-0.006550	0.118786
6	0	14.310903	-2.895013	0.208843
6	0	14.023174	-4.236406	0.385451
6	0	12.693122	-4.656346	0.540927
6	0	11.672805	-3.724480	0.517026
7	0	9.540898	-1.486368	0.436457
6	0	9.009068	-0.261066	0.330869
7	0	9.984660	0.672721	0.136457
6	0	9.727461	2.077755	-0.016420
6	0	7.566947	-0.205848	0.448389
6	0	7.113838	-1.528992	0.661446
6	0	5.741116	-1.724612	0.806941
6	0	4.829075	-0.654546	0.748624
6	0	5.327069	0.648042	0.531393
6	0	6.687707	0.884532	0.379919
6	0	9.507207	2.602738	-1.291883
6	0	9.237528	3.964154	-1.434844
6	0	9.185450	4.790551	-0.309799
6	0	9.402906	4.256505	0.962520
6	0	9.673866	2.896174	1.114179
5	0	8.326921	-2.607703	0.688491
6	0	8.229178	-3.645626	-0.564392
6	0	8.481968	-3.293471	2.158940
6	0	2.898039	-1.837684	1.835381
6	0	3.372778	-0.885176	0.913727
6	0	2.434936	-0.154757	0.154175
6	0	1.073136	-0.380272	0.310739
6	0	0.619286	-1.320067	1.261037

6	0	1.533937	-2.054545	2.017974
6	0	-0.109713	0.268638	-0.416963
6	0	-1.290776	-0.361400	0.328778
6	0	-0.844516	-1.308641	1.270842
6	0	-2.648318	-0.142028	0.143130
6	0	-3.595534	-0.863384	0.898850
6	0	-3.129826	-1.807979	1.834743
6	0	-1.768436	-2.035454	2.024962
6	0	-15.415797	1.286059	-0.710409
6	0	-15.122882	-0.044321	-0.470835
6	0	-13.801446	-0.497340	-0.256192
6	0	-12.753365	0.478177	-0.294671
6	0	-13.074944	1.834123	-0.540239
6	0	-14.382287	2.233437	-0.744865
6	0	-13.503213	-1.910084	-0.002106
6	0	-12.159996	-2.344620	0.213353
6	0	-11.124914	-1.346412	0.169103
6	0	-11.419844	-0.008233	-0.074559
6	0	-14.519863	-2.892303	0.040655
6	0	-14.238577	-4.225068	0.281325
6	0	-12.913821	-4.637857	0.491578
6	0	-11.892321	-3.707635	0.457105
7	0	-9.756225	-1.475576	0.338597
6	0	-9.220967	-0.254746	0.203118
7	0	-10.190603	0.671547	-0.048850
6	0	-9.929200	2.070981	-0.240527
6	0	-7.781700	-0.195999	0.349829
6	0	-7.333822	-1.512057	0.612279
6	0	-5.963953	-1.704126	0.786357
6	0	-5.049480	-0.637072	0.710503
6	0	-5.542961	0.659003	0.448086
6	0	-6.900364	0.891518	0.265299
6	0	-9.906439	2.925433	0.864173
6	0	-9.632733	4.280641	0.676170
6	0	-9.381991	4.773946	-0.606446
6	0	-9.402903	3.911603	-1.705235
6	0	-9.675230	2.555050	-1.525865
5	0	-8.548471	-2.588575	0.653428
6	0	-8.732145	-3.219905	2.144998
6	0	-8.429057	-3.670769	-0.559063
1	0	16.261485	1.622713	-0.450951
1	0	15.747791	-0.735970	-0.138015
1	0	12.095988	2.594698	-0.252085
1	0	14.419710	3.312275	-0.510038
1	0	15.348564	-2.606193	0.090229
1	0	14.831418	-4.962371	0.402343
1	0	12.462045	-5.708744	0.678959
1	0	10.646708	-4.040165	0.634334
1	0	5.357161	-2.733126	0.943442
1	0	4.636479	1.486164	0.511541
1	0	7.043642	1.897231	0.224306
1	0	9.548547	1.946242	-2.155450
1	0	9.065551	4.377156	-2.424498
1	0	8.973873	5.849841	-0.424373
1	0	9.359665	4.896904	1.838620
1	0	9.843367	2.464770	2.095792

1	0	7.293164	-4.216512	-0.483675
1	0	8.203372	-3.140074	-1.539591
1	0	9.036061	-4.388791	-0.609372
1	0	9.316715	-4.000845	2.248982
1	0	7.570860	-3.865431	2.385836
1	0	8.597632	-2.556382	2.965616
1	0	3.611651	-2.388111	2.441317
1	0	2.794745	0.572438	-0.567286
1	0	1.193411	-2.776786	2.755719
1	0	-2.994520	0.566849	-0.604800
1	0	-3.849973	-2.351492	2.439127
1	0	-1.438179	-2.764181	2.761014
1	0	-16.445816	1.592047	-0.870558
1	0	-15.942887	-0.752046	-0.449527
1	0	-12.289634	2.576765	-0.569218
1	0	-14.603293	3.280687	-0.931486
1	0	-15.553635	-2.608614	-0.117620
1	0	-15.047767	-4.949736	0.306502
1	0	-12.687767	-5.683393	0.680660
1	0	-10.870335	-4.017619	0.617252
1	0	-5.584112	-2.708698	0.958369
1	0	-4.851511	1.495955	0.415914
1	0	-7.252450	1.899301	0.073283
1	0	-10.101712	2.525497	1.854292
1	0	-9.613631	4.948965	1.532040
1	0	-9.168551	5.829401	-0.749427
1	0	-9.204787	4.292844	-2.702714
1	0	-9.693260	1.871101	-2.368685
1	0	-9.566363	-3.926661	2.244640
1	0	-7.824248	-3.779479	2.412029
1	0	-8.866528	-2.453309	2.920691
1	0	-7.497167	-4.241331	-0.438192
1	0	-8.380595	-3.200499	-1.550896
1	0	-9.237723	-4.412505	-0.594313
6	0	-0.205573	-0.193654	-1.909526
6	0	0.900659	0.250332	-2.876671
1	0	-1.171686	0.159300	-2.297202
1	0	-0.259930	-1.290097	-1.915904
6	0	0.660237	-0.265794	-4.303403
1	0	0.970137	1.346182	-2.903849
1	0	1.873120	-0.117792	-2.527053
6	0	1.750609	0.157065	-5.296214
1	0	0.592177	-1.363364	-4.284926
1	0	-0.316265	0.092418	-4.662316
1	0	1.817821	1.255399	-5.317604
1	0	2.727367	-0.199269	-4.936493
6	0	1.517436	-0.362084	-6.720872
6	0	2.610442	0.064242	-7.706308
1	0	0.541206	-0.006878	-7.080950
1	0	1.451708	-1.459067	-6.699357
1	0	2.679360	1.157263	-7.773313
1	0	3.593312	-0.309698	-7.393948
1	0	2.413585	-0.319173	-8.714095
6	0	-0.098665	1.817866	-0.321384
6	0	-0.133900	2.398233	1.099120
1	0	-0.957210	2.202384	-0.891668

1	0	0.795610	2.194710	-0.834913
6	0	-0.103546	3.932459	1.114544
1	0	-1.035776	2.048071	1.617472
1	0	0.719588	2.012814	1.672392
6	0	-0.139993	4.526894	2.528439
1	0	0.800340	4.286246	0.595732
1	0	-0.955410	4.321181	0.536058
1	0	-1.042744	4.172819	3.048029
1	0	0.712213	4.140225	3.106882
6	0	-0.112448	6.060497	2.552009
6	0	-0.148283	6.644251	3.968198
1	0	-0.965091	6.446804	1.975126
1	0	0.789742	6.414478	2.032653
1	0	-1.056147	6.335554	4.501108
1	0	0.711334	6.304128	4.558863
1	0	-0.128247	7.740136	3.951650

Compound 11

6	0	15.201947	1.540901	-0.560863
6	0	14.932188	0.186209	-0.632713
6	0	13.620705	-0.327361	-0.517159
6	0	12.557224	0.611913	-0.320044
6	0	12.855249	1.993429	-0.248836
6	0	14.153717	2.452188	-0.367008
6	0	13.347741	-1.765805	-0.594174
6	0	12.014582	-2.262103	-0.471184
6	0	10.964263	-1.299768	-0.270950
6	0	11.234488	0.063792	-0.203874
6	0	14.379318	-2.713215	-0.790645
6	0	14.120977	-4.070213	-0.863335
6	0	12.805513	-4.543676	-0.741824
6	0	11.770235	-3.648848	-0.548759
7	0	9.601057	-1.490670	-0.116587
6	0	9.044416	-0.282127	0.039707
7	0	9.995057	0.695884	-0.006591
6	0	9.708509	2.097122	0.125752
6	0	7.608003	-0.287607	0.220766
6	0	7.186433	-1.637807	0.184612
6	0	5.825140	-1.893460	0.344910
6	0	4.893539	-0.856824	0.539057
6	0	5.360122	0.474896	0.564834
6	0	6.708053	0.771843	0.406444
6	0	9.431004	2.854254	-1.014742
6	0	9.138509	4.211896	-0.881048
6	0	9.120879	4.804047	0.384026
6	0	9.393837	4.038226	1.519929
6	0	9.688194	2.680106	1.394832
5	0	8.416762	-2.669498	-0.053175
6	0	8.289235	-3.429032	-1.489768
6	0	8.641002	-3.638484	1.238333
6	0	3.042844	-2.285720	1.463016
6	0	3.450168	-1.151865	0.719722
6	0	2.477476	-0.307227	0.163394

6	0	1.129875	-0.612456	0.357545
6	0	0.722270	-1.746641	1.109841
6	0	1.700238	-2.582783	1.660247
6	0	-1.129897	-0.612440	0.357577
6	0	-0.722286	-1.746635	1.109853
6	0	-2.477500	-0.307214	0.163433
6	0	-3.450189	-1.151842	0.719780
6	0	-3.042859	-2.285694	1.463075
6	0	-1.700251	-2.582768	1.660280
6	0	-15.201931	1.540942	-0.561081
6	0	-14.932194	0.186238	-0.632780
6	0	-13.620720	-0.327343	-0.517171
6	0	-12.557226	0.611935	-0.320147
6	0	-12.855225	1.993465	-0.249113
6	0	-14.153684	2.452234	-0.367340
6	0	-13.347776	-1.765796	-0.594058
6	0	-12.014620	-2.262100	-0.471055
6	0	-10.964288	-1.299760	-0.270891
6	0	-11.234501	0.063807	-0.203901
6	0	-14.379369	-2.713211	-0.790430
6	0	-14.121042	-4.070216	-0.863026
6	0	-12.805581	-4.543683	-0.741518
6	0	-11.770288	-3.648853	-0.548541
7	0	-9.601086	-1.490663	-0.116491
6	0	-9.044439	-0.282116	0.039751
7	0	-9.995070	0.695899	-0.006620
6	0	-9.708521	2.097143	0.125651
6	0	-7.608029	-0.287593	0.220817
6	0	-7.186454	-1.637790	0.184672
6	0	-5.825161	-1.893441	0.344972
6	0	-4.893559	-0.856806	0.539120
6	0	-5.360149	0.474913	0.564899
6	0	-6.708080	0.771858	0.406505
6	0	-9.688417	2.680239	1.394683
6	0	-9.394070	4.038367	1.519711
6	0	-9.120905	4.804085	0.383787
6	0	-9.138323	4.211823	-0.881237
6	0	-9.430813	2.854173	-1.014863
5	0	-8.416775	-2.669491	-0.053103
6	0	-8.640962	-3.638508	1.238389
6	0	-8.289282	-3.429003	-1.489714
1	0	16.225164	1.893727	-0.654434
1	0	15.762941	-0.492921	-0.782131
1	0	12.058404	2.708686	-0.098693
1	0	14.356387	3.517996	-0.308634
1	0	15.406535	-2.382720	-0.889149
1	0	14.941099	-4.766593	-1.015134
1	0	12.597433	-5.608309	-0.798874
1	0	10.755166	-4.005202	-0.455204
1	0	5.465193	-2.918542	0.295781
1	0	4.655711	1.281715	0.745323
1	0	7.039229	1.804195	0.442093
1	0	9.447862	2.377860	-1.990029
1	0	8.922867	4.805019	-1.764973
1	0	8.892132	5.861181	0.484912
1	0	9.376561	4.496039	2.504641

1	0	9.901400	2.070279	2.267216
1	0	7.378667	-4.044955	-1.490562
1	0	8.196186	-2.733381	-2.335207
1	0	9.117975	-4.109778	-1.724965
1	0	9.488008	-4.331496	1.151530
1	0	7.747586	-4.264195	1.376242
1	0	8.778610	-3.079888	2.174532
1	0	3.801673	-2.916863	1.914318
1	0	2.780352	0.550037	-0.429602
1	0	1.414874	-3.452830	2.245918
1	0	-2.780379	0.550038	-0.429579
1	0	-3.801682	-2.916832	1.914395
1	0	-1.414884	-3.452819	2.245943
1	0	-16.225143	1.893775	-0.654689
1	0	-15.762957	-0.492896	-0.782129
1	0	-12.058363	2.708725	-0.099073
1	0	-14.356335	3.518053	-0.309102
1	0	-15.406586	-2.382714	-0.888929
1	0	-14.941176	-4.766600	-1.014751
1	0	-12.597513	-5.608323	-0.798502
1	0	-10.755222	-4.005208	-0.454984
1	0	-5.465217	-2.918524	0.295837
1	0	-4.655744	1.281736	0.745391
1	0	-7.039257	1.804210	0.442156
1	0	-9.901778	2.070492	2.267085
1	0	-9.376957	4.496267	2.504385
1	0	-8.892165	5.861225	0.484620
1	0	-8.922522	4.804866	-1.765177
1	0	-9.447510	2.377693	-1.990110
1	0	-9.487960	-4.331530	1.151599
1	0	-7.747533	-4.264211	1.376249
1	0	-8.778543	-3.079942	2.174610
1	0	-7.378724	-4.044941	-1.490539
1	0	-8.196242	-2.733343	-2.335146
1	0	-9.118038	-4.109734	-1.724899
6	0	-0.000011	1.284902	-0.879585
6	0	0.000054	2.556822	-0.017275
1	0	-0.877216	1.272289	-1.536757
1	0	0.877151	1.272233	-1.536809
6	0	0.000042	3.837844	-0.860476
1	0	-0.879005	2.540610	0.640515
1	0	0.879174	2.540574	0.640430
6	0	0.000131	5.119543	-0.017255
1	0	0.878568	3.839768	-1.523018
1	0	-0.878560	3.839824	-1.522918
1	0	-0.878150	5.118474	0.645105
1	0	0.878475	5.118406	0.645023
6	0	0.000144	6.404187	-0.855918
6	0	0.000242	7.678996	-0.006091
1	0	-0.877901	6.404595	-1.517436
1	0	0.878120	6.404517	-1.517526
1	0	-0.884268	7.723803	0.641223
1	0	0.884820	7.723724	0.641137
1	0	0.000253	8.578139	-0.632714
7	0	-0.000015	0.053614	-0.108799