

**Access tetracoordinate boron-doped polycyclic aromatic
hydrocarbons with aggregation-induced emission under mild
conditions**

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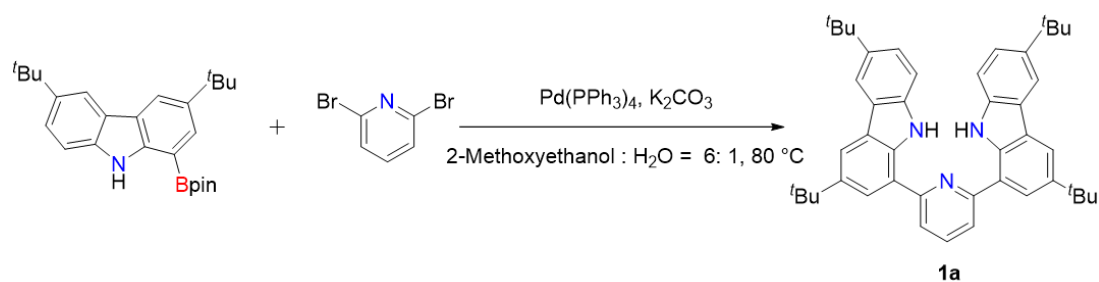
1. Experimental section

1.1 General information

All reactions were carried out under an atmosphere of dry nitrogen. Dichloromethane was freshly distilled over calcium hydrogen and stored under nitrogen prior to use. All starting materials were purchased from Energy Chemical and Leyan and used without further purification. Proton nuclear magnetic resonance (^1H NMR) and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on Bruker Avance 400 or 500 MHz spectrometers. All Photophysical property measurements were under nitrogen atmosphere. UV/vis and fluorescence measurements were performed on a Jasco V-770 UV/vis spectrophotometer and a F97 Pro fluorescence spectrophotometer, respectively. Quantum efficiencies were determined using an absolute PL quantum yield spectrometer C11347. Phosphorescence and photoluminescence decay curves were recorded on an Edinburgh Instruments FLS980 spectrophotometer equipped with 365 nm picosecond pulsed LEDs and decay curves were analyzed using the Edinburgh Instruments F980 software. Bpin-carbazole¹ and 7-Bpin-indole² were synthesized according to the reported procedure.

1.2 Synthetic details

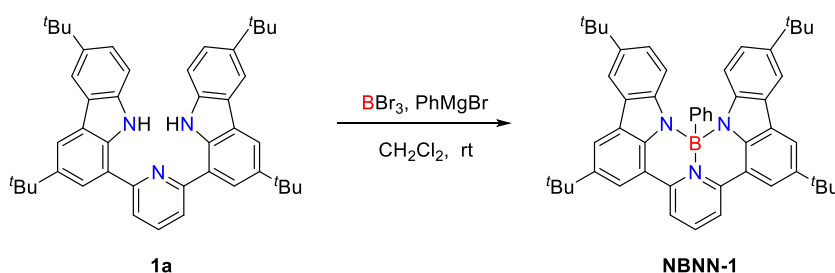
Synthesis of Compound NBNN-1



A mixture of 2-Methoxyethanol (48 ml) and water (8 ml) was stirred and degassed by nitrogen for 1 hour. 2,6-dibromopyridine (830 mg, 3.53 mmol), Bpin-carbazole (3.12 g, 7.70 mmol), $\text{Pd(PPh}_3)_4$ (200 mg, 0.173 mmol) and K_2CO_3 (1.45 g, 10.51 mmol) were added to the mixed solvents. The reaction mixture was heated to $80\text{ }^\circ\text{C}$ and stirred for 16 hours. The reaction mixture was quenched with water and then the mixture was washed with brine and CH_2Cl_2 for three times. The combined organic layers were dried

over magnesium sulfate and then the solvents were evaporated under reduced pressure. Purification of the crude product by silica gel column chromatography (petroleum ether/ethyl acetate = 50:1) afforded the product **1a** as a white solid in 90% yield (2.01 g, 3.18 mmol). ¹H NMR (500 MHz, CDCl₃) δ 10.26 (s, 2H, -NH), 8.29 (s, 2H, carbazole), 8.16 (s, 2H, carbazole), 8.10 (s, 2H, carbazole), 8.03 (t, *J* = 8.7 Hz, 1H, Py), 7.98 (d, *J* = 8.7 Hz 2H, Py), 7.27 (d, *J* = 8.9 Hz, 2H, carbazole), 6.83 (d, *J* = 8.9 Hz, 2H, carbazole), 1.61 (s, 18H, ^tBu), 1.45 (s, 18H, ^tBu). ¹³C NMR (126 MHz, CDCl₃) δ 157.68(Py), 142.47, 142.23, 138.48, 137.92, 136.61(Py), 125.30, 124.14, 122.82, 121.86, 120.85(Py), 119.06, 117.98, 116.12, 110.93, 35.05 (^tBu), 34.84 (^tBu), 32.35 (^tBu), 32.17 (^tBu). HRMS(ESI) (*m/z*): [M+H]⁺ calcd for C₄₅H₅₂N₃: 634.4146; found: 634.4158.

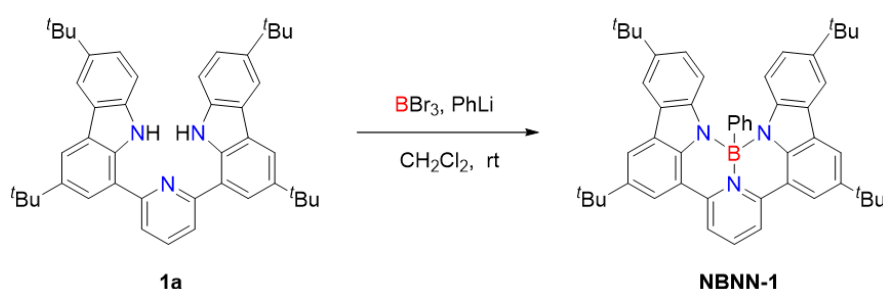
Method 1



Boron tribromide (0.1 mL) was added to a solution of **1a** (100 mg, 0.157 mmol) in CH₂Cl₂ (2 mL) under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 2 hours. Phenylmagnesium bromide (1 M in tetrahydrofuran, 4 mL, 4.0 mmol) was dripped into the reaction mixture and the reaction mixture was stirred for 1.5 hours. The reaction mixture was quenched with water and then the mixture was washed with brine and CH₂Cl₂ for three times. The combined organic layers were dried over magnesium sulfate and then the solvents were evaporated under reduced pressure. Purification of the crude product by alumina column chromatography (petroleum ether/ethyl acetate = 30:1) afforded the product **NBNN-1** as an orange solid in 78% yield (88 mg, 0.122 mmol). The product was confirmed by X-ray diffraction analysis. ¹H NMR (400 MHz, CD₂Cl₂) δ 8.39 (d, *J* = 1.5 Hz, 2H, carbazole), 8.35 (d, *J* = 8.1, 1H, Py), 8.23 – 8.18 (m, 2H, carbazole), 8.15 (d, *J* = 1.6 Hz, 1H, carbazole), 8.08 (t, *J* = 8.1 Hz, 1H, Py), 8.00 (d, *J* = 8.1, 1H, Py), 7.95 (d, *J* = 1.6 Hz, 1H, carbazole),

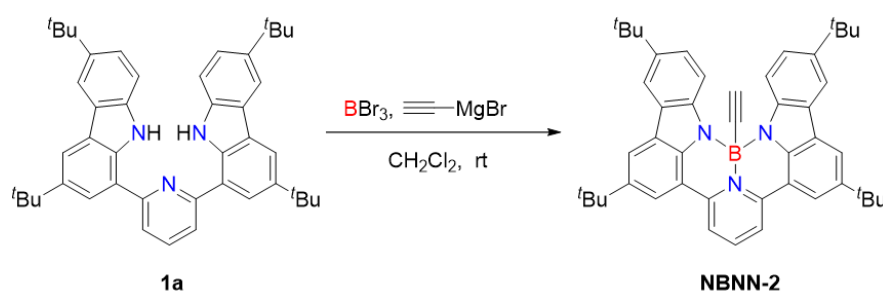
7.18 (ddd, $J = 17.2, 8.7, 2.1$ Hz, 2H, carbazole), 6.88 (d, $J = 7.4$ Hz, 2H, Ph), 6.86 – 6.80 (m, 1H, Ph), 6.73 (td, $J = 7.4, 1.1$ Hz, 2H, Ph), 6.17 (d, $J = 7.3$ Hz, 2H, carbazole), 1.59 (s, 9H, t Bu), 1.53 (s, 9H, t Bu), 1.44 (s, 18H, t Bu). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 152.64(Py), 150.14(Py), 144.49, 144.05, 142.75, 142.62, 142.46, 142.14, 139.63, 139.01, 131.58(Py), 126.98(Ph), 126.62(Ph), 126.06, 125.50, 125.48, 124.84, 123.69, 123.12, 121.43, 121.22, 120.07(Py), 118.77, 118.17, 117.89, 117.07, 116.69, 116.43, 115.92, 112.23, 35.42 (t Bu), 35.37 (t Bu), 34.97 (t Bu), 34.93 (t Bu), 32.31 (t Bu), 32.13 (t Bu). HRMS(ESI) (m/z): $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{51}\text{H}_{55}\text{BN}_3$: 720.4489; found: 720.4484.

Method 2



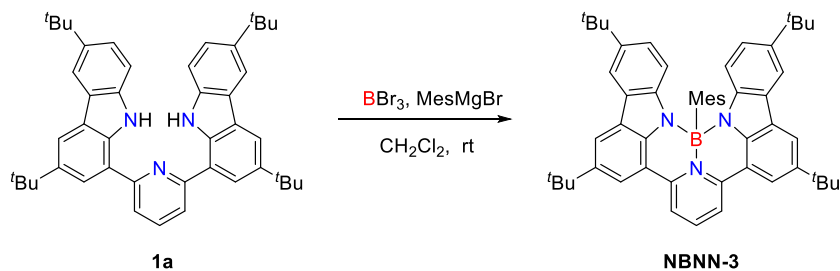
Boron tribromide (0.1 mL) was added to a solution of **1a** (100 mg, 0.157 mmol) in CH_2Cl_2 (2 mL) under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 2 hours. Phenyllithium (1 M in ethyl ether, 4 mL, 4.0 mmol) was dripped into the reaction mixture and the reaction mixture was stirred for 1.5 hours. The reaction mixture was quenched with water and then the mixture was washed with brine and CH_2Cl_2 for three times. The combined organic layers were dried over magnesium sulfate and then the solvents were evaporated under reduced pressure. Purification of the crude product by alumina column chromatography (petroleum ether/ethyl acetate = 30:1) afforded the product **NBNN-1** as an orange solid in 57% yield (64 mg, 0.089 mmol)

Synthesis of Compound NBNN-2



Boron tribromide (0.1 mL) was added to a solution of **1a** (300 mg, 0.437 mmol) in CH₂Cl₂ (6 mL) under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 2 hours. Ethynylmagnesium bromide (0.5 M in tetrahydrofuran, 8 mL, 4.0 mmol) was dripped into the reaction mixture and the reaction mixture was stirred for 1.5 hours. The reaction mixture was quenched with water and then the mixture was washed with brine and CH₂Cl₂ for three times. The combined organic layers were dried over magnesium sulfate and then the solvents were evaporated under reduced pressure. Purification of the crude product by alumina column chromatography (petroleum ether/ethyl acetate = 30:1) afforded the product **NBNN-2** as an orange solid in 58% yield (169 mg, 0.253 mmol). ¹H NMR (500 MHz, CDCl₃) δ 8.34 (s, 1H, carbazole), 8.31 (s, 1H, carbazole), 8.23 (d, *J* = 7.8 Hz, 1H, Py), 8.20 (s, 1H, carbazole), 8.15 (s, 1H, carbazole), 8.12 (d, *J* = 7.8 Hz, 1H, Py), 8.08 (m, 2H, Py, carbazole), 8.01 (s, 1H, carbazole), 7.57 (d, *J* = 8.5 Hz, 1H, carbazole), 7.45 (d, *J* = 8.5 Hz, 1H, carbazole), 7.11 (d, *J* = 8.8 Hz, 1H, carbazole), 6.81 (d, *J* = 8.8 Hz, 1H, carbazole), 1.89 (s, 1H, -C≡H), 1.58 (s, 9H, ^tBu), 1.55 (s, 13H, ^tBu, H₂O), 1.51 (s, 9H, ^tBu), 1.40 (s, 9H, ^tBu). ¹³C NMR (126 MHz, CDCl₃) δ 152.56(Py), 149.29(Py), 144.27, 142.90, 142.76, 142.62, 142.56, 142.31, 141.83, 139.29, 138.51(Py), 126.47, 125.90, 125.73, 124.59, 123.57, 123.45, 121.32, 120.89, 119.74(Py), 118.09, 117.68, 117.44, 116.49, 116.31, 116.26, 115.93, 111.67, 85.16 (-C≡H), 35.32 (^tBu), 35.17 (^tBu), 34.97 (^tBu), 34.77 (^tBu), 32.40 (^tBu), 32.32 (^tBu), 32.25 (^tBu), 32.11 (^tBu). HRMS(ESI) (*m/z*): [M+H]⁺ calcd for C₄₇H₅₁BN₃: 668.4176; found: 668.4176.

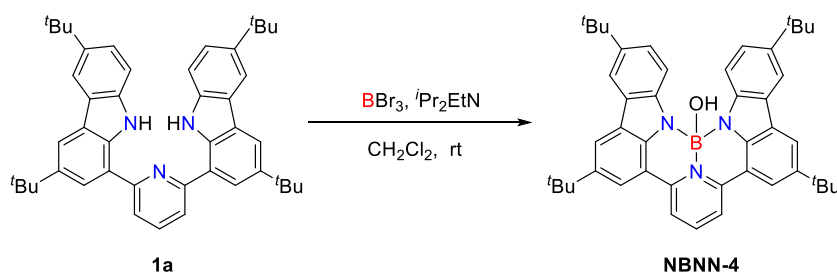
Synthesis of Compound NBNN-3



Boron tribromide (0.1 mL) was added to a solution of **1a** (100 mg, 0.157 mmol) in CH₂Cl₂ (2 mL) under nitrogen atmosphere. The reaction mixture was stirred at room

temperature for 2 hours. 2,4,6-trimethylphenylmagnesium bromide (1 M in tetrahydrofuran, 4 ml, 4.0 mmol) was dripped into the reaction mixture and the reaction mixture was stirred for 1.5 hours. The reaction mixture was quenched with water and then the mixture was washed with brine and CH₂Cl₂ for three times. The combined organic layers were dried over magnesium sulfate and then the solvents were evaporated under reduced pressure. Purification of the crude product by alumina column chromatography (petroleum ether/ethyl acetate = 50:1) afforded the product **NBNN-3** as an orange solid in 69% yield (82 mg, 0.108 mmol). ¹H NMR (500 MHz, CDCl₃) δ 8.32 (s, 1H, carbazole), 8.19 (s, 1H, carbazole), 8.17 (s, 1H, carbazole), 8.05 (d, *J* = 7.9 Hz, 1H, Py), 8.01 (s, 1H, carbazole), 7.94 (s, 1H, carbazole), 7.88 (t, *J* = 7.9 Hz, 1H, Py), 7.84 (s, 1H, carbazole), 7.75 (d, *J* = 7.9 Hz, 1H, Py), 7.32 (d, *J* = 8.8 Hz, 1H, carbazole), 7.01 (d, *J* = 8.8 Hz, 1H, carbazole), 6.95 (d, *J* = 8.9 Hz, 1H, carbazole), 6.41 (s, 1H, Mes), 6.38 (s, 1H, Mes), 6.23 (d, *J* = 8.9 Hz, 1H, carbazole), 2.05 (s, 3H, -CH₃), 1.53 (s, 9H, ^tBu), 1.49 (s, 9H, ^tBu), 1.46 (s, 9H, ^tBu), 1.37 (s, 3H, -CH₃), 1.32 (s, 9H, ^tBu), 1.00 (s, 3H, -CH₃). ¹³C NMR (126 MHz, CDCl₃) δ 153.81(Py), 151.08(Py), 143.70, 143.45, 143.17, 142.97, 142.18, 141.99, 141.85, 141.79, 141.56, 139.34, 137.93, 135.40(Py), 130.12, 129.79, 126.63, 125.54, 125.24, 124.51, 124.20, 124.02, 120.94, 120.14, 119.55(Py), 118.12, 117.87, 116.79, 116.36, 115.92, 113.95, 113.48, 112.96, 35.22 (^tBu), 35.14 (^tBu), 34.86 (^tBu), 34.66 (^tBu), 32.37 (^tBu), 32.31 (^tBu), 32.17 (^tBu), 32.04 (^tBu), 22.50 (-CH₃), 21.99 (-CH₃), 20.74 (-CH₃). HRMS(ESI) (*m/z*): [M+H]⁺ calcd for C₅₄H₆₁BN₃: 762.4959; found: 762.4951.

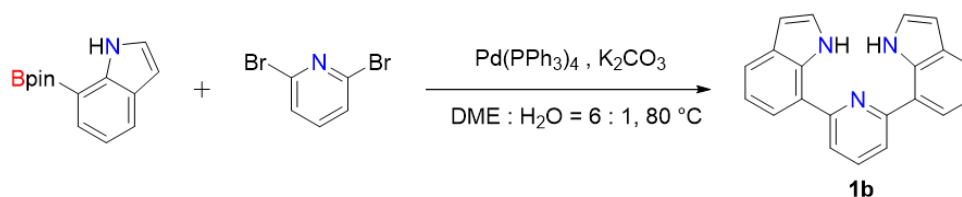
Synthesis of Compound NBNN-4



Boron tribromide (0.1 mL) was added to a solution of **1a** (100 mg, 0.157 mmol) in CH₂Cl₂ (2 mL) under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 2 hours. The reaction mixture was quenched with N,N-

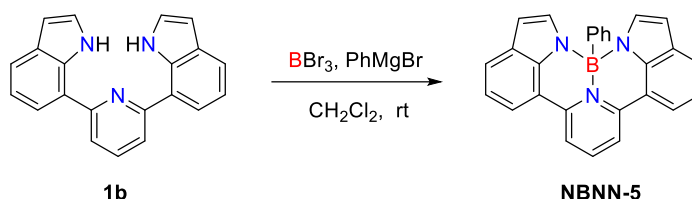
diisopropylethylamine (0.34 ml, 1.96 mmol) and then the mixture was washed with brine and CH₂Cl₂ for three times. The combined organic layers were dried over magnesium sulfate and then the solvents were evaporated under reduced pressure. Purification of the crude product by alumina column chromatography (petroleum ether/ethyl acetate = 10:1) afforded the product **NBNN-4** as a yellow solid in 48% yield (50 mg, 0.076 mmol). ¹H NMR (500 MHz, DMSO-d₆) δ 8.70 (d, *J* = 8.0 Hz, 1H, Py), 8.67 (d, *J* = 8.0 Hz, 1H, Py), 8.50 (s, 1H, carbazole), 8.43 (s, 1H, carbazole), 8.41 (s, 1H, carbazole), 8.36 (s, 1H, carbazole), 8.35 – 8.31 (m, 1H, Py), 8.30 (s, 1H, carbazole), 8.24 (s, 1H, carbazole), 7.45 (d, *J* = 8.6 Hz, 1H, carbazole), 7.33 (d, *J* = 8.6 Hz, 1H, carbazole), 7.06 (d, *J* = 8.7 Hz, 1H, carbazole), 6.72 (d, *J* = 8.7 Hz, 1H, carbazole), 4.53 (s, 1H, -OH), 1.57 (s, 9H, 'Bu), 1.54 (s, 9H, 'Bu), 1.48 (s, 9H, 'Bu), 1.37 (s, 9H, 'Bu). ¹³C NMR (126 MHz, CDCl₃) δ 151.60(Py), 149.19(Py), 143.30, 143.00, 142.65, 142.58, 142.21, 141.96, 138.57, 138.52, 126.47, 125.62, 124.65, 123.70, 123.48, 120.98, 120.80, 119.83(Py), 118.20, 117.91, 116.93, 116.41, 116.38, 115.80, 115.38, 112.14, 35.29 ('Bu), 35.20 ('Bu), 34.99 ('Bu), 34.78 ('Bu), 32.42 ('Bu), 32.36 ('Bu), 32.24 ('Bu), 32.13 ('Bu). HRMS(ESI) (*m/z*): [M-OH]⁺ calcd for C₄₅H₄₉BN₃: 642.4020; found: 642.4022.

Synthesis of Compound NBNN-5



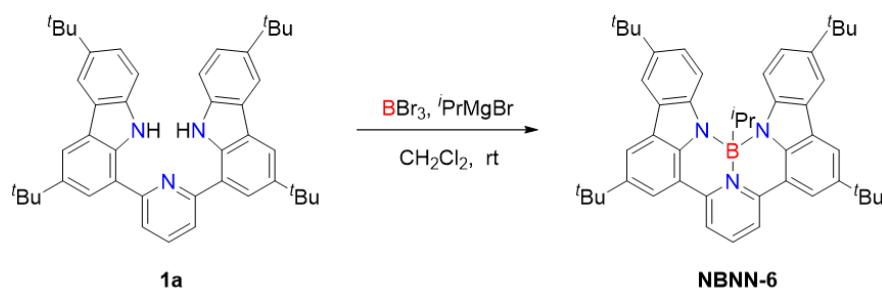
A mixture of 1,2-dimethoxyethane (DME, 24 ml) and water (4 ml) was stirred and degassed by nitrogen for 1 hour. 2,6-dibromopyridine (592 mg, 2.52 mmol), 7-Bpin-indole (1.34 g, 5.51 mmol), Pd(PPh₃)₄ (144 mg, 0.124 mmol) and K₂CO₃ (1.03 g, 7.45 mmol) were added to the mixed solvents. The reaction mixture was heated to 80 °C and stirring for 16 hours. The reaction mixture was quenched with water and then the mixture was washed with brine and CH₂Cl₂ for three times. The combined organic layers were dried over magnesium sulfate and then the solvents were evaporated under reduced pressure. Purification of the crude product by silica gel column

chromatography (petroleum ether/ethyl acetate = 50:1) afforded the product **1b** as a white solid in 46% yield (355 mg, 1.15 mmol). ^1H NMR (500 MHz, CDCl_3) δ 10.36 (s, 2H, -NH), 7.96 (t, $J = 7.8$ Hz, 1H, Py), 7.93 – 7.71 (m, 6H, indole, Py), 7.31 (t, $J = 7.5$ Hz, 2H, indole), 7.22 (m, 2H, indole), 6.67 (d, $J = 9.7$ Hz, 2H, indole). ^{13}C NMR (126 MHz, CDCl_3) δ 157.35(Py), 138.17, 133.99(Py), 129.59, 125.07, 122.44, 120.65(Py), 119.95, 119.35, 102.62. HRMS(ESI) (m/z): $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{21}\text{H}_{16}\text{N}_3$: 310.1344; found: 310.1356.



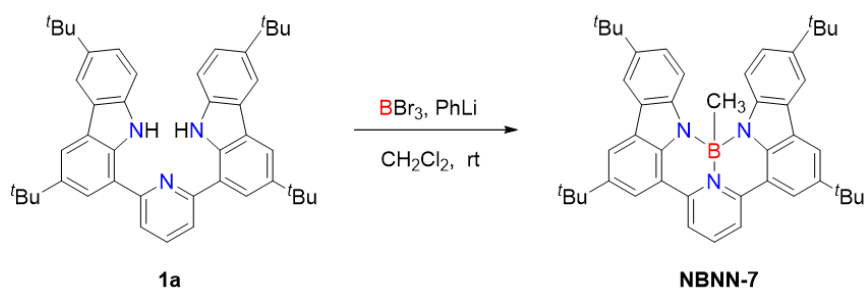
Boron tribromide (0.1 mL) was added to a solution of **1b** (150 mg, 0.485 mmol) in CH_2Cl_2 (6 mL) under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 2 hours. Phenylmagnesium bromide (1 M in tetrahydrofuran, 4 mL, 4.0 mmol) was dripped into the reaction mixture and the reaction mixture was stirred for 1.5 hours. The reaction mixture was quenched with water and then the mixture was washed with brine and CH_2Cl_2 for three times. The combined organic layers were dried over magnesium sulfate and then the solvents were evaporated under reduced pressure. Purification of the crude product by alumina column chromatography (petroleum ether/ethyl acetate = 50:1) afforded the product **NBNN-5** as a yellow-green solid in 46% yield (88 mg, 0.223 mmol). ^1H NMR (500 MHz, CDCl_3) δ 8.04 (d, $J = 8.0$ Hz, 2H, indole), 7.88 (t, $J = 7.8$ Hz, 1H, Py), 7.83 (m, 4H, indole), 7.68 (d, $J = 7.8$ Hz, 2H, Py), 7.18 (t, $J = 7.6$ Hz, 2H, indole), 6.89 (t, $J = 7.3$ Hz, 1H, Ph), 6.79 (m, 4H, Ph), 6.15 (d, $J = 7.5$ Hz, 2H, indole). ^{13}C NMR (126 MHz, CDCl_3) δ 151.23(Py), 139.95, 137.01, 130.51(Py), 129.67, 128.83(Ph), 127.37(Ph), 127.27(Ph), 125.24, 119.70, 118.85(Py), 117.83, 115.05, 104.21. HRMS(ESI) (m/z): $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{27}\text{H}_{19}\text{N}_3$: 396.1672; found: 396.1682.

Synthesis of Compound NBNN-6



Boron tribromide (0.1 mL) was added to a solution of **1a** (300 mg, 0.437 mmol) in CH₂Cl₂ (6 mL) under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 2 hours. Isopropylmagnesium chloride (2 M in tetrahydrofuran, 2 mL, 4.0 mmol) was dripped into the reaction mixture and the reaction mixture was stirred for 1.5 hours. The reaction mixture was quenched with water and then the mixture was washed with brine and CH₂Cl₂ for three times. The combined organic layers were dried over magnesium sulfate and then the solvents were evaporated under reduced pressure. Purification of the crude product by alumina column chromatography (petroleum ether/ethyl acetate = 20:1). Although we saw yellow product spots on both silica plate and alumina plate, we did not get the stable product **NBNN-6** by column chromatography.

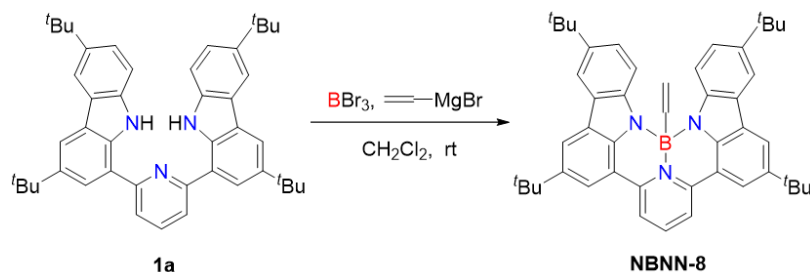
Synthesis of Compound NBNN-7



Boron tribromide (0.1 mL) was added to a solution of **1a** (100 mg, 0.157 mmol) in CH₂Cl₂ (2 mL) under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 2 hours. Methyl lithium diethyl ether (1.6 M in diethyl ether, 2.5 mL, 4.0 mmol) was dripped into the reaction mixture and the reaction mixture was stirred for 1.5 hours. The reaction mixture was quenched with water and then the mixture was washed with brine and CH₂Cl₂ for three times. The combined organic layers were dried over magnesium sulfate and then the solvents were evaporated under reduced pressure. Purification of the crude product by alumina column chromatography (petroleum

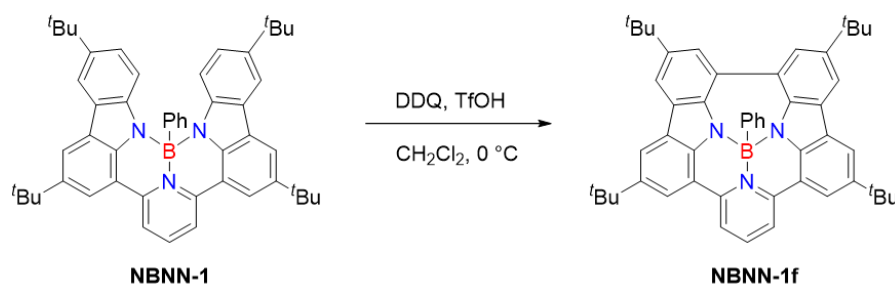
ether/ethyl acetate = 25:1). Although we saw orange product spots on both silica plate and alumina plate, we did not get the stable product **NBNN-7** by column chromatography.

Synthesis of Compound NBNN-8



Boron tribromide (0.1 mL) was added to a solution of **1a** (300 mg, 0.437 mmol) in CH_2Cl_2 (6 mL) under nitrogen atmosphere. The reaction mixture was stirred at room temperature for 2 hours. Vinylmagnesium bromide (2 M in tetrahydrofuran, 2 mL, 4.0 mmol) was dripped into the reaction mixture and the reaction mixture was stirred for 1.5 hours. The reaction mixture was quenched with water and then the mixture was washed with brine and CH_2Cl_2 for three times. The combined organic layers were dried over magnesium sulfate and then the solvents were evaporated under reduced pressure. We saw lighter orange product spots on both silica plate and alumina plate, but we did not get the stable product **NBNN-8** by column chromatography.

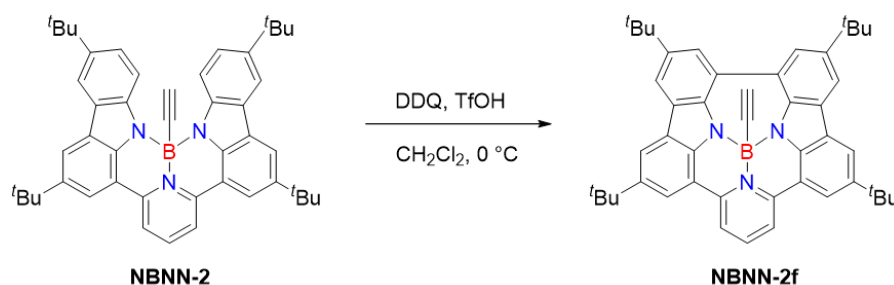
Synthesis of Compound NBNN-1f



2,3-dichloro-5,6-dicyano-1,4-benzoquinone (56.8 mg, 0.250 mmol) was added to a solution of compound **NBNN-1** (72 mg, 0.10 mmol) in CH_2Cl_2 (20 mL), after stirring for 5 min at room temperature, triflic acid (1.10 mL) was added under nitrogen atmosphere at 0 °C. Then the mixture was stirred for 15 min at the same temperature. After quenching with triethylamine, the reaction mixture was concentrated under

reduced pressure. Purification of the crude product by alumina column chromatography (petroleum ether/ethyl acetate = 20:1) afforded the product **NBNN-1f** as a red solid in 78% yield (56 mg, 0.078 mmol), which was confirmed by X-ray diffraction analysis. ^1H NMR (500 MHz, CDCl_3) δ 8.45 (s, 2H, carbazole), 8.21 (s, 2H, carbazole), 8.06 (s, 2H, carbazole), 7.97 (d, $J = 7.3$ Hz, 2H, Py), 7.94 – 7.87 (m, 1H, Py), 7.84 (s, 2H, carbazole), 6.80 (t, $J = 7.3$ Hz, 1H, Ph), 6.71 (t, $J = 7.6$ Hz, 2H, Ph), 6.49 (d, $J = 6.7$ Hz, 2H, Ph), 1.58 (s, 18H, $t\text{Bu}$), 1.52 (s, 18H, $t\text{Bu}$). ^{13}C NMR (126 MHz, CDCl_3) δ 151.49(Py), 142.41, 141.91, 140.84, 140.30, 139.56(Py), 129.31, 127.24(Ph), 126.94(Ph), 126.41, 125.08, 121.97, 121.79, 121.05(Py), 118.54, 118.44, 116.59, 113.91, 35.19 ($t\text{Bu}$), 35.10 ($t\text{Bu}$), 32.33 ($t\text{Bu}$), 32.27 ($t\text{Bu}$). HRMS(ESI) (m/z): $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{51}\text{H}_{53}\text{BN}_3$: 718.4333; found: 718.4381.

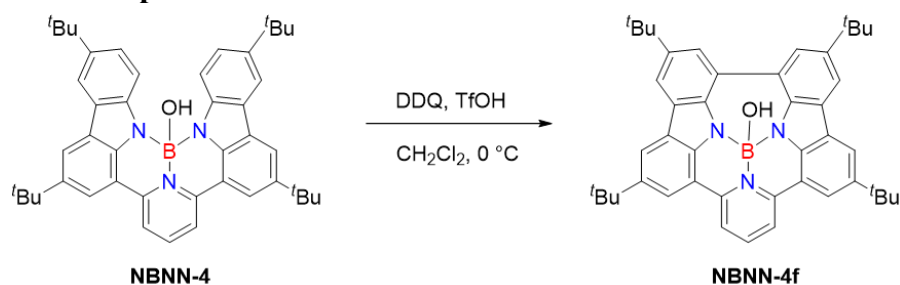
Synthesis of Compound **NBNN-2f**



2,3-dichloro-5,6-dicyano-1,4-benzoquinone (28.4 mg, 0.125 mmol) was added to a solution of compound **NBNN-2** (33 mg, 0.05 mmol) in CH_2Cl_2 (10 mL), after stirring for 5 min at room temperature, triflic acid (0.55 mL) was added under nitrogen atmosphere at 0 °C. Then the mixture was stirred for 15 min at the same temperature. After quenching with triethylamine, the reaction mixture was concentrated under reduced pressure. Purification of the crude product by alumina column chromatography (petroleum ether/ethyl acetate = 20:1) afforded the product **NBNN-2f** as a red solid in 58% yield (19 mg, 0.029 mmol). ^1H NMR (500 MHz, CDCl_3) δ 8.45 (s, 2H, carbazole), 8.20 (s, 2H, carbazole), 8.06 (s, 2H, carbazole), 7.92 (m, 3H, Py), 7.85 (s, 2H, carbazole), 1.86 (s, 1H, $-\text{C}\equiv\text{H}$), 1.59 (s, 18H, $t\text{Bu}$), 1.53 (s, 18H, $t\text{Bu}$). ^{13}C NMR (126 MHz, CDCl_3) δ 150.79(Py), 142.96, 142.39, 140.64, 140.47, 139.23(Py), 127.00, 125.55, 122.13, 121.95, 121.30(Py), 118.81, 118.65, 116.83, 113.42, 86.93, 35.25 ($t\text{Bu}$),

35.15 (tBu), 32.34 (tBu), 32.27 (tBu). HRMS(ESI) (m/z): [M+H]⁺ calcd for C₄₇H₄₉BN₃: 666.4020; found: 666.4019.

Synthesis of Compound NBNN-4f



2,3-dichloro-5,6-dicyano-1,4-benzoquinone (28.4 mg, 0.125 mmol) was added to a solution of compound **NBNN-4** (33 mg, 0.05 mmol) in CH₂Cl₂ (10 mL), after stirring for 5 min at room temperature, triflic acid (0.55 mL) was added under nitrogen atmosphere at 0 °C. Then the mixture was stirred for 15 min at the same temperature. After quenching with triethylamine, the reaction mixture was concentrated under reduced pressure. Purification of the crude product by alumina column chromatography (petroleum ether/ethyl acetate = 4:1) afforded the mixed product **NBNN-4f** as a red solid. We found that the stability of product **NBNN-4f** was not good, so we did not get clean NMR spectrum (**Figure S3.15** and **Figure S3.16**), but we got a HRMS spectrum. HRMS(ESI) (m/z): [M-OH]⁺ calcd for C₄₅H₄₇BN₃: 640.3863; found: 640.3872.

2. Electrochemical Properties

Electrochemical measurements were through a three-electrode system with a glassy carbon work electrode, a Pt wire reference electrode and a Pt wire counter electrode. **NBNN-1**, **NBNN-3**, **NBNN-4**, **NBNN-1f**, **NBNN-2f**, and **1a** were measured in CH₃CN (0.1 mol/L ⁿBu₄NBF₄ vs Fc/Fc⁺) at a scan rate of 100 mV/s. The solubility of **NBNN-2** in CH₃CN is not good, so it was measured in CH₂Cl₂ (0.1 mol/L ⁿBu₄NBF₄ vs Fc/Fc⁺) at a scan rate of 100 mV/s. No obvious peak can be found of **NBNN-5** and **1b** in either CH₃CN or CH₂Cl₂.

Table S2.1 Electrochemical Data.

	E _{HOMO} (eV) ^a	E _{LUMO} (eV) ^b	E _{red} (eV)	E _{ox} (eV)
NBNN-1	-5.10	-2.79	-2.02	0.30
NBNN-1f	-4.93	-3.01	-1.93	0.13
NBNN-2	-5.06	-2.62	-2.16	0.26
NBNN-2f	-4.99	-2.96	-1.96	0.19
NBNN-3	-5.07	-2.74	-2.09	0.27
NBNN-4	-5.08	-2.70	-2.06	0.28
1a	-5.06	-2.69	N/A	0.22

^a Calculated from the first oxidation peak using $E_{\text{HOMO}} = -E_{\text{ox}} - 4.80 \text{ eV}$. ^b Estimated according to $E_{\text{LUMO}} = E_{\text{HOMO}} + \text{the UV/vis absorption edge}$.

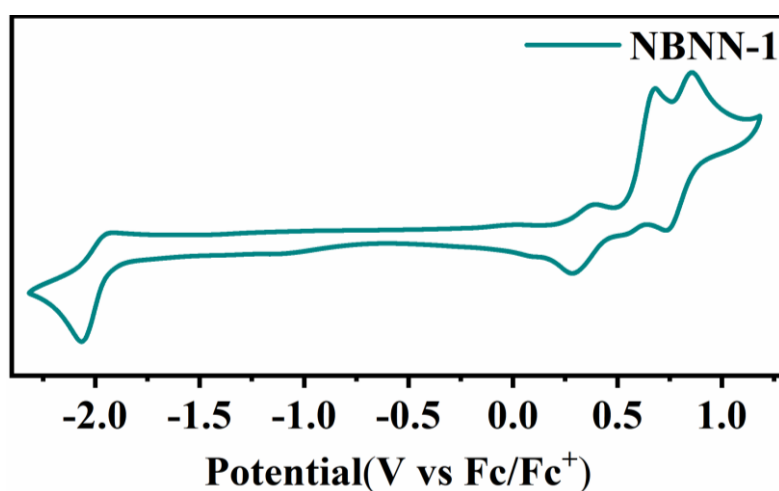


Figure S2.1 Cyclic voltammetry curve of **NBNN-1**

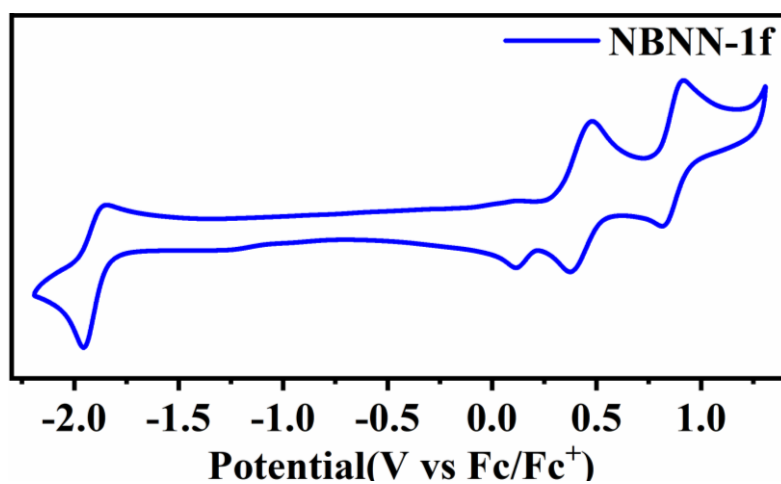


Figure S2.2 Cyclic voltammetry curve of NBNN-1f

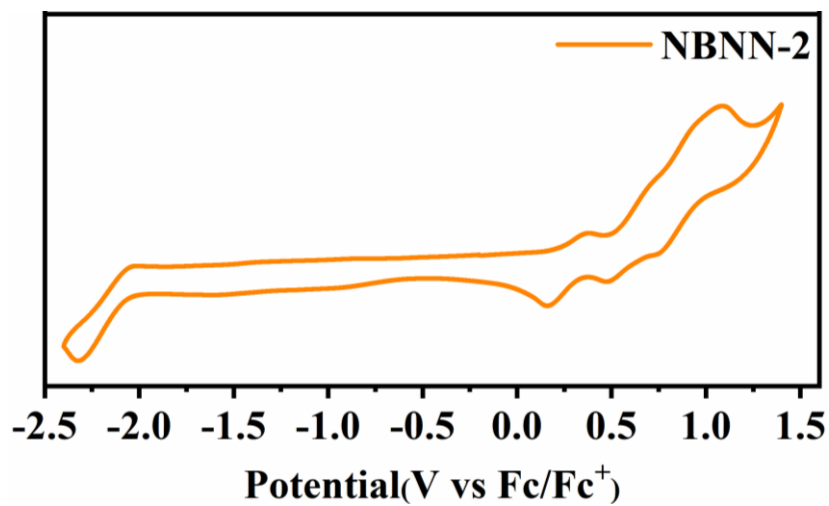


Figure S2.3 Cyclic voltammetry curve of NBNN-2

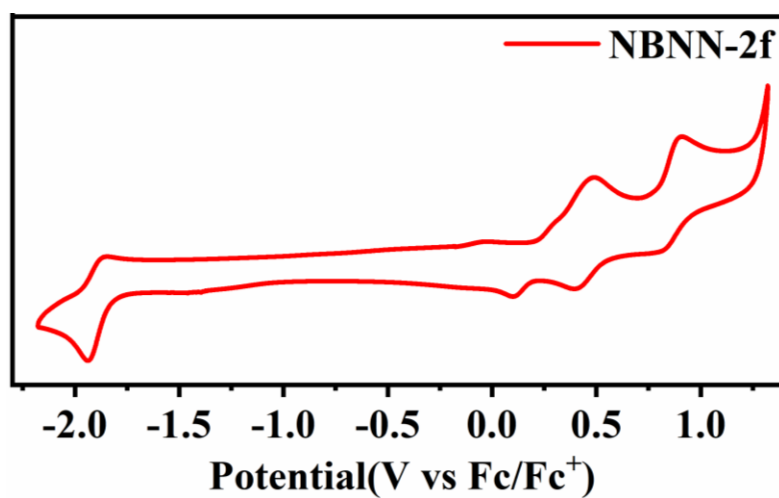


Figure S2.4 Cyclic voltammetry curve of NBNN-2f

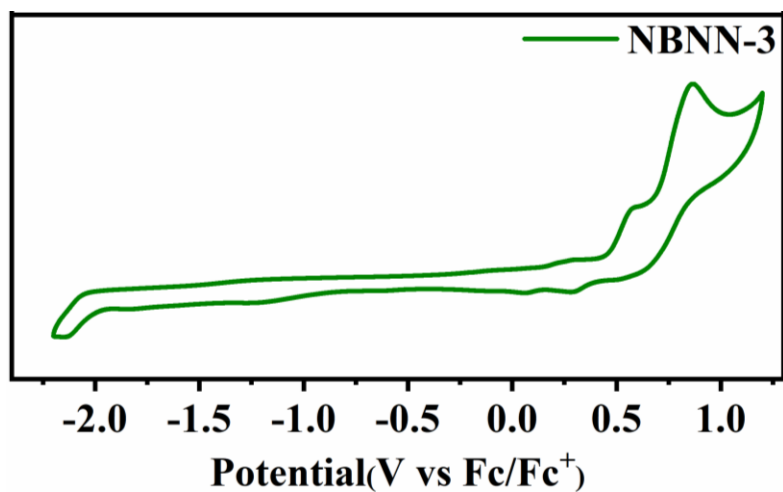


Figure S2.5 Cyclic voltammetry curve of NBNN-3

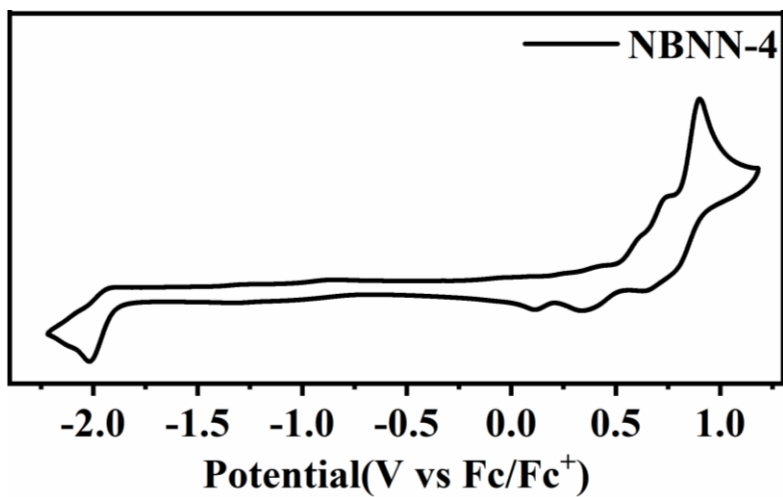


Figure S2.6 Cyclic voltammetry curve of NBNN-4

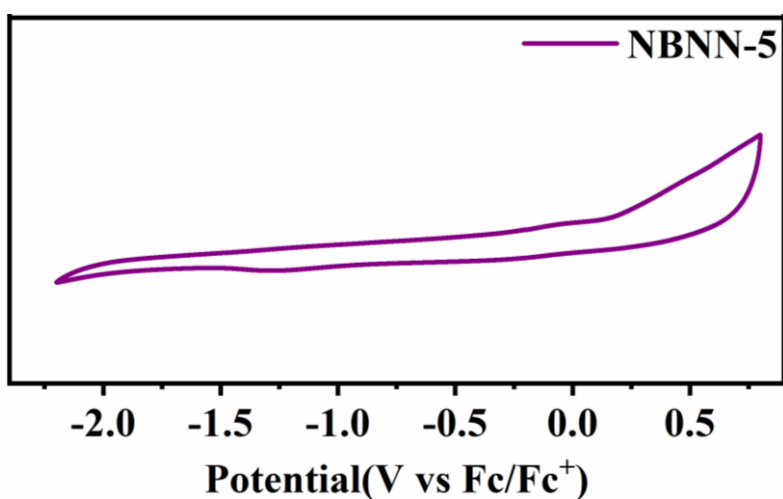


Figure S2.7 Cyclic voltammetry curve of NBNN-5

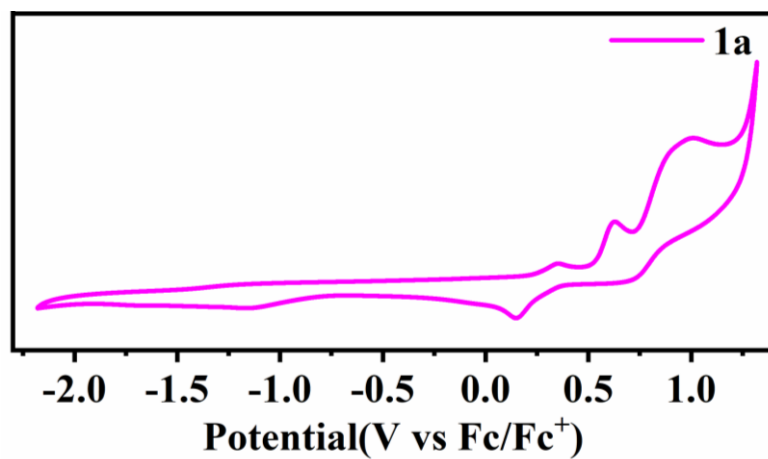


Figure S2.8 Cyclic voltammetry curve of **1a**

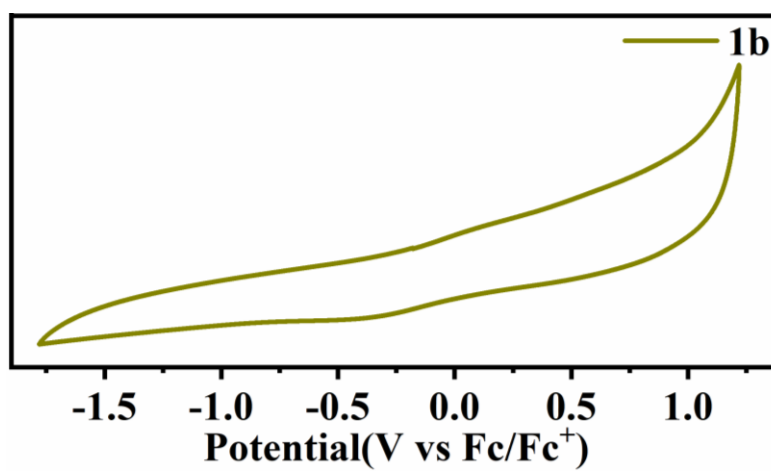
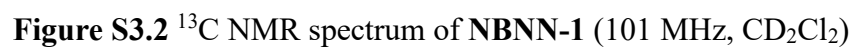
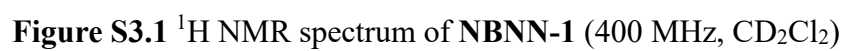


Figure S2.9 Cyclic voltammetry curve of **1b**

^1H and ^{13}C NMR spectra of **NBNN-1** in CD_2Cl_2 

^1H and ^{13}C NMR spectra of NBNN-2 in CDCl_3

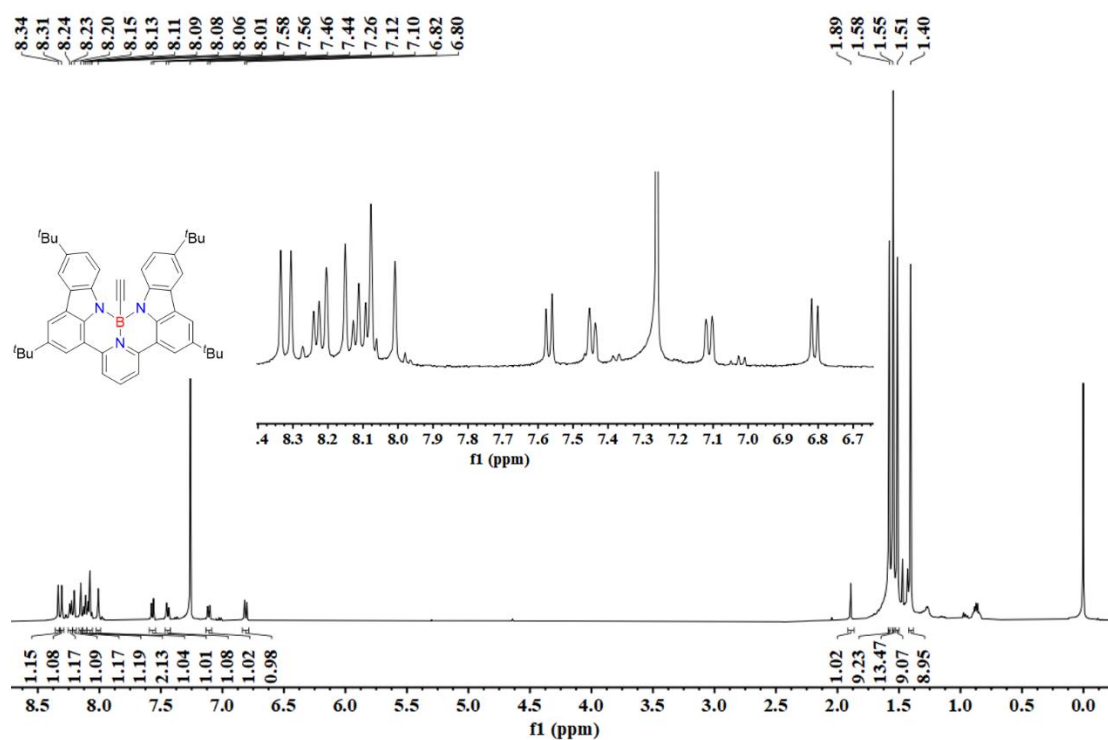


Figure S3.3 ^1H NMR spectrum of NBNN-2 (500 MHz, CDCl_3)

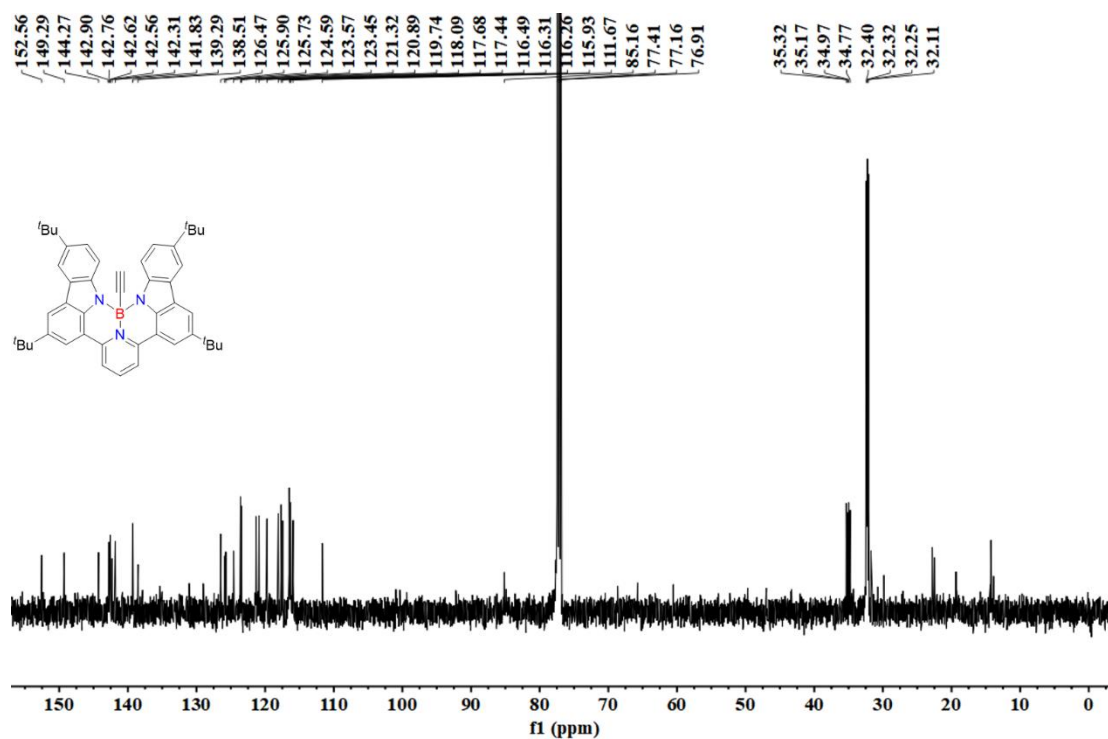


Figure S3.4 ^{13}C NMR spectrum of NBNN-2 (126 MHz, CDCl_3)

^1H and ^{13}C NMR spectra of **NBNN-3** in CDCl_3

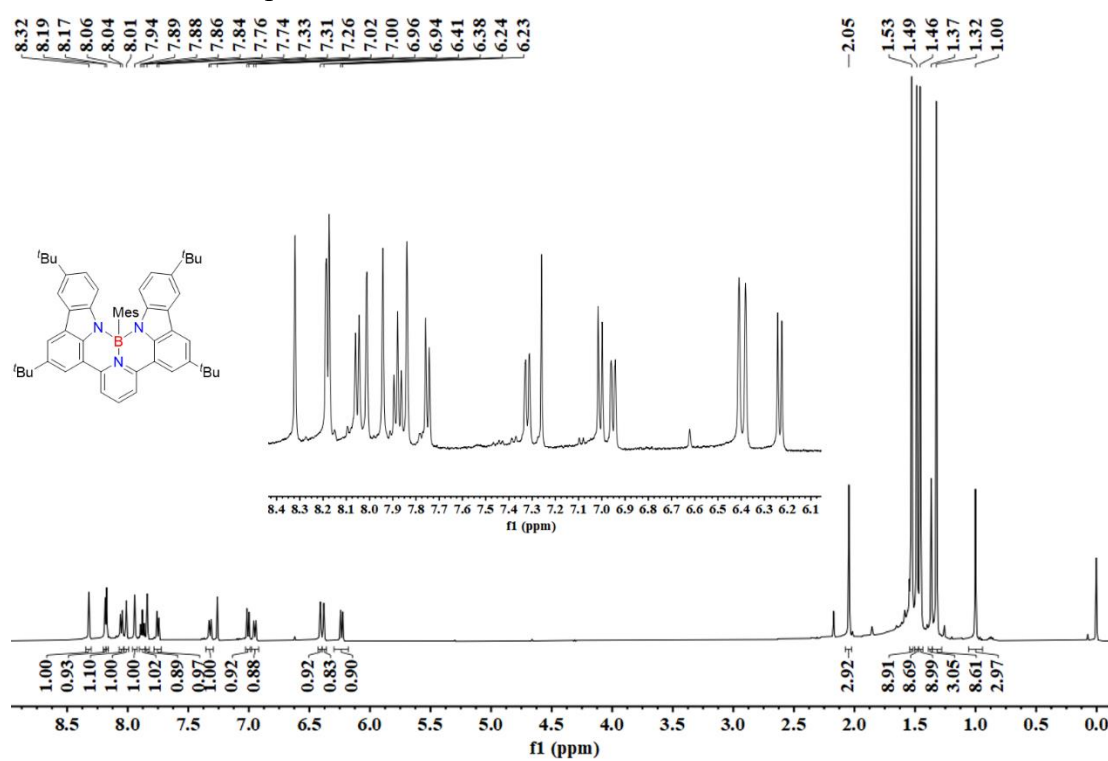


Figure S3.5 ^1H NMR spectrum of **NBNN-3** (500 MHz, CDCl_3)

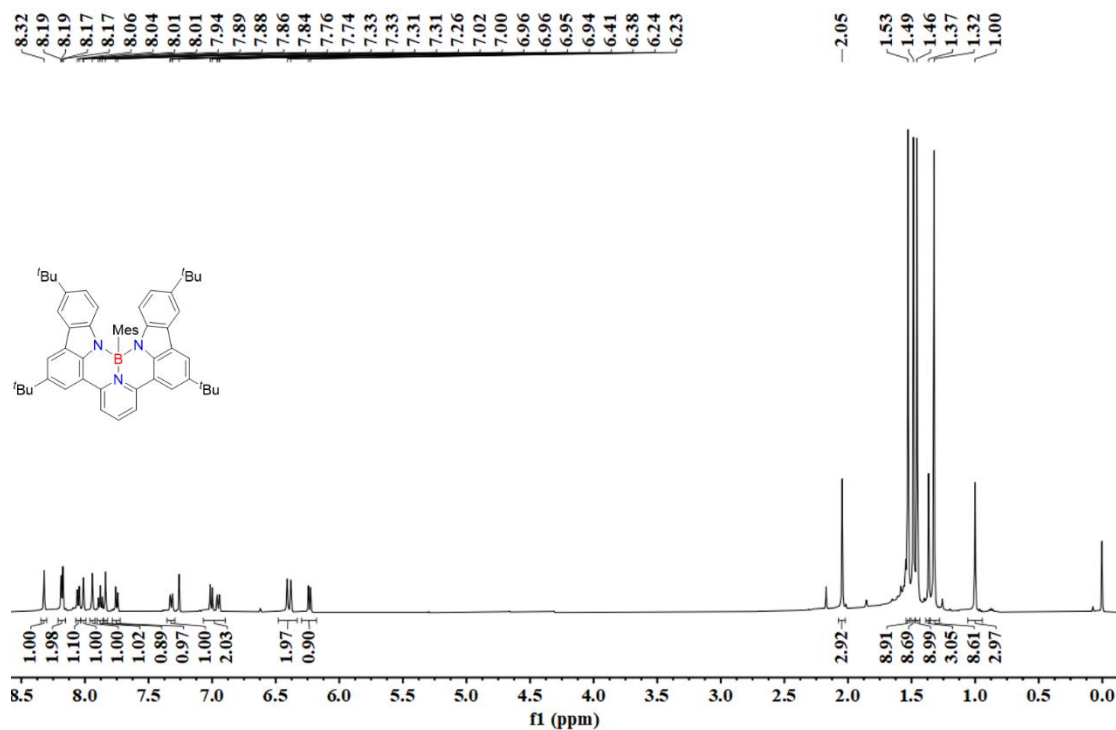


Figure S3.6 ^{13}C NMR spectrum of **NBNN-3** (126 MHz, CDCl_3)

^1H and ^{13}C NMR spectra of NBNN-4

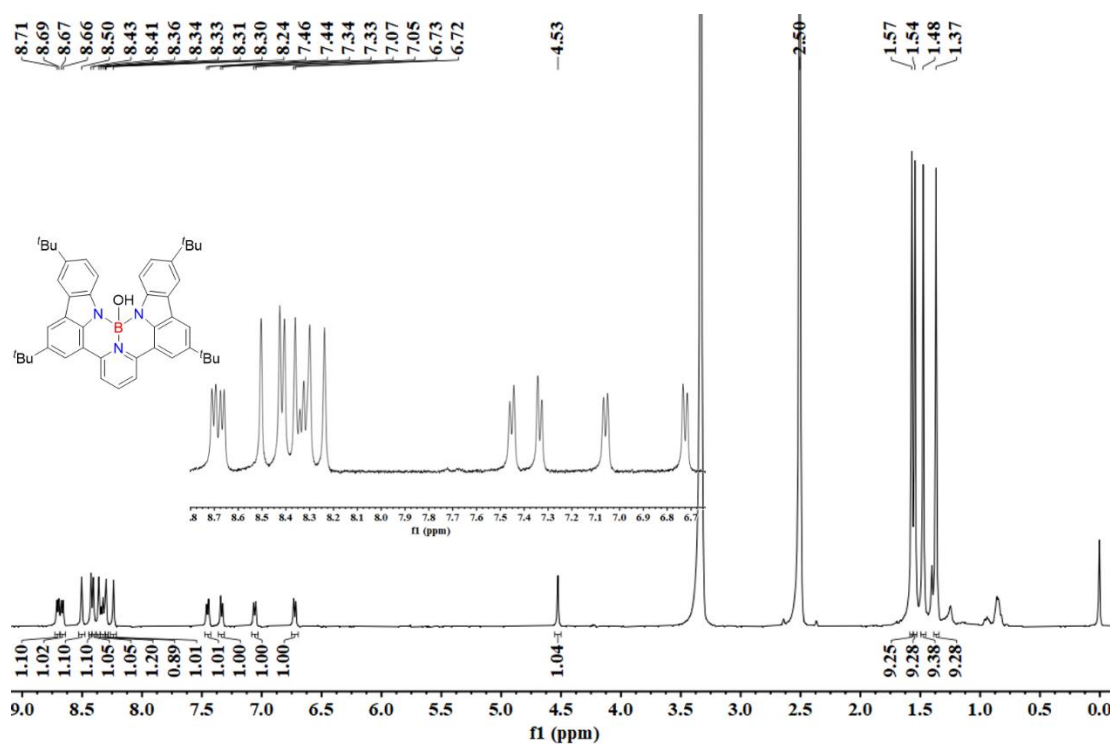


Figure S3.7 ^1H NMR spectrum of NBNN-4 (500 MHz, DMSO- d_6)

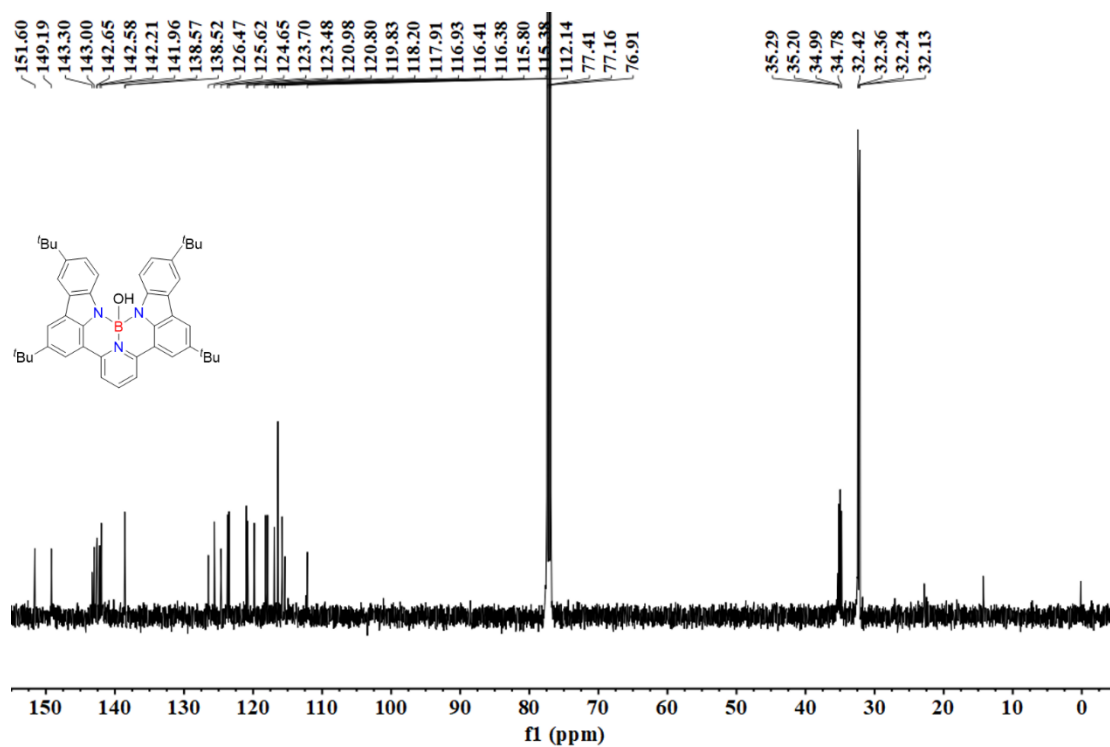


Figure S3.8 ^{13}C NMR spectrum of NBNN-4 (126 MHz, CDCl_3)

^1H and ^{13}C NMR spectra of **NBNN-5** in CDCl_3

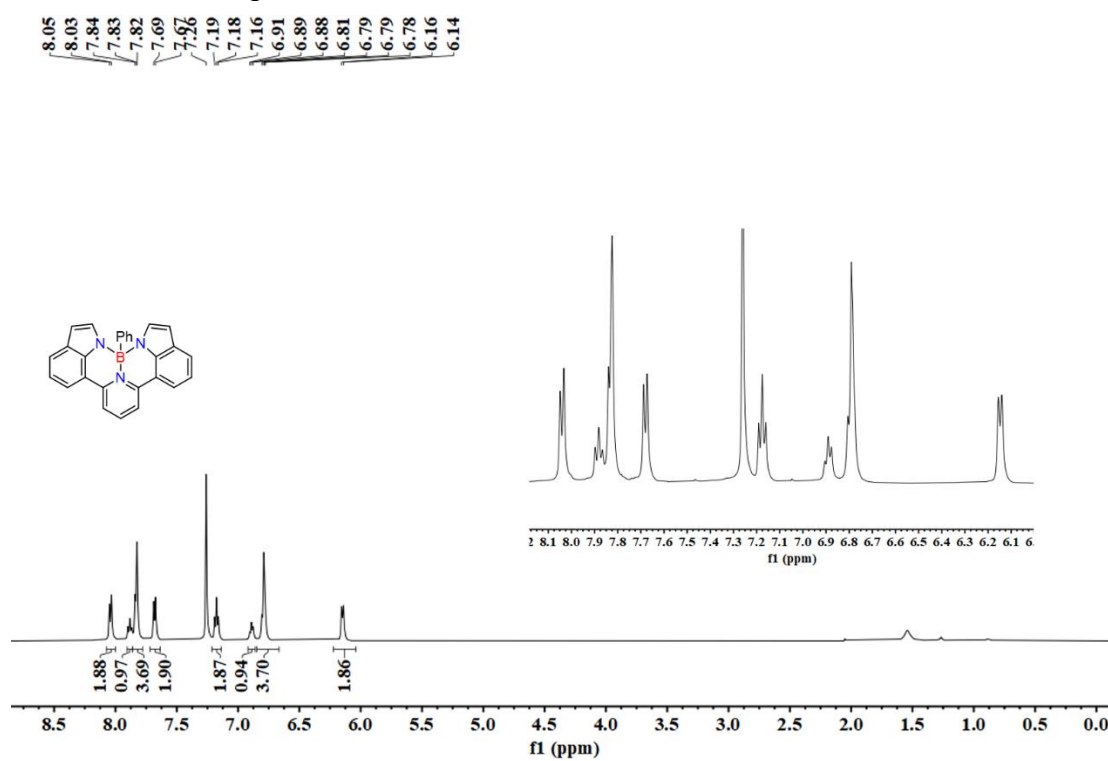


Figure S3.9 ^1H NMR spectrum of **NBNN-5** (500 MHz, CDCl_3)

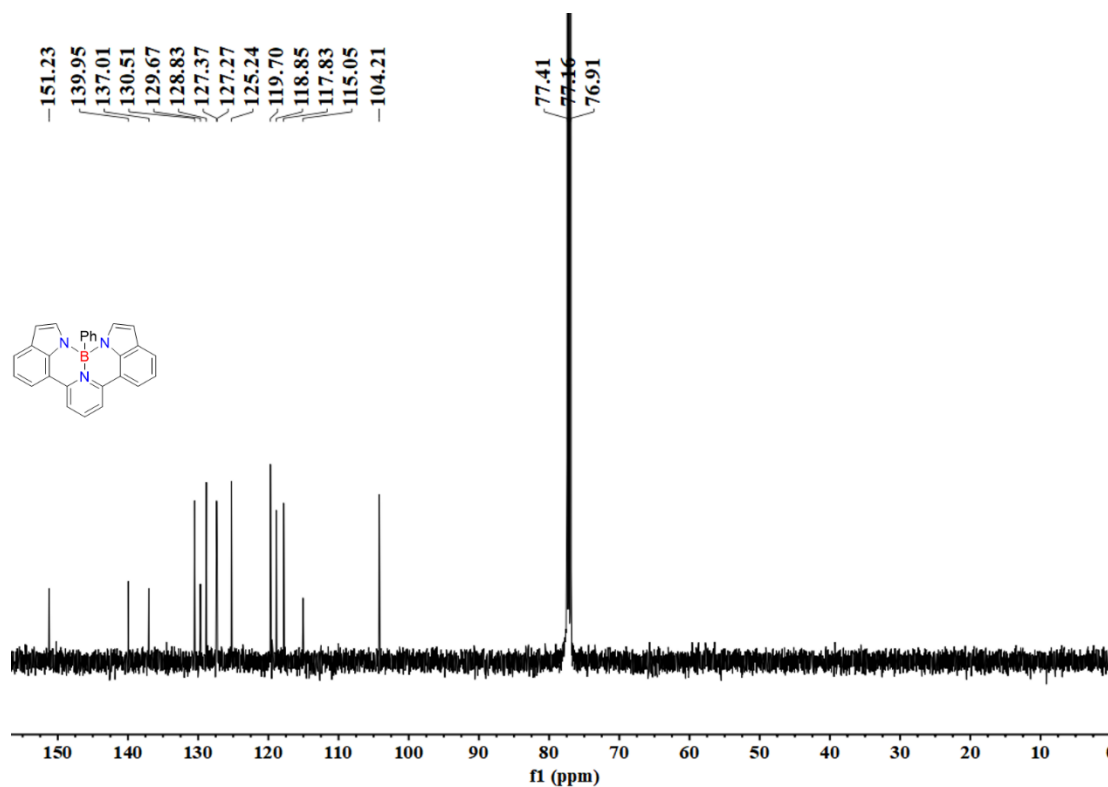


Figure S3.10 ^{13}C NMR spectrum of **NBNN-5** (126 MHz, CDCl_3)

^1H and ^{13}C NMR spectra of **NBNN-1f** in CDCl_3

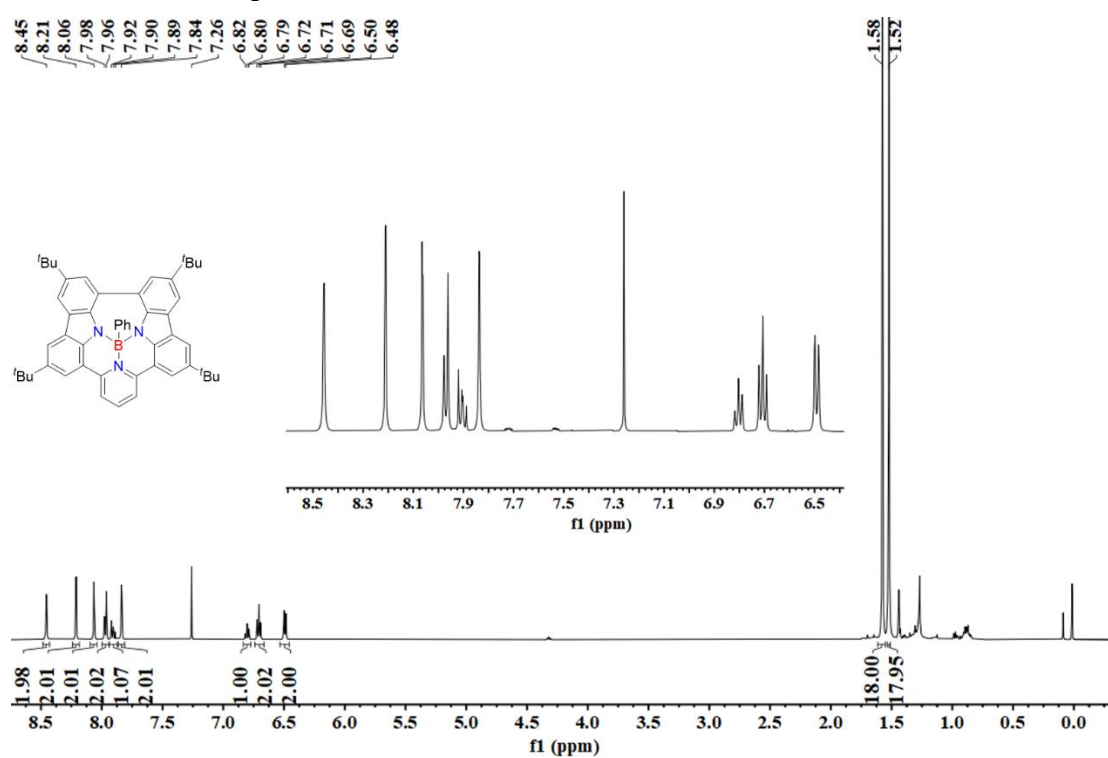


Figure S3.11 ^1H NMR spectrum of **NBNN-1f** (500 MHz, CDCl_3)

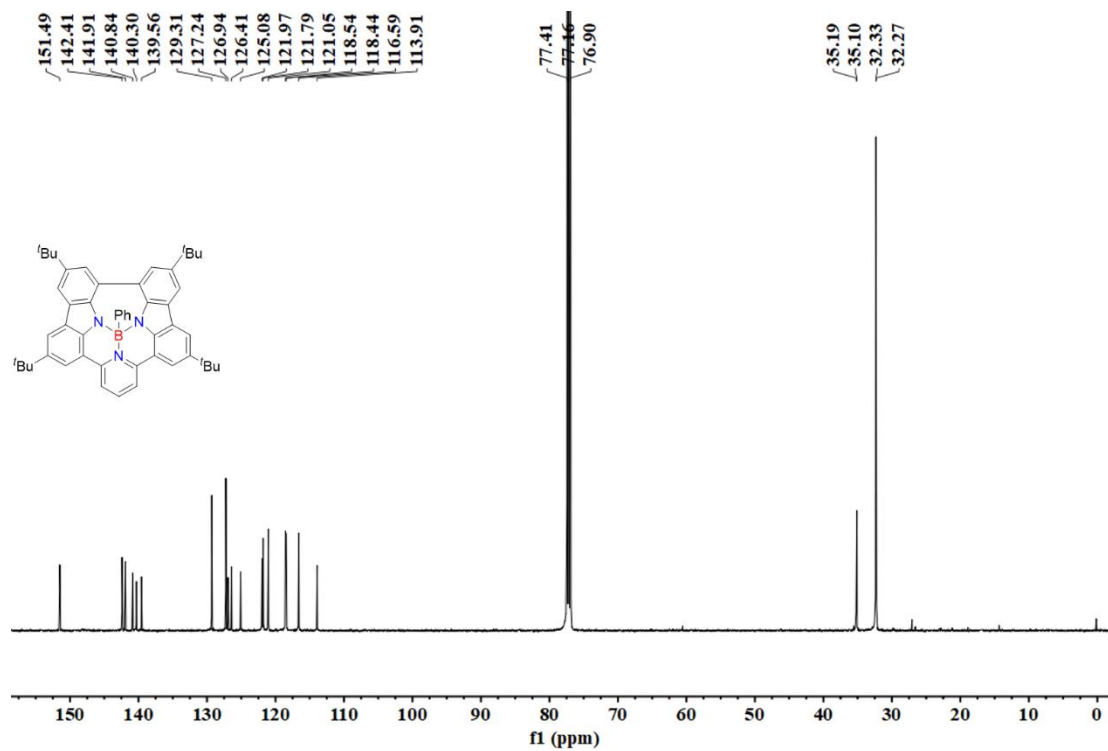


Figure S3.12 ^{13}C NMR spectrum of **NBNN-1f** (126 MHz, CDCl_3)

^1H and ^{13}C NMR spectra of **NBNN-2f** in CDCl_3

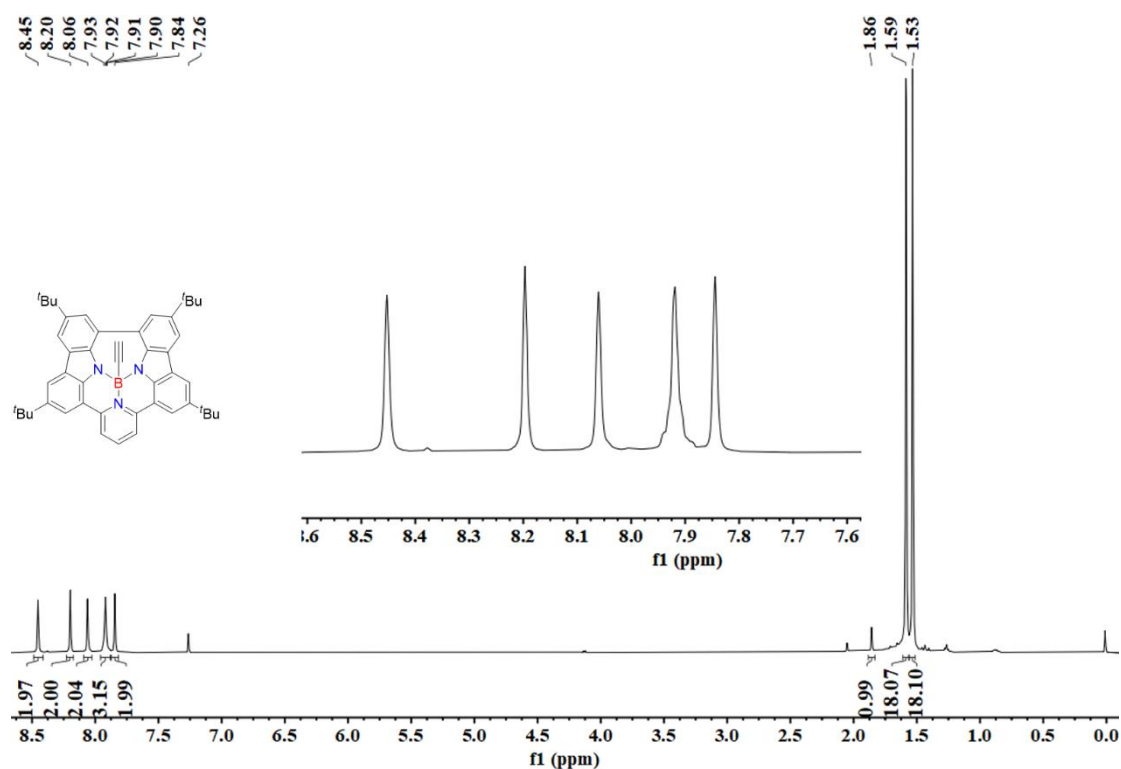


Figure S3.13 ^1H NMR spectrum of **NBNN-2f** (500 MHz, CDCl_3)

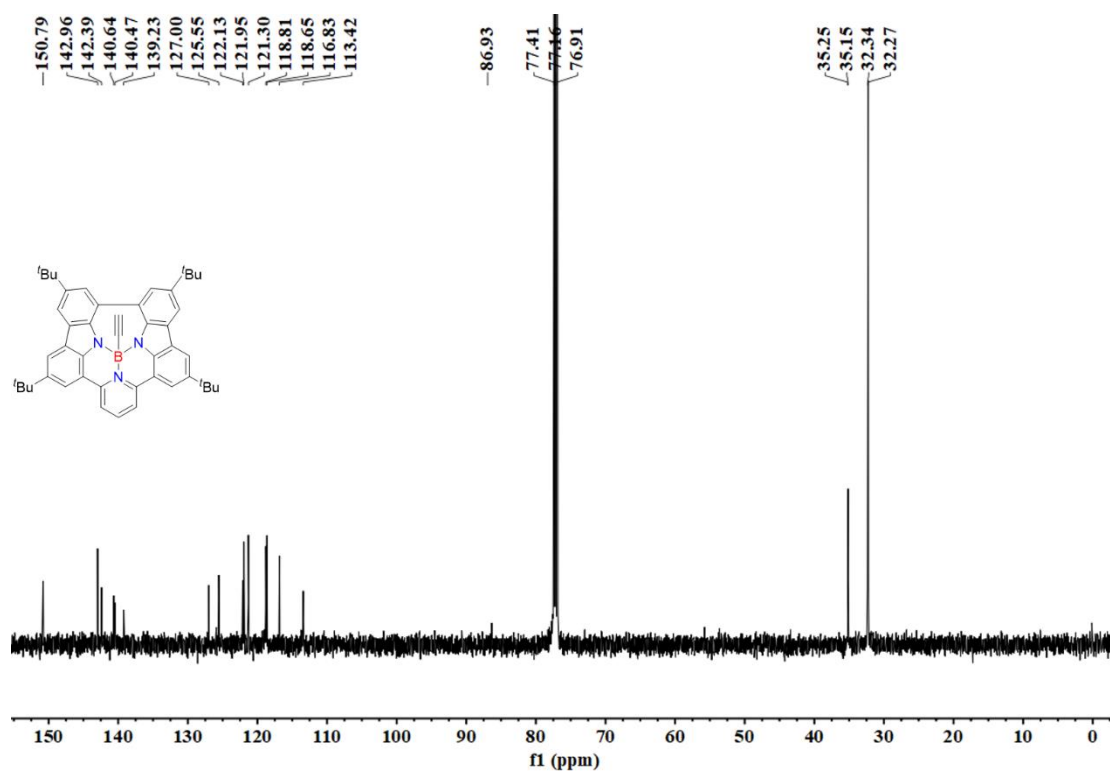


Figure S3.14 ^{13}C NMR spectrum of **NBNN-2f** (126 MHz, CDCl_3)

^1H and ^{13}C NMR spectra of **NBNN-4f** in CDCl_3 (the stability of **NBNN-4f** was not good, so we did not get clean NMR spectra)

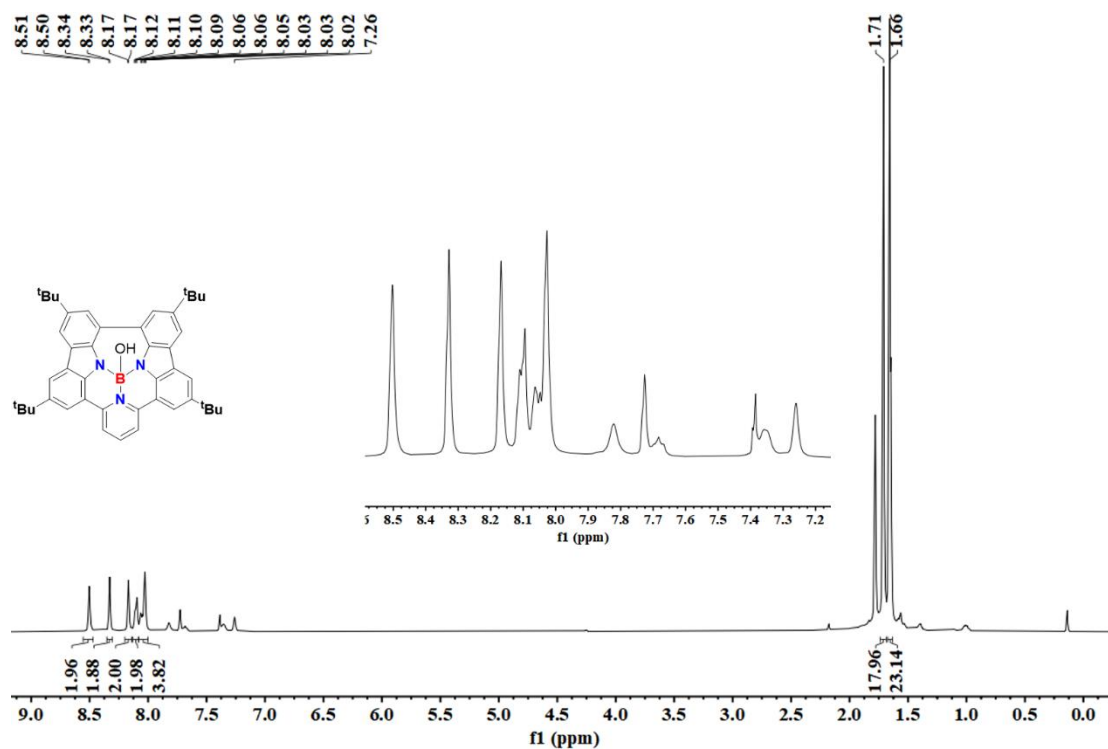


Figure S3.15 ^1H NMR spectrum of **NBNN-4f** (500 MHz, CDCl_3)

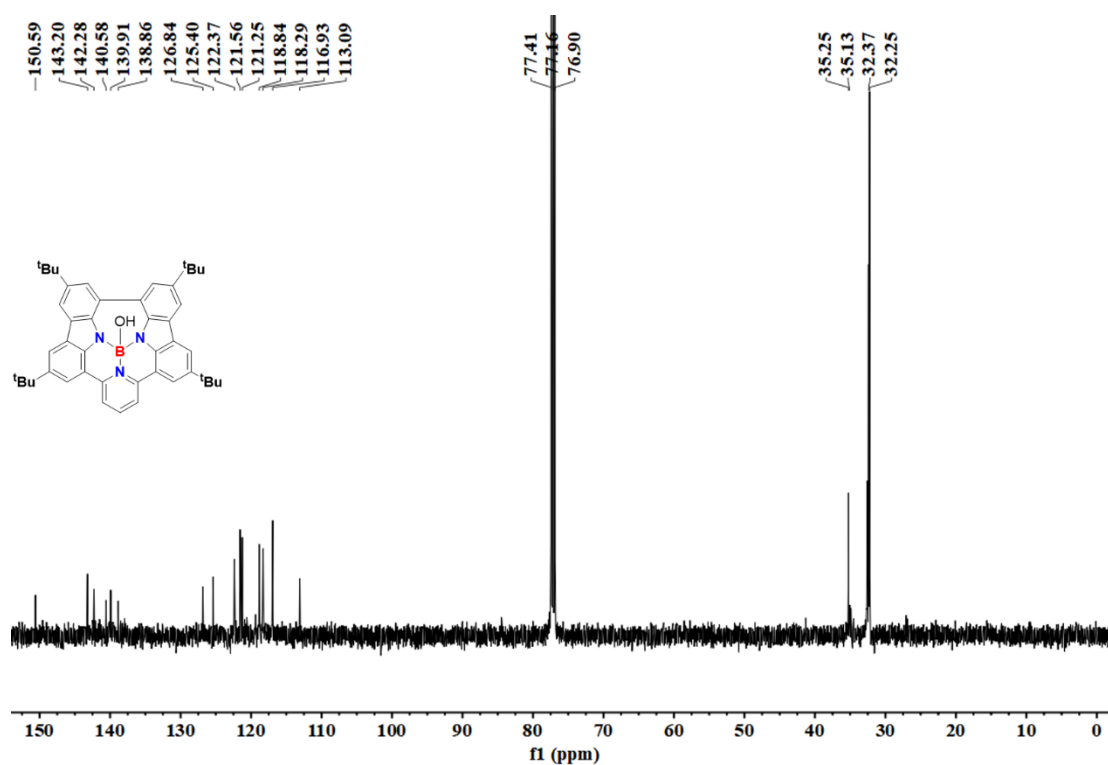


Figure S3.16 ^{13}C NMR spectrum of **NBNN-4f** (126 MHz, CDCl_3)

^1H and ^{13}C NMR spectra of **1a** in CDCl_3

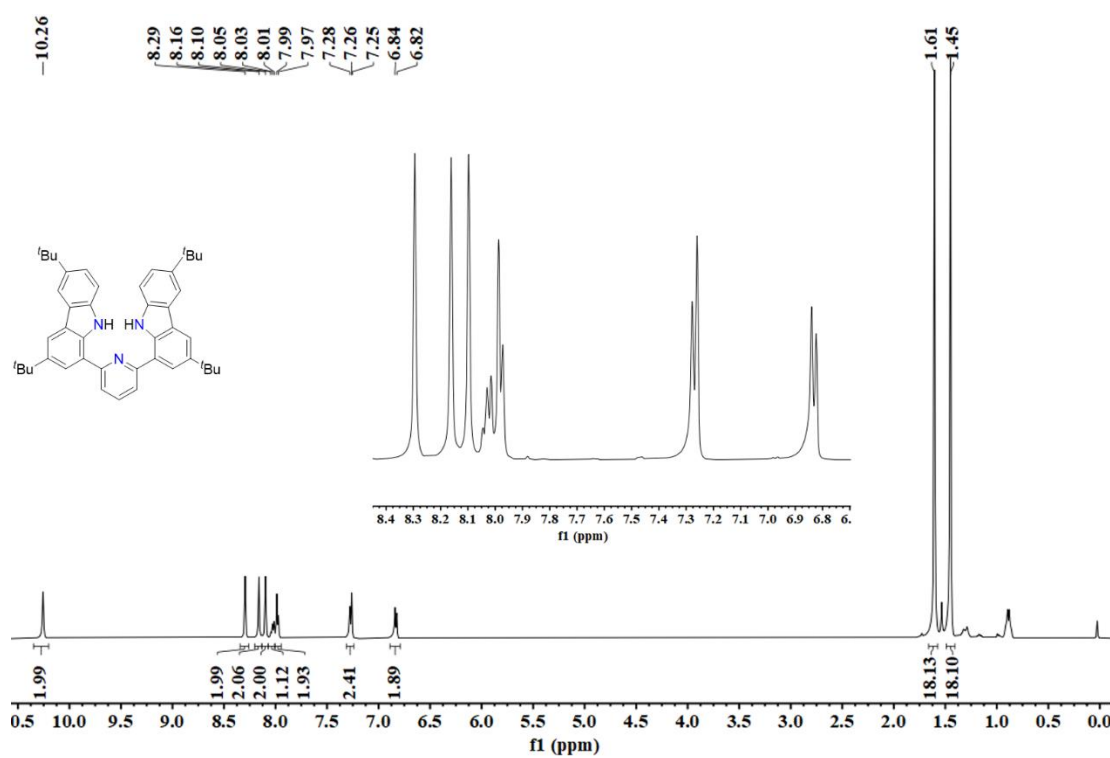


Figure S3.17 ^1H NMR spectrum of **1a** (500 MHz, CDCl_3)

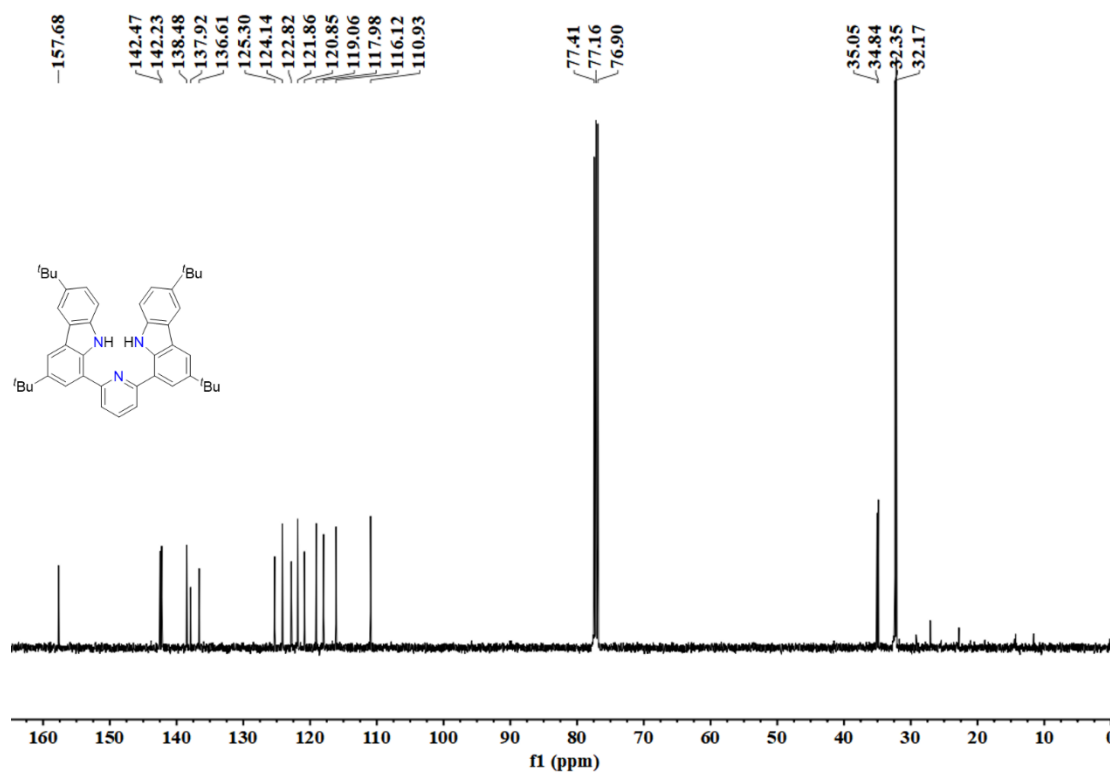


Figure S3.18 ^{13}C NMR spectrum of **1a** (126 MHz, CDCl_3)

^1H and ^{13}C NMR spectra of **1b** in CDCl_3

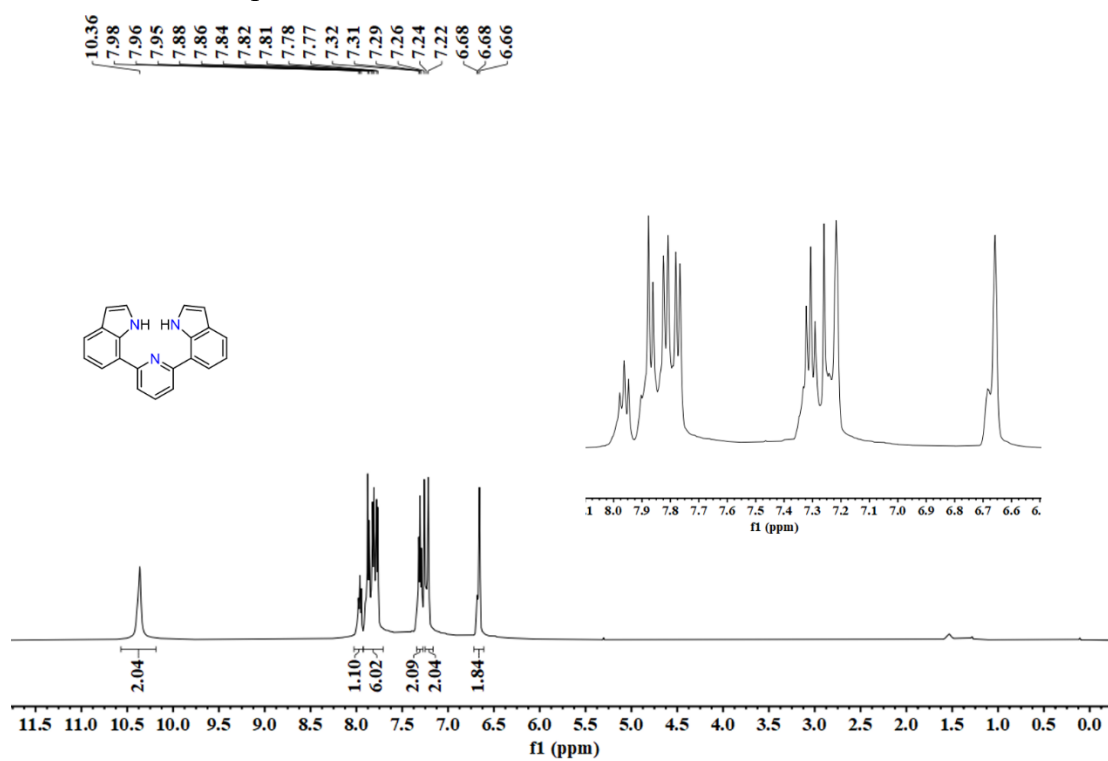


Figure S3.19 ^1H NMR spectrum of **1b** (500 MHz, CDCl_3)

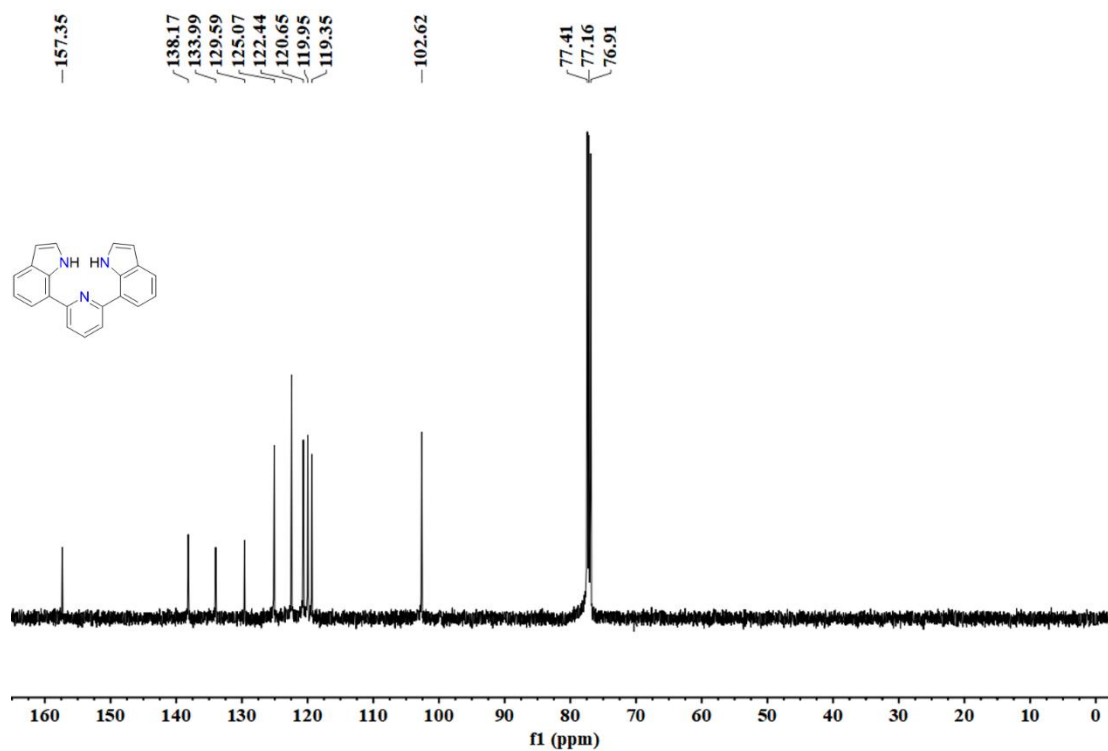


Figure S3.20 ^{13}C NMR spectrum of **1b** (126 MHz, CDCl_3)

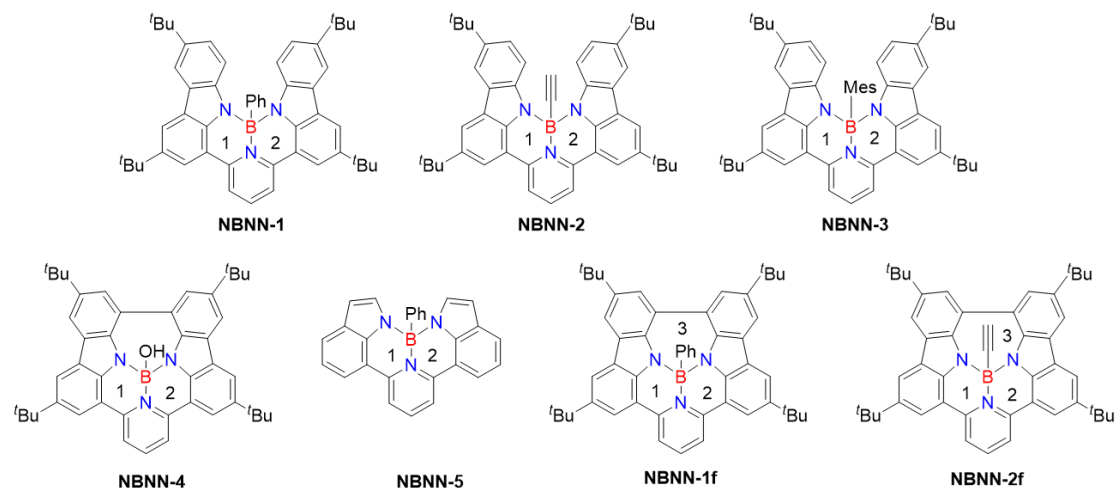
4. Computational Results

All calculations were performed using the Gaussian 16 suite of programs.³. Initial input coordinates were taken from the corresponding crystal structure data if applicable, while all others were generated in GausView 6.0. DFT and TD-DFT calculations were performed using the B3LYP/6-311g(d,p) level⁴ of theory based on optimized structures.

Table S4.1 HOMO and LUMO energy levels.

Compounds	LUMO/eV	HOMO/eV
NBNN-1	-2.24	-5.31
NBNN-2	-2.26	-5.33
NBNN-3	-2.23	-5.29
NBNN-4	-2.15	-5.27
NBNN-5	-2.36	-5.55
NBNN-1f	-2.33	-4.98
NBNN-2f	-2.34	-4.99

Table S4.2 NICS(1) values (in ppm) of NBNN-PAHs were calculated at B3LTP/6-311+g(d,p) level using optimized structures.



NBNN-1		NBNN-2		NBNN-3		NBNN-4		NBNN-5		NBNN-1f			NBNN-2f		
1	2	1	2	1	2	1	2	1	2	1	2	3	1	2	3
9.7	4.9	10.4	4.9	7.3	2.5	9.7	5.4	7.7	5.8	12.8	11.8	14.6	12.6	12.0	15.7

Table S4.3 TD-DFT calculated electronic transitions for **NBNN-1** along with their corresponding excitation energies and oscillator strengths (iso = 0.02).

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
NBNN-1	T1	HOMO → LUMO (88%) H-1 → L+1 (6%)	576 nm, 2.15 eV	0
	T2	H-1 → LUMO (58%) HOMO → L+1 (33%)	560 nm, 2.21 eV	0
	T3	H-1 → LUMO (37%) HOMO → L+1 (43%)	500 nm, 2.48 eV	0
	S1	HOMO → LUMO (98%)	497 nm, 2.49 eV	0.1508
	S2	H-1 → LUMO (98%)	478 nm, 2.60 eV	0.0437
	S3	H-1 → L+1 (97%)	432 nm, 2.87 eV	0.0168

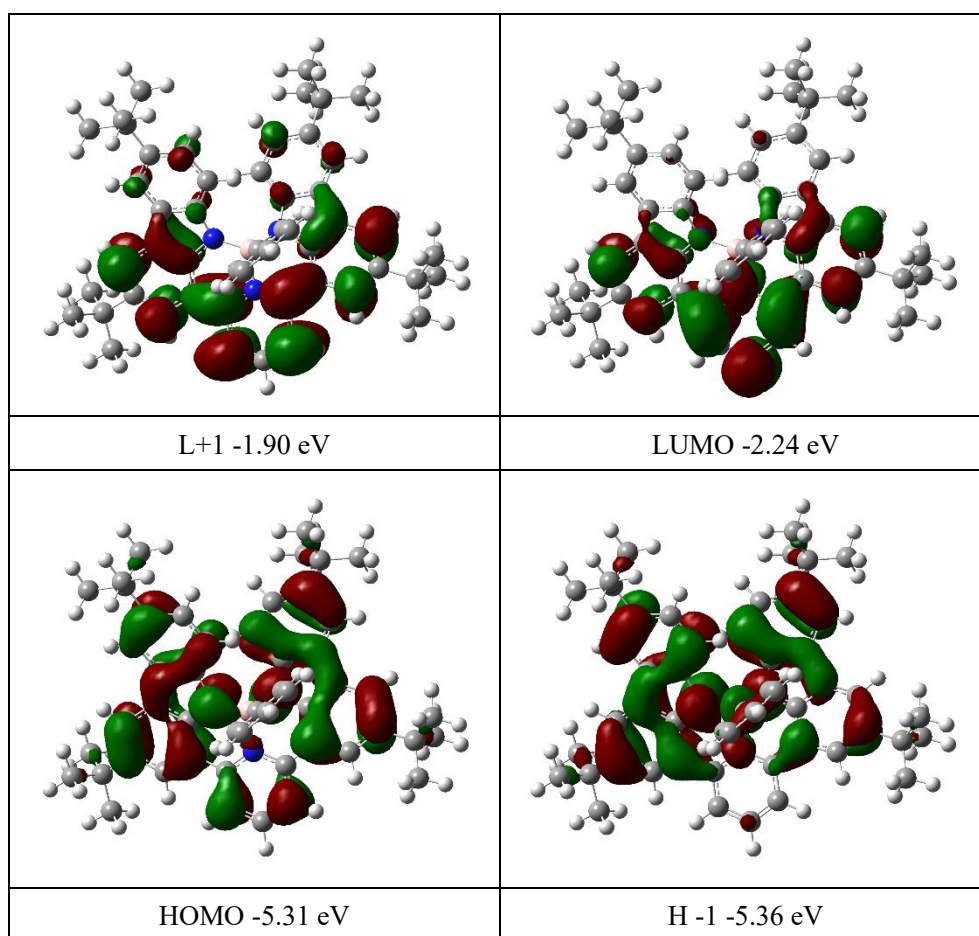


Table S4.4 TD-DFT calculated electronic transitions for **NBNN-2** along with their corresponding excitation energies and oscillator strengths (iso = 0.02).

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
NBNN-2	T1	HOMO $\rightarrow$ LUMO (88%) H-1 $\rightarrow$ L+1 (5%)	578 nm, 2.15 eV	0
	T2	H-1 $\rightarrow$ LUMO (53%) HOMO $\rightarrow$ L+1 (37%)	551 nm, 2.25 eV	0
	T3	H-1 $\rightarrow$ LUMO (40%) HOMO $\rightarrow$ L+1 (37%)	495 nm, 2.50 eV	0
	S1	HOMO $\rightarrow$ LUMO (98%)	500 nm, 2.49 eV	0.1530
	S2	H-1 $\rightarrow$ LUMO (97%)	468 nm, 2.65 eV	0.0473
	S3	H-1 $\rightarrow$ L+1 (75%) HOMO $\rightarrow$ L+1 (21%)	423 nm, 2.93 eV	0.0269

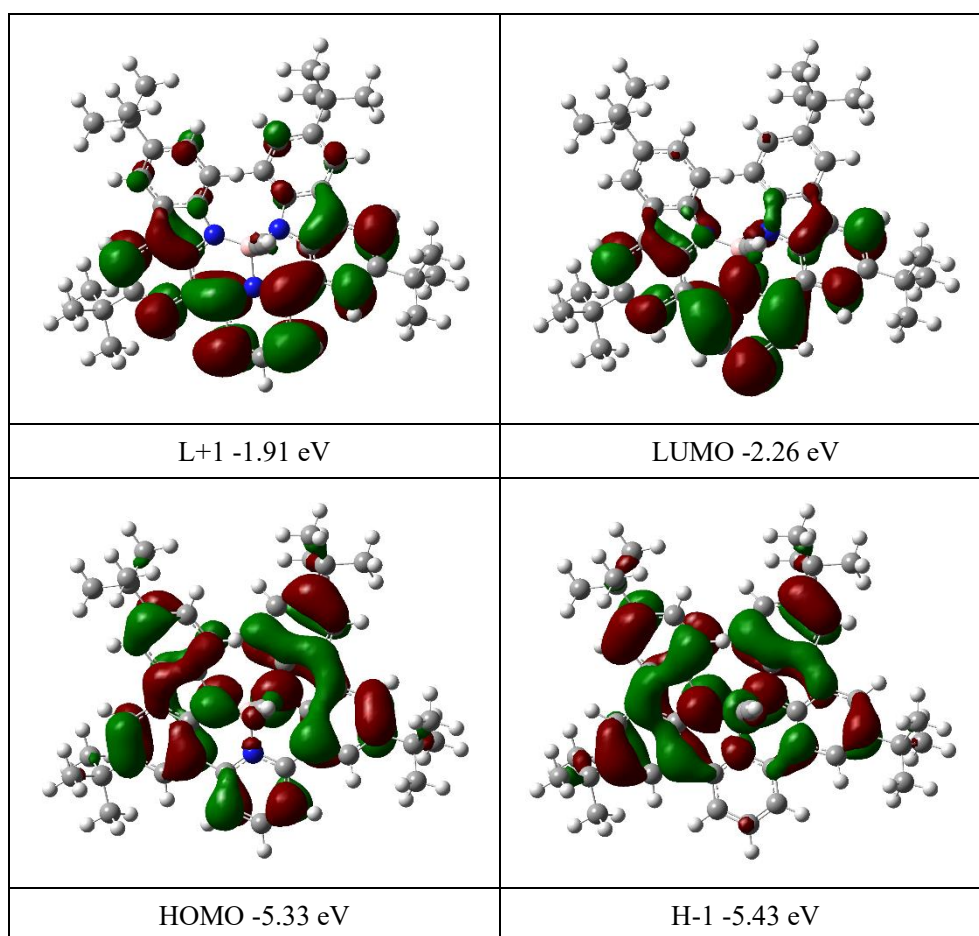
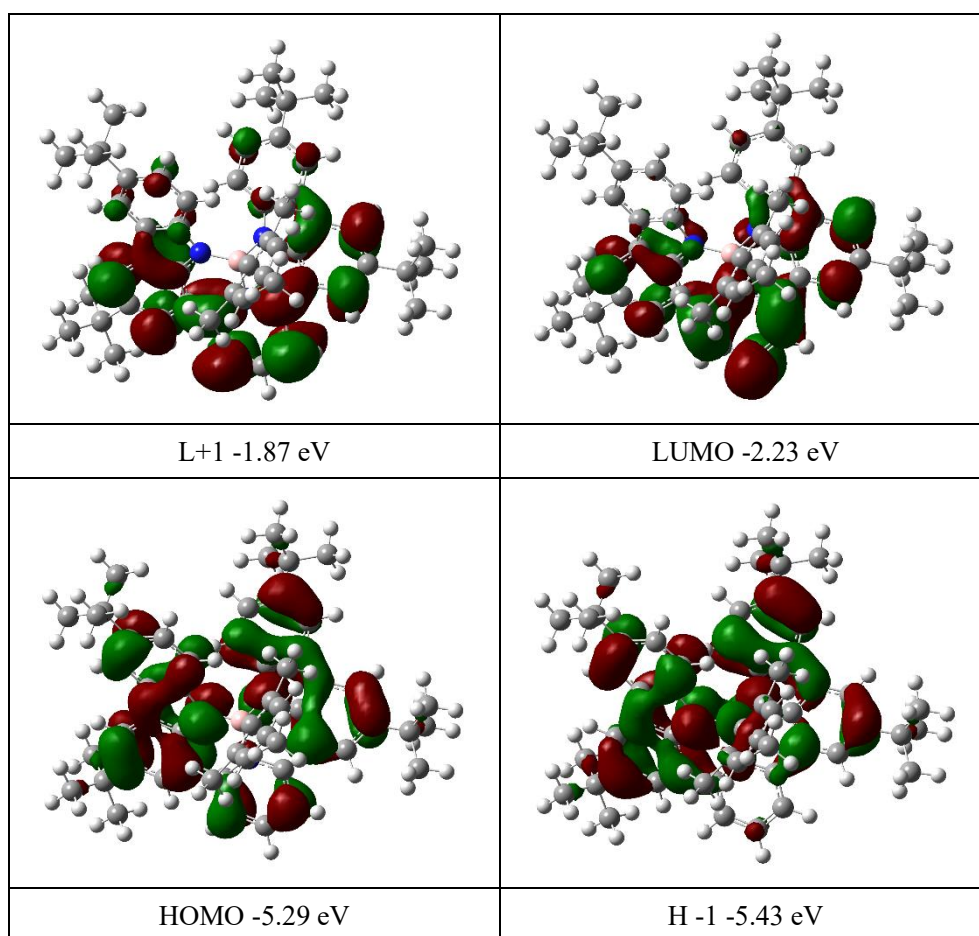


Table S4.5 TD-DFT calculated electronic transitions for **NBNN-3** along with their corresponding excitation energies and oscillator strengths (iso = 0.02).

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
NBNN-3	T1	HOMO → LUMO (89%) H-1 → L+1 (4%)	583 nm, 2.13 eV	0
	T2	H-1 → LUMO (46%) HOMO → L+1 (43%)	550 nm, 2.25 eV	0
	T3	H-1 → LUMO (47%), HOMO → L+1 (33%) H-2 → LUMO (5%)	496 nm, 2.50 eV	0
	S1	HOMO → LUMO (98%)	502nm, 2.47 eV	0.1419
	S2	H-1 → LUMO (97%)	465 nm, 2.67 eV	0.0416
	S3	HOMO → L+1 (86%) H-1 → L+1 (5%)	421 nm, 2.95 eV	0.0679



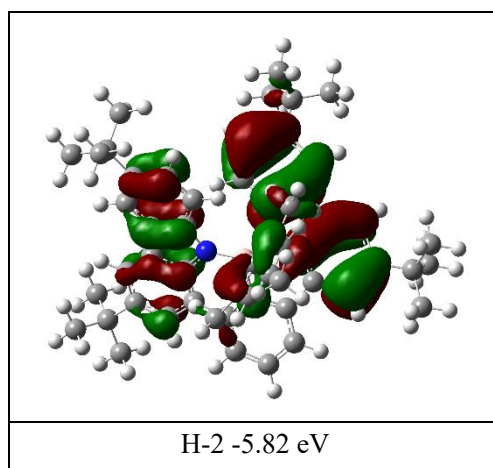
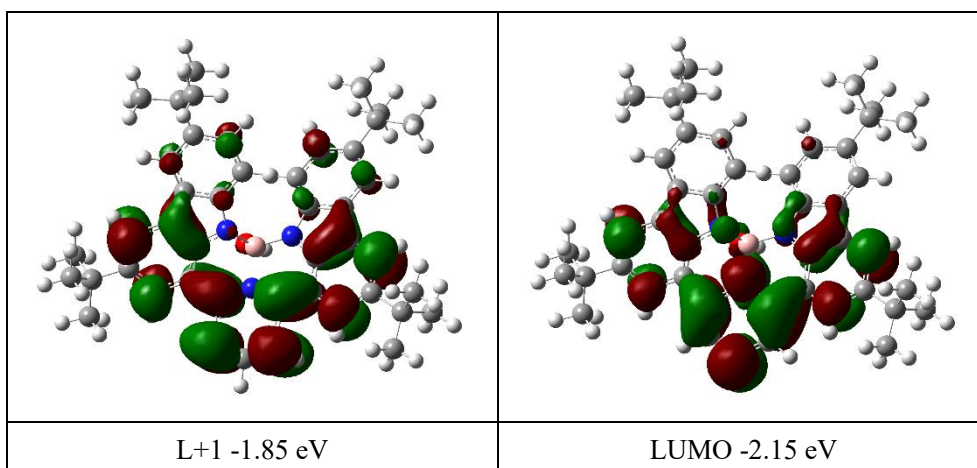


Table S4.6 TD-DFT calculated electronic transitions for **NBNN-4** along with their corresponding excitation energies and oscillator strengths (iso = 0.02).

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
NBNN-4	T1	HOMO → LUMO (87%)	563 nm, 2.20 eV	0
	T2	H-1 → LUMO (27%), HOMO → L+1(54%) H-4 → L+1 (4%), H-1 → L+1 (4%)	537 nm, 2.32 eV	0
	T3	H-2 → LUMO (16%), H-2 → L+1 (11%) H-1 → LUMO (48%), HOMO → L+1 (10%)	480 nm, 2.58 eV	0
	S1	HOMO → LUMO (97%)	484 nm, 2.56 eV	0.1680
	S2	H-1 → LUMO (84%), HOMO → L+1 (13%)	439 nm, 2.82 eV	0.0379
	S3	H-1 → LUMO (12%), HOMO → L+1 (77%) H-1 → L+1 (5%)	420 nm, 2.95 eV	0.0934



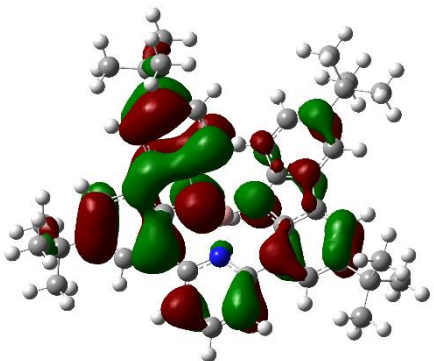
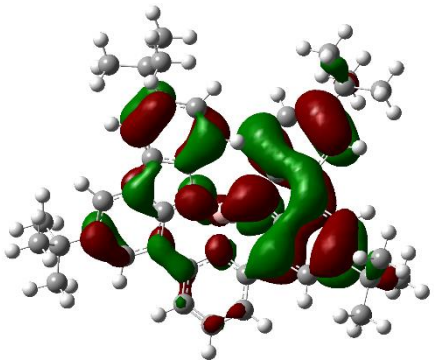
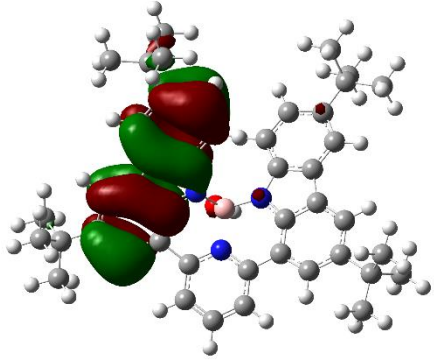
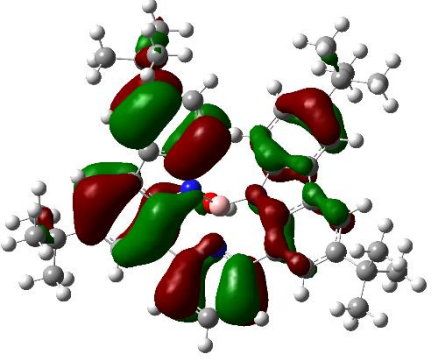
	
HOMO -5.27 eV	H-1 -5.49 eV
	
H-2 -5.75 eV	H-4 -6.48 eV

Table S4.7 TD-DFT calculated electronic transitions for **NBNN-5** along with their corresponding excitation energies and oscillator strengths (iso = 0.02).

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
NBNN-5	T1	HOMO → LUMO (86%) H-1 → L+1 (8%)	576 nm, 2.15 eV	0
	T2	H-1 → LUMO (45%) HOMO → L+1 (46%)	550 nm, 2.25 eV	0
	T3	H-1 → LUMO (47%), HOMO → L+1 (39%) H-3 → L+1 (5%)	463 nm, 2.68 eV	0
	S1	HOMO → LUMO (98%)	467 nm, 2.67 eV	0.1762
	S2	H-1 → LUMO (96%)	438 nm, 2.84 eV	0.0111
	S3	H-3 → LUMO (18%), H-2 → LUMO (44%) H-1 → L+1 (10%), HOMO → L+1 (26%)	396 nm, 3.13 eV	0.0213

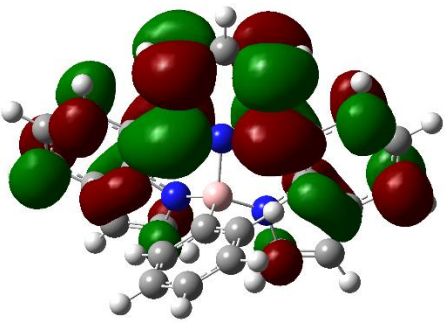
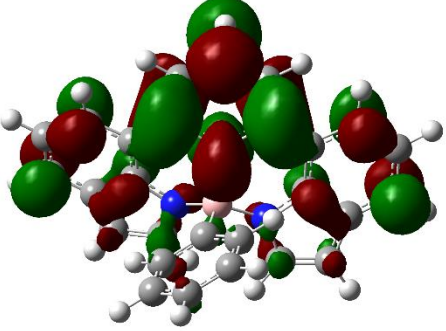
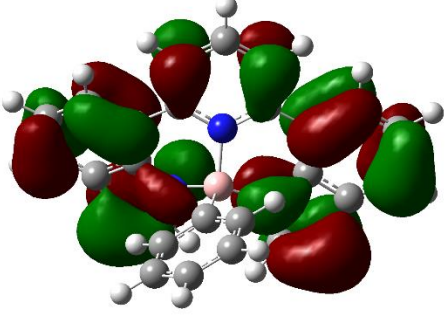
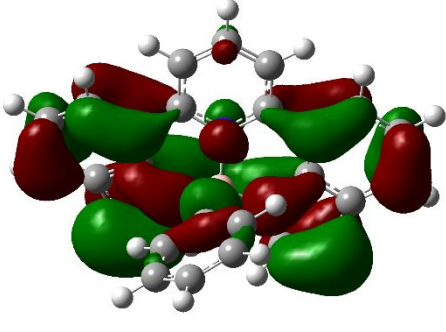
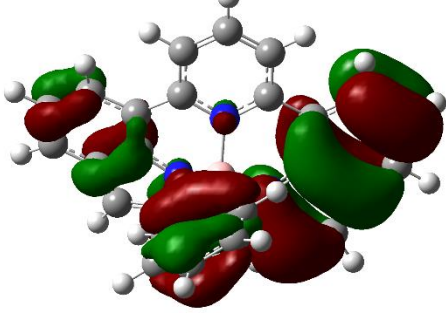
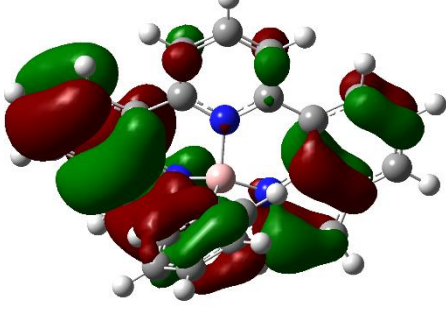
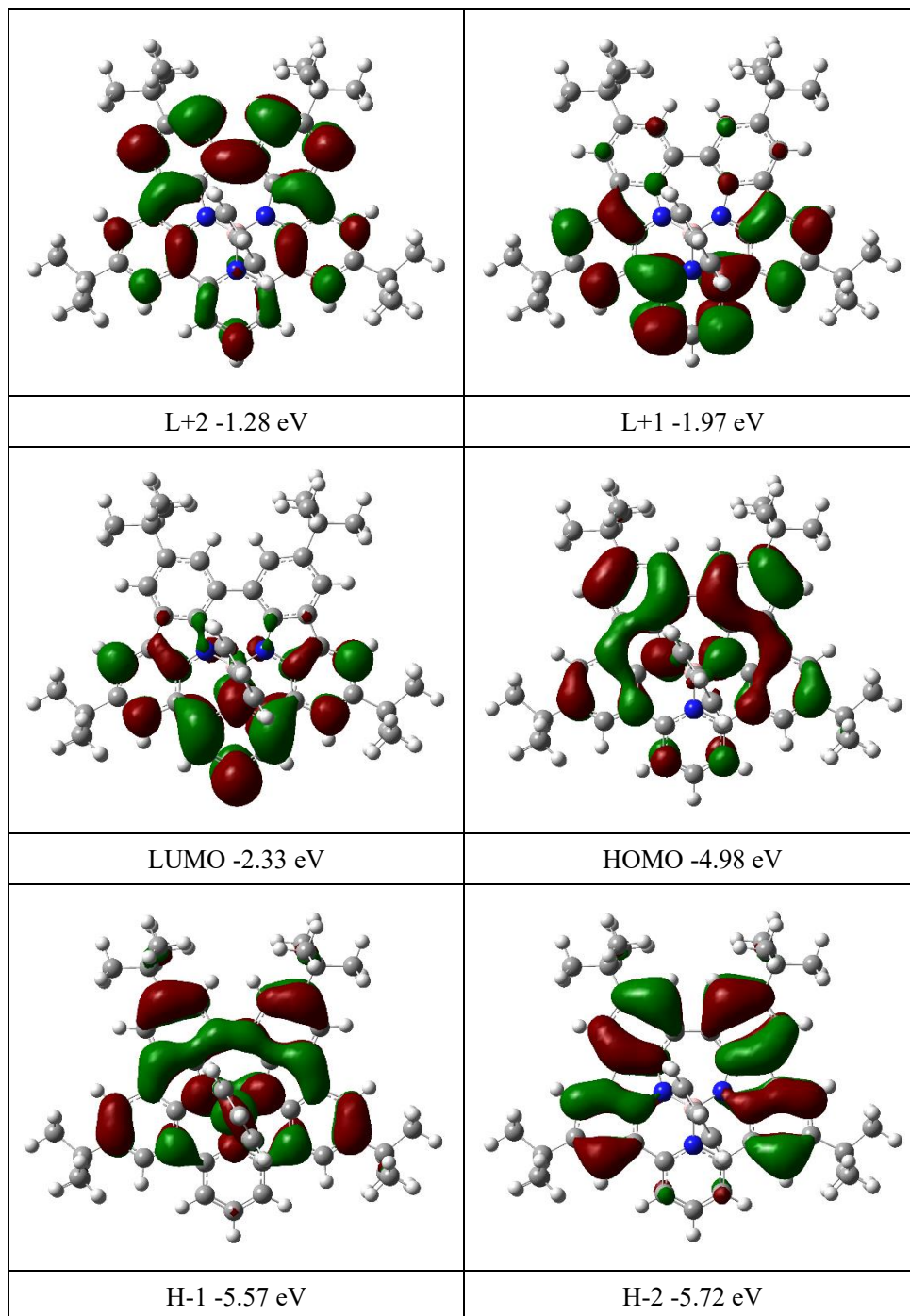
	
L+1 -1.93 eV	LUMO -2.36 eV
	
HOMO -5.55 eV	H-1 -5.76 eV
	
H-2 -6.12 eV	H-3 -6.15 eV

Table S4.8 TD-DFT calculated electronic transitions for **NBNN-1f** along with their corresponding excitation energies and oscillator strengths (iso = 0.020).

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
NBNN-1f	T1	HOMO → LUMO (94%)	654 nm, 1.89 eV	0
	T2	H-1 → LUMO (15%) HOMO → L+1 (74%)	584 nm, 2.12 eV	0
	T3	H-3 → L+1 (10%), H-2 → LUMO (31%) HOMO → L+2 (37%), H-2 → L+2 (9%)	516 nm, 2.40 eV	0

	S1	HOMO → LUMO (99%)	607 nm, 2.04 eV	0.0280
	S2	HOMO → L+1 (97%)	494 nm, 2.51 eV	0.0454
	S3	H-1 → LUMO (96%)	461 nm, 2.69 eV	0.0413



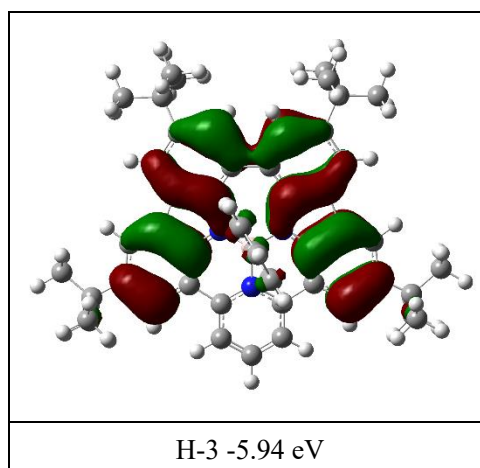
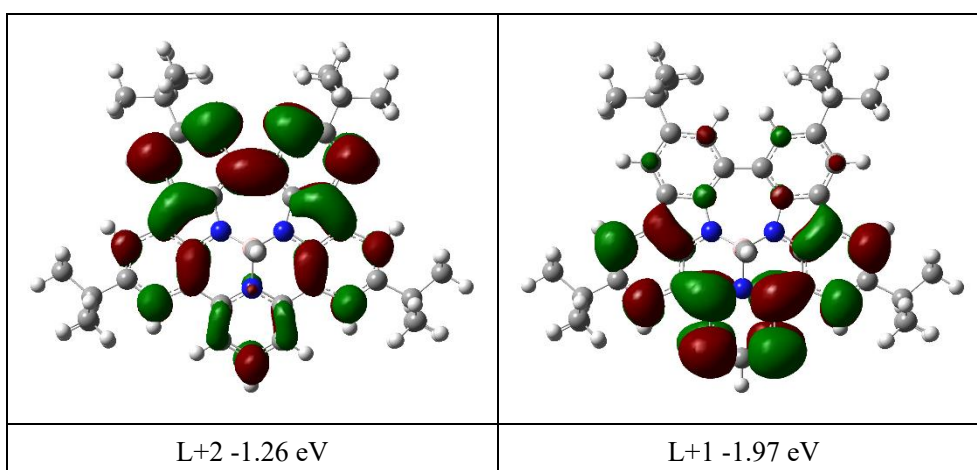
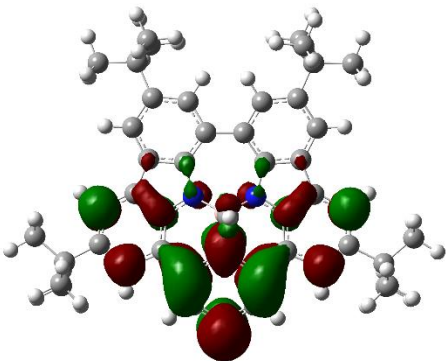
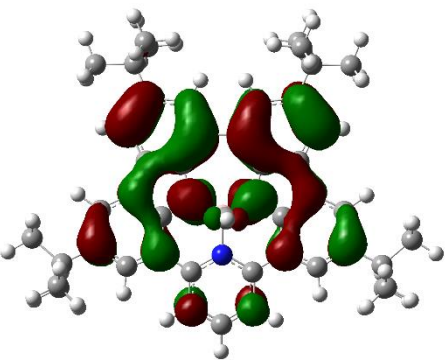
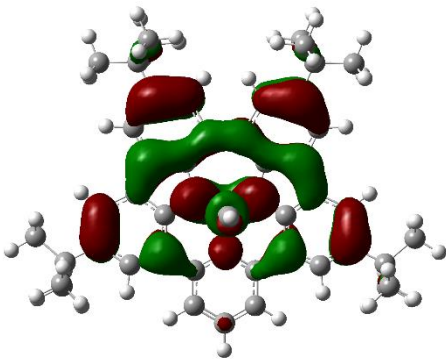
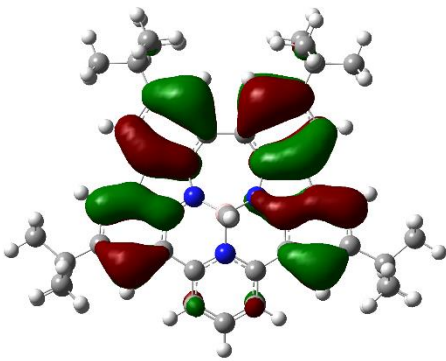
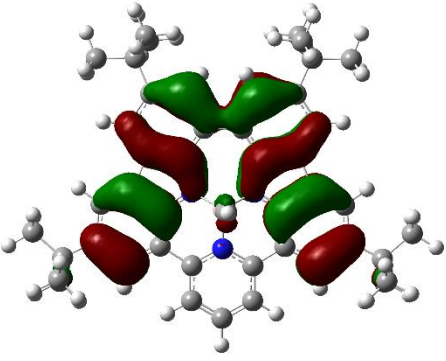
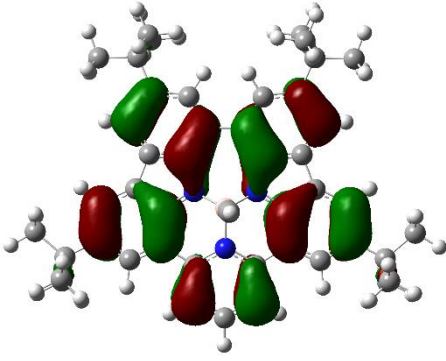


Table S4.9 TD-DFT calculated electronic transitions for **NBNN-2f** along with their corresponding excitation energies and oscillator strengths (iso = 0.02).

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
NBNN-2f	T1	HOMO → LUMO (94%)	652 nm, 1.90 eV	0
	T2	H-1 → LUMO (10%), HOMO → L+1 (78%) H-4 → L+1 (5%)	575 nm, 2.16 eV	0
	T3	H-3 → L+1 (10%), H-2 → LUMO (36%) HOMO → L+2 (33%), H-2 → L+2 (9%)	515 nm, 2.41 eV	0
	S1	HOMO → LUMO (99%)	605 nm, 2.05 eV	0.0292
	S2	HOMO → L+1 (98%)	488 nm, 2.54 eV	0.0482
	S3	H-1 → LUMO (96%)	440 nm, 2.81 eV	0.0497



	
LUMO -2.34 eV	HOMO -4.99 eV
	
H-1 -5.68 eV	H-2 -5.71 eV
	
H-3 -5.93 eV	H-4 -6.34 eV

DFT calculated UV/vis spectra

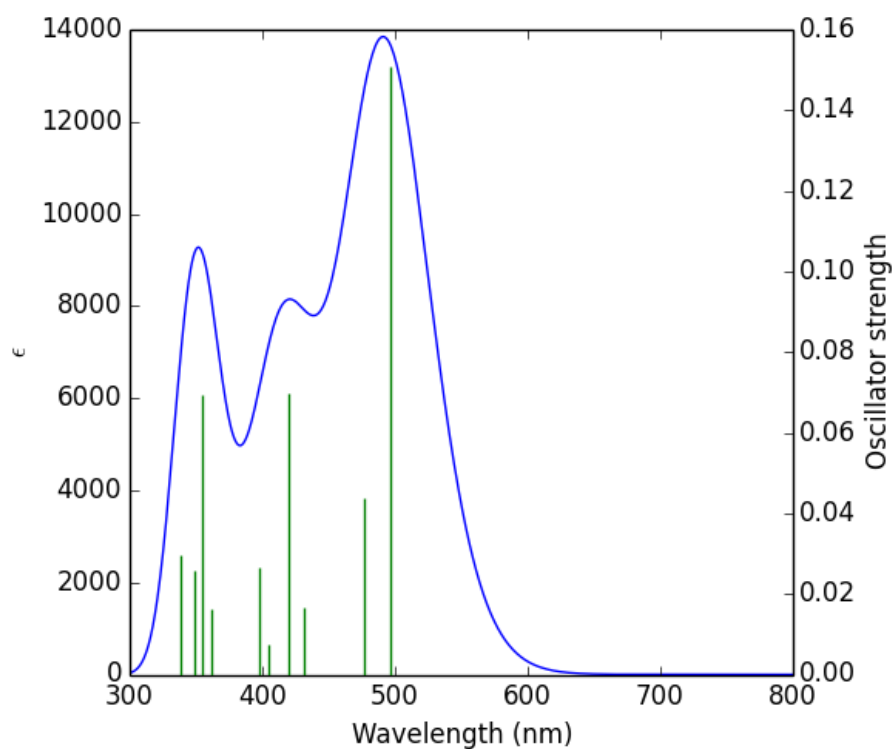


Figure S4.1 DFT calculated UV/vis spectra of NBNN-1

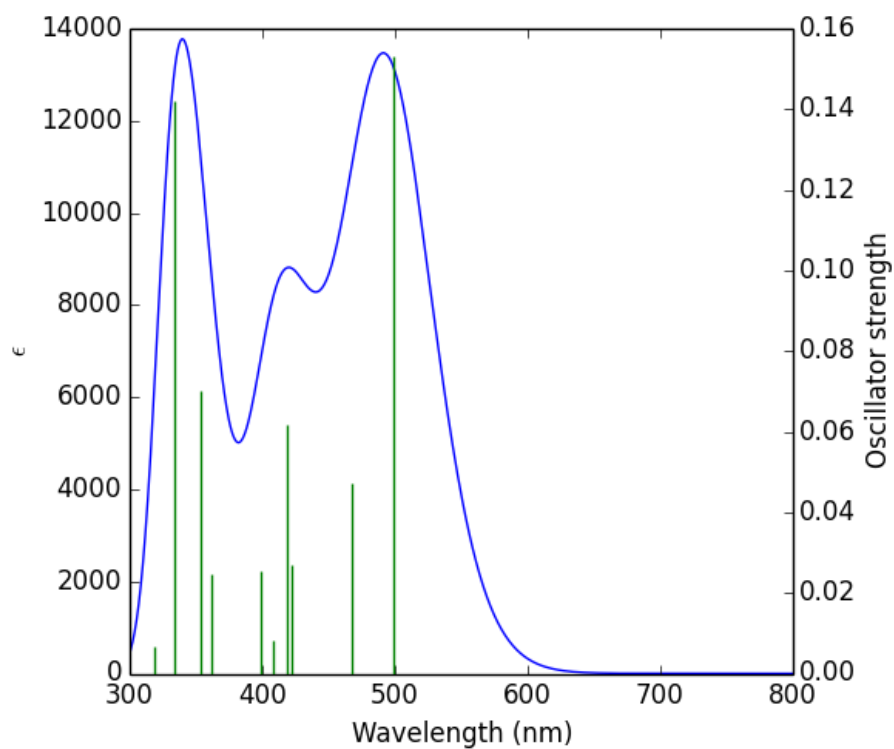


Figure S4.2 DFT calculated UV/vis spectra of NBNN-2

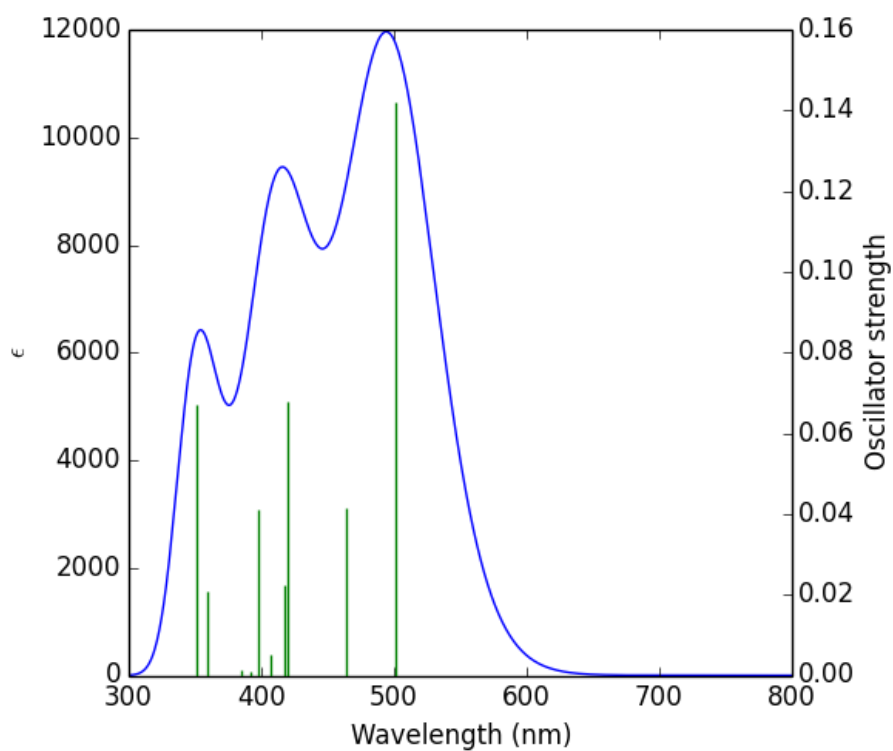


Figure S4.3 DFT calculated UV/vis spectra of NBNN-3

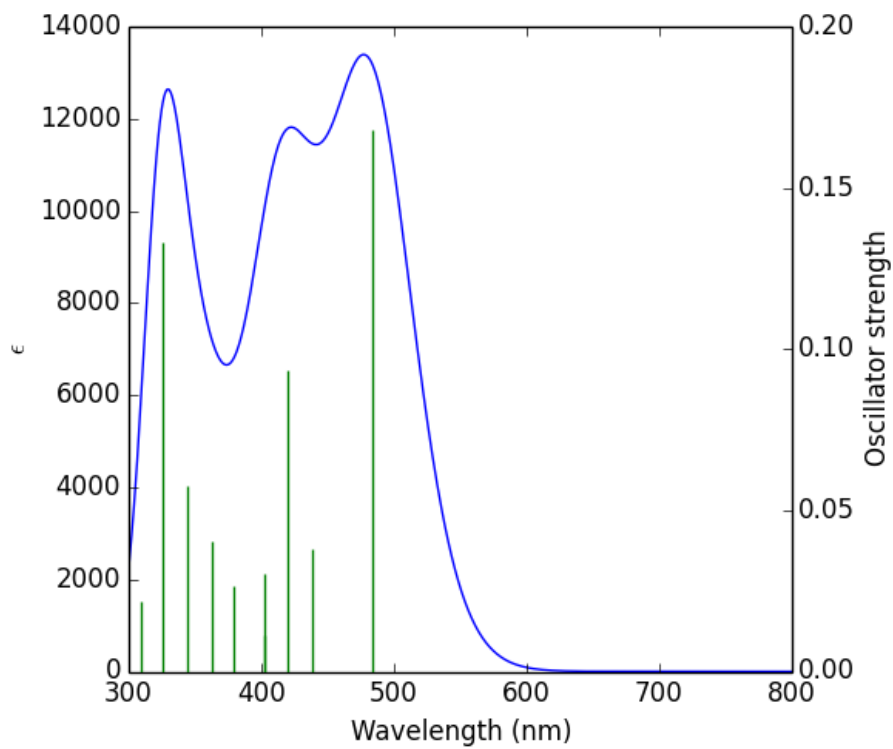


Figure S4.4 DFT calculated UV/vis spectra of NBNN-4

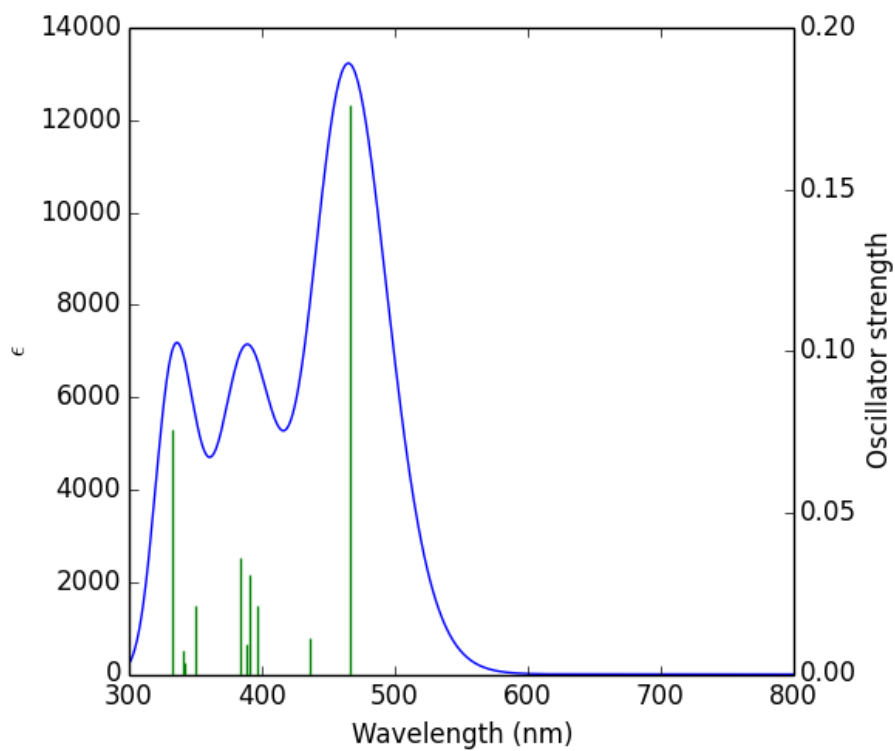


Figure S4.5 DFT calculated UV/vis spectra of **NBNN-5**

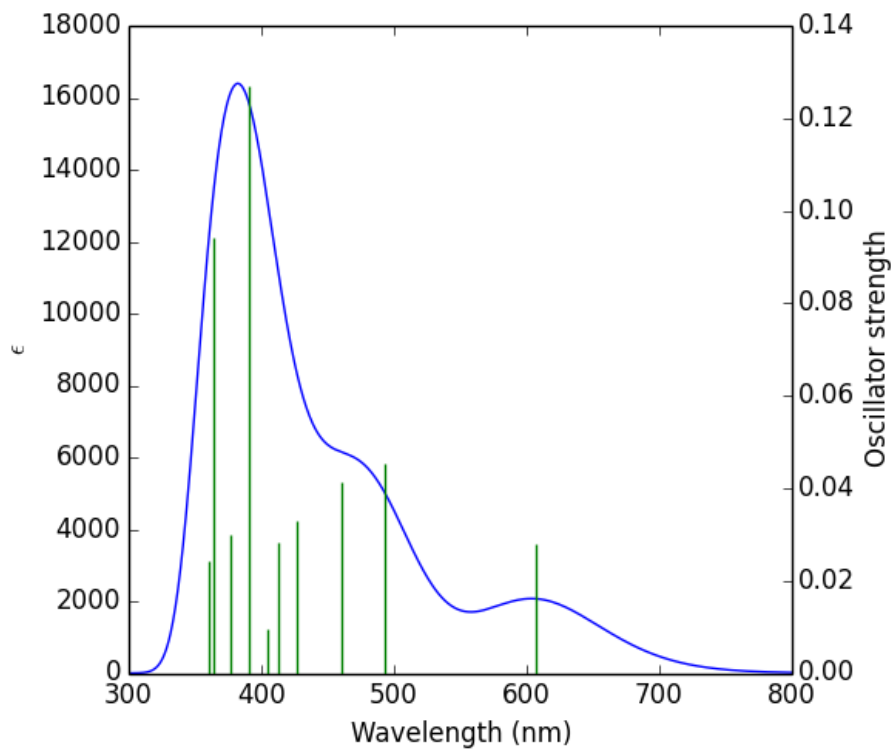


Figure S4.6 DFT calculated UV/vis spectra of **NBNN-1f**

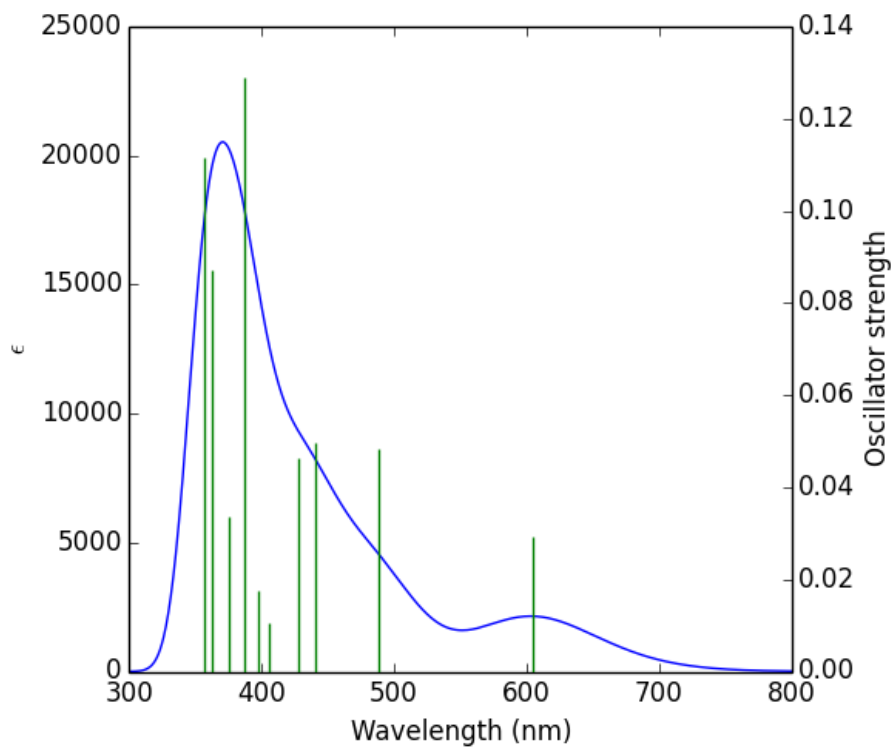


Figure S4.7 DFT calculated UV/vis spectra of **NBNN-2f**

Cartesian coordinates of DFT calculated structure

NBNN-1

Atom	X	Y	Z
N	1.23171800	-0.09406800	-0.28880400
N	-1.30201600	-0.39469100	0.28502000
N	0.29543100	-2.39561600	-0.01453400
C	0.45668200	-0.84459300	2.13567600
C	-4.10961500	5.35228300	0.98971400
H	-3.11179900	5.56695800	1.37883900
H	-4.75136800	6.20691700	1.22667400
H	-4.03393600	5.27461100	-0.09840900
C	2.69569000	-2.02087100	0.13249300
C	-1.98363800	0.75893600	0.69452800
C	1.45393500	1.21010000	-0.75869000
C	-0.75459300	-3.17038000	-0.44041600

C	2.84786900	1.43906400	-0.90724800
C	-3.32921700	0.70491200	0.25633500
C	2.46265500	-0.68319900	-0.19741100
C	-2.22440100	-1.20253900	-0.31884900
C	3.32233600	2.66713800	-1.37923500
H	4.39049100	2.81112100	-1.47966100
C	1.56184900	-2.93634600	0.06396200
C	4.04160100	-2.41459500	0.26492200
H	4.25609200	-3.43243100	0.55625400
C	2.43200400	3.68196900	-1.72425100
C	-0.58030300	-4.54927400	-0.59526900
H	-1.42591600	-5.16156500	-0.86820500
C	5.10752300	-1.54034000	0.02808500
C	-3.77474200	2.86703300	1.25413900
C	1.05132900	3.41674000	-1.58927800
H	0.33571400	4.18176200	-1.86777500
C	-4.20862800	1.75849500	0.53105700
H	-5.23072100	1.69218600	0.18105700
C	4.82301100	-0.22635600	-0.39912900
H	5.63572700	0.45442600	-0.62605700
C	-0.32654000	-1.64398000	2.98489400
H	-1.11174800	-2.26521300	2.56272100
C	-2.03846100	-2.52974400	-0.70599300
C	1.43928600	-0.04971600	2.74249700
H	2.06764800	0.58845400	2.13051400
C	3.51064300	0.20958300	-0.52078900
C	0.54957000	2.20972600	-1.12128900
H	-0.51736600	2.05733000	-1.05311200
C	-3.49201800	-0.57271700	-0.40250000

C	1.74239100	-4.31230600	-0.08831800
H	2.73793400	-4.72486900	-0.02279400
C	-1.53373800	1.85760800	1.43002300
H	-0.51762100	1.91317500	1.79532000
C	-3.13765100	-3.18085600	-1.29888800
H	-3.01059600	-4.19429700	-1.64834900
C	-4.38327200	-2.56635100	-1.46644300
C	6.57808600	-1.97092600	0.19910000
C	2.89247000	5.05318300	-2.25189700
C	-2.43152500	2.88138500	1.69517000
H	-2.07332900	3.72632600	2.27176500
C	0.66049900	-5.12394700	-0.38077700
H	0.79149000	-6.19502500	-0.48327000
C	-4.55185200	-1.25431000	-0.98576600
H	-5.51948900	-0.77079700	-1.05881300
C	-5.57220200	-3.28259700	-2.13737300
C	-4.69464000	4.05418000	1.59355100
C	1.63444500	-0.05055100	4.12377300
H	2.40186000	0.57998200	4.56073800
C	0.84952800	-0.86012500	4.94016500
H	1.00031700	-0.86561200	6.01433200
C	-0.13577200	-1.66036300	4.36396800
H	-0.75820400	-2.29114500	4.99020300
C	2.32016000	5.28314400	-3.67014100
H	2.67067500	4.51089600	-4.36031500
H	2.63797200	6.25665900	-4.05710000
H	1.22806600	5.26321400	-3.67509400
C	2.38356500	6.16833600	-1.30889700
H	1.29352400	6.17385600	-1.23887600

H	2.69996800	7.15091100	-1.67345300
H	2.78171700	6.03503800	-0.29926200
C	4.42598500	5.16269600	-2.33408500
H	4.89519700	5.03676800	-1.35439800
H	4.70427100	6.15164600	-2.70847600
H	4.85037300	4.42075900	-3.01612200
C	-6.74940000	-3.38267000	-1.13928400
H	-6.46010900	-3.95188500	-0.25167800
H	-7.60226200	-3.88654600	-1.60477900
H	-7.08699400	-2.39815500	-0.80779600
C	-6.02209800	-2.47880300	-3.37968000
H	-6.33157200	-1.46492600	-3.11590200
H	-6.87035700	-2.97029100	-3.86648500
H	-5.20994000	-2.40012800	-4.10744200
C	-5.21897200	-4.70886700	-2.59768400
H	-4.40827100	-4.71124200	-3.33165600
H	-6.09138800	-5.16720500	-3.07084200
H	-4.92832600	-5.34775500	-1.75885700
C	6.71515800	-3.43361800	0.66008900
H	6.22979500	-3.60395400	1.62501100
H	7.77325200	-3.68287100	0.77579300
H	6.29239900	-4.13184500	-0.06796900
C	7.32429800	-1.82431400	-1.14752900
H	6.86798800	-2.45406600	-1.91617600
H	8.37106600	-2.12456200	-1.03774600
H	7.31162100	-0.79417900	-1.51057100
C	-6.11750200	3.86924800	1.03529700
H	-6.73073300	4.73560800	1.29792300
H	-6.60471500	2.98274900	1.45057000

H	-6.11832600	3.78282800	-0.05482100
C	7.25540400	-1.07232600	1.26030200
H	7.23573200	-0.01886000	0.97188600
H	8.30252600	-1.36174900	1.39380400
H	6.75042600	-1.16291600	2.22573800
C	-4.79960300	4.20715100	3.12893900
H	-3.82438100	4.38748300	3.58660900
H	-5.21784500	3.30401800	3.58157000
H	-5.44957500	5.05000900	3.38498200
B	0.14031700	-0.83258900	0.53775400

NBNN-2

Atom	X	Y	Z
N	1.28038800	-0.20162600	-0.05566200
N	-1.26309400	-0.41886200	0.51468200
N	0.29211300	-2.46490100	0.31570700
C	-3.94835600	5.40351800	1.00880400
H	-2.93912800	5.61633100	1.36837900
H	-4.56939100	6.28024700	1.21868400
H	-3.89596400	5.27512700	-0.07587300
C	2.69571800	-2.12418700	0.51254400
C	-1.91479700	0.76472200	0.88261000
C	1.54287200	1.09139900	-0.53669500
C	-0.77333600	-3.23691100	-0.07716300
C	2.94447400	1.30355400	-0.61089100
C	-3.26896000	0.71386400	0.47321600
C	2.49937600	-0.79682500	0.12659200
C	-2.21022800	-1.24127300	-0.02720600
C	3.45695600	2.51412200	-1.08714000

H	4.53037700	2.64655000	-1.13075400
C	1.54831300	-3.02226400	0.43493100
C	4.02743200	-2.53190400	0.72330800
H	4.21217200	-3.54261000	1.05707300
C	2.59730600	3.52796700	-1.50633200
C	-0.61644200	-4.62146900	-0.19028700
H	-1.46928000	-5.23076600	-0.44651500
C	5.11508300	-1.67729900	0.51618300
C	-3.65390900	2.92683700	1.38030600
C	1.20879900	3.27876000	-1.44317800
H	0.51782500	4.04294000	-1.78006700
C	-4.12301800	1.79563400	0.71618500
H	-5.15315100	1.73368800	0.38990100
C	4.87028700	-0.37050600	0.04373300
H	5.70253500	0.29543000	-0.15428300
C	-2.05122800	-2.58806100	-0.35228600
C	3.57197700	0.07735600	-0.15760800
C	0.66993900	2.08763500	-0.97497100
H	-0.40070800	1.94448200	-0.96354400
C	-3.46699200	-0.59207000	-0.11925200
C	1.70797100	-4.40439200	0.32404800
H	2.69624300	-4.82996900	0.41294900
C	-1.42887900	1.88356900	1.56115000
H	-0.40463100	1.93126300	1.90500900
C	-3.17272400	-3.24765700	-0.89234500
H	-3.07126000	-4.27978200	-1.19156800
C	-4.41056100	-2.61998700	-1.06689500
C	6.56950000	-2.12101200	0.77154200
C	3.10078600	4.88181700	-2.03964500

C	-2.30258100	2.93529200	1.79635300
H	-1.91862000	3.79825900	2.32793500
C	0.61589300	-5.20674700	0.04378000
H	0.73171400	-6.28193500	-0.02988500
C	-4.54845100	-1.28266000	-0.64937400
H	-5.50928700	-0.78689300	-0.72906400
C	-5.62443900	-3.34782800	-1.67799800
C	-4.54497200	4.14572200	1.68252300
C	2.61157200	5.08263900	-3.49292300
H	2.99289400	4.29123900	-4.14396500
H	2.96007800	6.04394000	-3.88400300
H	1.52134200	5.07173100	-3.55913200
C	2.55117500	6.02382900	-1.15332100
H	1.45902900	6.04113900	-1.14559400
H	2.89816200	6.99447300	-1.52202300
H	2.89001800	5.91076600	-0.11986800
C	4.63755500	4.97580500	-2.03758500
H	5.04955700	4.86960200	-1.03024700
H	4.94644400	5.95288200	-2.41909200
H	5.09217700	4.21382500	-2.67669600
C	-6.78269700	-3.37744000	-0.65354200
H	-6.48492800	-3.90646600	0.25582000
H	-7.65285200	-3.88907300	-1.07663600
H	-7.09741400	-2.37189800	-0.36551400
C	-6.08581400	-2.59911900	-2.95018200
H	-6.37361700	-1.56818300	-2.73186500
H	-6.95141800	-3.09959200	-3.39548800
H	-5.28716100	-2.57079100	-3.69637500
C	-5.30434000	-4.80124300	-2.07301300

H	-4.50879100	-4.85449500	-2.82152700
H	-6.19368400	-5.26692800	-2.50572000
H	-5.00771100	-5.40271700	-1.20900900
C	6.66377800	-3.57200600	1.27807800
H	6.13043500	-3.70928600	2.22276500
H	7.71148000	-3.83151300	1.45149900
H	6.26644800	-4.28478300	0.54980600
C	7.38232900	-2.02113400	-0.54034500
H	6.95582100	-2.66675300	-1.31294300
H	8.41852700	-2.33039000	-0.37123000
H	7.40066200	-1.00151000	-0.93166500
C	-5.98193000	3.96318600	1.16073700
H	-6.57350300	4.85250100	1.39472100
H	-6.47723600	3.10637000	1.62575600
H	-6.00620000	3.82697400	0.07598900
C	7.20697900	-1.20206400	1.83991800
H	7.21619400	-0.15677300	1.52287900
H	8.24219000	-1.50113600	2.03218400
H	6.65455100	-1.25925400	2.78161900
C	-4.61651300	4.37017600	3.21102900
H	-3.62928100	4.55292600	3.64117700
H	-5.04173300	3.49649000	3.71236900
H	-5.24607700	5.23580000	3.44069400
B	0.16092900	-0.88327400	0.77807700
C	0.48411800	-0.82283400	2.32984400
C	0.68862900	-0.76501000	3.51856100
H	0.86976700	-0.70841900	4.56466200

NBNN-3

Atom	X	Y	Z
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N	1.15958600	0.09878400	-0.31248700
N	-1.28990000	-0.49593600	0.30748000
N	0.49611700	-2.26254100	-0.26129600
C	0.57788800	-0.97431100	2.11796600
C	-4.61556200	4.82501600	1.74173900
H	-3.67218900	5.03358600	2.25131500
H	-5.34252100	5.57749000	2.06373100
H	-4.44932400	4.94968200	0.66815300
C	2.84310500	-1.67450000	-0.11166600
C	-2.09557900	0.51313400	0.85214400
C	1.18140600	1.40442200	-0.82379900
C	-0.45188800	-3.02518800	-0.89303700
C	2.51623700	1.77473700	-1.13949400
C	-3.39281000	0.45312600	0.28547400
C	2.44310700	-0.35930800	-0.36906900
C	-2.08873900	-1.22608700	-0.53119400
C	2.79863300	3.04028100	-1.66191400
H	3.82565400	3.29405500	-1.89116800
C	1.80591000	-2.69255300	-0.23033600
C	4.22971800	-1.92615400	-0.11881100
H	4.57515900	-2.92277200	0.11589400
C	1.77203900	3.95561800	-1.88860000
C	-0.15310900	-4.34196200	-1.25496800
H	-0.92478100	-4.96069700	-1.68680200
C	5.16744800	-0.94185200	-0.44726900
C	-4.09639500	2.36167100	1.60181800
C	0.45507400	3.55549200	-1.57372700
H	-0.36322900	4.24462200	-1.74817100
C	-4.37646000	1.37620700	0.65836400

H	-5.35757500	1.30622500	0.20653800
C	4.70356000	0.33217700	-0.84313300
H	5.41248400	1.08696000	-1.16424400
C	0.03683500	-2.06844100	2.85505700
C	-1.76259100	-2.43638500	-1.14450000
C	1.37891800	-0.06162600	2.86006400
C	3.34845900	0.63119300	-0.81807700
C	0.14205400	2.30818300	-1.04886000
H	-0.88504800	2.05519500	-0.82942400
C	-3.39439100	-0.68141000	-0.61182400
C	2.10832800	-4.01840300	-0.55011900
H	3.13327300	-4.35474300	-0.49601900
C	-1.80100700	1.48882800	1.80702100
H	-0.83097500	1.53986000	2.27910500
C	-2.75333200	-3.03415100	-1.94632300
H	-2.51159700	-3.94833900	-2.46746800
C	-4.03033200	-2.48558200	-2.10880300
C	6.68505300	-1.21350400	-0.42934500
C	2.01937500	5.36095000	-2.46714000
C	-2.79874700	2.38537000	2.16158000
H	-2.55863400	3.13298600	2.90869800
C	1.11365700	-4.85519400	-1.02615100
H	1.33776300	-5.88668800	-1.27256600
C	-4.34522500	-1.30697900	-1.40795700
H	-5.34126700	-0.88462100	-1.47814400
C	-5.09907100	-3.13692400	-3.00881800
C	-5.13586800	3.40283000	2.05556700
C	1.66604400	-0.29479500	4.21153500
H	2.28007500	0.42902300	4.74008200

C	1.18874700	-1.39993000	4.90261300
C	0.35534300	-2.26351100	4.20135300
H	-0.07979700	-3.11348600	4.72004000
C	1.24801900	5.51723100	-3.79845000
H	1.58320400	4.77767500	-4.53077100
H	1.41199300	6.51403600	-4.22032300
H	0.17227500	5.38623200	-3.66158000
C	1.52652200	6.42891100	-1.46297100
H	0.45964100	6.32604900	-1.25252700
H	1.69271700	7.43448700	-1.86251900
H	2.06275900	6.34634600	-0.51364000
C	3.51035000	5.62353900	-2.74732100
H	4.11254800	5.55762200	-1.83692600
H	3.63606100	6.63091800	-3.15353200
H	3.91634700	4.91995600	-3.47936900
C	-6.33801200	-3.50671400	-2.16020700
H	-6.07216500	-4.21567900	-1.37138900
H	-7.10667200	-3.96763800	-2.78840000
H	-6.78178000	-2.62973100	-1.68365200
C	-5.51593200	-2.14031500	-4.11552900
H	-5.92900000	-1.21964700	-3.69708200
H	-6.27916700	-2.58450000	-4.76224400
H	-4.65866900	-1.86800900	-4.73711600
C	-4.59280900	-4.42045100	-3.69229100
H	-3.73005400	-4.22653800	-4.33566800
H	-5.38427500	-4.83661000	-4.32114300
H	-4.31580600	-5.18799600	-2.96400300
C	7.02220500	-2.64724000	0.01957500
H	6.65123700	-2.85631000	1.02667700

H	8.10717000	-2.78039900	0.03390900
H	6.61031500	-3.39608700	-0.66295400
C	7.26986400	-1.00774100	-1.84610800
H	6.80557300	-1.69141100	-2.56211300
H	8.34796800	-1.19636700	-1.84430000
H	7.11276100	0.01070600	-2.20835400
C	-6.49012000	3.22419500	1.34529200
H	-7.19256800	3.98478100	1.69691800
H	-6.93218400	2.24596400	1.55354300
H	-6.39835800	3.33599200	0.26136100
C	7.36883600	-0.23464000	0.55389000
H	7.20729600	0.80706700	0.26735900
H	8.44896600	-0.41007000	0.57795900
H	6.97929900	-0.36581000	1.56697900
C	-5.37337300	3.27001800	3.57799400
H	-4.45563400	3.43152400	4.14780400
H	-5.74896500	2.27385400	3.82711000
H	-6.10957300	4.00672800	3.91512500
B	0.19456300	-0.81085400	0.51410200
C	-0.92513800	-3.09027200	2.27627000
H	-1.69130700	-2.64070500	1.64686900
H	-0.41086200	-3.85384100	1.68612400
H	-1.43954500	-3.61103200	3.08637400
C	1.96253400	1.22833800	2.31354300
H	2.86000900	1.05351100	1.71644400
H	1.26868900	1.79048700	1.69073100
H	2.25335800	1.87727600	3.14235800
C	1.54945300	-1.64915400	6.34645700
H	0.72452200	-2.11832100	6.88896000

H	2.41373600	-2.31824900	6.42670100
H	1.80783900	-0.71959600	6.85932100
NBNN-4			
Atom	X	Y	Z
N	-1.29132100	-0.19630300	-0.01677800
N	1.26243700	-0.42745100	-0.59324200
N	-0.30762800	-2.46549000	-0.40749400
C	3.97370700	5.38522100	-1.03144200
H	2.97158400	5.60166100	-1.40825500
H	4.60087300	6.26041600	-1.22890400
H	3.90190100	5.25521400	0.05189000
C	-2.70856100	-2.12090300	-0.59541000
C	1.92567600	0.75556400	-0.94355700
C	-1.55578200	1.09306400	0.46860300
C	0.75299000	-3.25055500	-0.03146000
C	-2.95693200	1.30061300	0.55068800
C	3.27248100	0.69722000	-0.51179400
C	-2.50856300	-0.79485300	-0.20467100
C	2.19668200	-1.25607400	-0.03488700
C	-3.47027000	2.50795000	1.03406400
H	-4.54380000	2.63754700	1.08348300
C	-1.56100600	-3.01996000	-0.55230800
C	-4.04190800	-2.52695900	-0.79829600
H	-4.22954900	-3.53593600	-1.13547500
C	-2.61116700	3.52296000	1.45202200
C	0.60494900	-4.63920800	0.02322000
H	1.45864600	-5.25536900	0.26087400
C	-5.12953000	-1.67559300	-0.57806900
C	3.67871900	2.91015800	-1.41174200

C	-1.22226000	3.27906800	1.37872700
H	-0.53170900	4.04489600	1.71285800
C	4.13376100	1.77655700	-0.74125700
H	5.15843600	1.71171500	-0.39878400
C	-4.88167100	-0.37166800	-0.10119600
H	-5.71227400	0.29315900	0.10756000
C	2.02567100	-2.60366400	0.28165400
C	-3.58198800	0.07526200	0.09259900
C	-0.68299300	2.09107800	0.90276900
H	0.38818600	1.95161300	0.88272900
C	3.45417900	-0.61211700	0.08091800
C	-1.71692900	-4.40788100	-0.49946200
H	-2.70248000	-4.83426600	-0.61260900
C	1.45383300	1.87439900	-1.63271300
H	0.43461200	1.91842500	-1.99315300
C	3.13343300	-3.26812600	0.84186100
H	3.02004300	-4.30018200	1.13781400
C	4.37063200	-2.64519900	1.04270800
C	-6.58538900	-2.12029600	-0.82306800
C	-3.11581400	4.87332200	1.99324000
C	2.33465600	2.92394900	-1.85144900
H	1.96289700	3.78898100	-2.38825900
C	-0.62509200	-5.21807500	-0.24435000
H	-0.73855700	-6.29570900	-0.21568900
C	4.52304400	-1.30834700	0.63040200
H	5.48368000	-0.81622900	0.73192500
C	5.56806100	-3.37883400	1.67918400
C	4.57859400	4.12687600	-1.69674300
C	-2.61760500	5.07114800	3.44387400

H	-2.99175000	4.27616200	4.09470300
H	-2.96680000	6.02991500	3.84062200
H	-1.52691400	5.06369300	3.50266000
C	-2.57648400	6.02047500	1.10724700
H	-1.48447400	6.04178800	1.09227200
H	-2.92456500	6.98863800	1.48151100
H	-2.92180400	5.90951700	0.07571500
C	-4.65288800	4.96192600	2.00199200
H	-5.07133800	4.85785800	0.99711100
H	-4.96265500	5.93650500	2.38922800
H	-5.10037000	4.19588200	2.64125700
C	6.74816900	-3.41225700	0.68009500
H	6.46818500	-3.93948800	-0.23599400
H	7.60683500	-3.92784000	1.12141300
H	7.07318800	-2.40775600	0.39996000
C	6.00486000	-2.63336500	2.96189300
H	6.30206100	-1.60356000	2.75100800
H	6.85813400	-3.13827600	3.42557700
H	5.19016300	-2.60206300	3.69035900
C	5.23343600	-4.83129100	2.06561100
H	4.42160100	-4.88200600	2.79651600
H	6.11127100	-5.30107200	2.51698100
H	4.95300500	-5.43075400	1.19482800
C	-6.68186800	-3.56839500	-1.33746800
H	-6.15676600	-3.69888000	-2.28774500
H	-7.73066200	-3.82877300	-1.50305400
H	-6.27660000	-4.28477200	-0.61714100
C	-7.38665900	-2.02990300	0.49660000
H	-6.95198500	-2.67948300	1.26129000

H	-8.42397700	-2.33971900	0.33516200
H	-7.40270800	-1.01269100	0.89425000
C	6.00569800	3.93952700	-1.15023700
H	6.60355900	4.82761900	-1.37240200
H	6.50698500	3.08219500	-1.60789400
H	6.01066100	3.80163000	-0.06547400
C	-7.23441000	-1.19626300	-1.88002100
H	-7.24210000	-0.15290200	-1.55668500
H	-8.27098000	-1.49575500	-2.06446900
H	-6.69058100	-1.24687400	-2.82708700
C	4.67745600	4.35367000	-3.22338100
H	3.69849400	4.54009400	-3.67053500
H	5.10941700	3.47983900	-3.71880300
H	5.31324100	5.21791600	-3.44048600
B	-0.17482400	-0.84461400	-0.86084000
O	-0.53595700	-0.72529100	-2.23628500
H	0.19558000	-0.95374400	-2.81551900

NBNN-5

Atom	X	Y	Z
C	1.34120800	1.72954200	0.45179400
C	1.38118300	2.93160100	1.16352400
C	0.20934900	3.53568400	1.58079400
C	-1.00382200	2.97351000	1.22582500
C	-1.04054800	1.77172400	0.51758600
N	0.13400200	1.11800900	0.20783500
H	0.24075000	4.45944500	2.14677000
H	2.33631800	3.38172600	1.38552500
H	-1.93021900	3.47239700	1.46613800
C	-2.29963700	1.25154000	-0.01683900

C	-2.24020400	0.23483600	-0.97570200
C	-3.56634200	1.81145400	0.20635800
C	-3.34202400	-0.18167100	-1.76656900
C	-4.68048900	1.38984700	-0.52985500
H	-3.70419300	2.58813900	0.94769700
C	-4.58273000	0.41906200	-1.52701000
C	-2.82068800	-1.20111600	-2.63140000
C	-1.49452600	-1.35258300	-2.30975700
H	-5.64187000	1.84683400	-0.32604300
H	-5.46062600	0.13316900	-2.09603200
H	-3.35358100	-1.74800400	-3.39341900
H	-0.77114700	-2.02397800	-2.74271800
C	2.56606400	1.11835100	-0.06414500
C	2.48676200	-0.11483600	-0.71929400
C	3.84217500	1.69515200	0.01575400
C	3.61310700	-0.79804700	-1.25390900
C	4.96313600	1.05494200	-0.52700500
H	3.98438600	2.65666600	0.49135700
C	4.86652200	-0.18425900	-1.15651400
C	3.10636200	-2.04215700	-1.75003000
C	1.75915800	-2.04867900	-1.49168100
H	5.92944000	1.53902000	-0.44686100
H	5.75353100	-0.66552500	-1.55371600
H	3.66520200	-2.83419500	-2.22310800
H	1.04219900	-2.83298600	-1.67442200
N	1.36559800	-0.86628000	-0.88583800
N	-1.12643300	-0.47730200	-1.29945700
B	0.01922900	-0.47838700	-0.27143200
C	0.38818800	-2.21694100	3.23153800

C	-0.79810400	-2.94012300	3.35028900
C	-1.73750100	-2.88355100	2.32506700
C	-1.49481600	-2.10337500	1.19410100
C	-0.31184400	-1.36412400	1.04913700
C	0.62303200	-1.44698400	2.09604200
H	1.13131500	-2.25887900	4.02110200
H	-0.98458700	-3.54418400	4.23175100
H	-2.66201300	-3.44606100	2.40383100
H	-2.24376000	-2.07835500	0.41031300
H	1.56272000	-0.90707600	2.02262000

NBNN-1f

Atom	X	Y	Z
C	-0.00025800	-5.17724600	-1.03813100
C	-1.19249300	-4.51898800	-0.79500300
C	-1.19082400	-3.16684200	-0.44192900
C	1.19567200	-3.13126900	-0.59661000
C	1.19285300	-4.48018600	-0.96033900
H	-0.00268100	-6.22529000	-1.31478400
H	-2.13374300	-5.03590300	-0.90282100
H	2.12761400	-4.96665100	-1.19383500
C	2.44145700	-2.36152300	-0.53359900
C	3.73151900	-2.90014600	-0.65028400
C	2.36241800	-0.97100000	-0.42830500
C	4.88975400	-2.10228300	-0.67399500
H	3.84929900	-3.97389100	-0.71486000
C	3.49133500	-0.13036900	-0.45911300
C	4.75407000	-0.70742800	-0.58505400
C	2.96353400	1.21143800	-0.31615900
C	1.54695000	1.08843600	-0.23099600

H	5.63013400	-0.07283400	-0.60331900
C	3.58415400	2.45722000	-0.24101100
C	0.71349200	2.22764300	-0.13806200
C	2.80487700	3.59556500	-0.05640800
H	4.66214500	2.51867000	-0.30965700
C	1.40717100	3.44260600	-0.01189500
H	0.82724900	4.34222300	0.12817300
C	-2.44217700	-2.42133700	-0.28411800
C	-3.72678600	-2.98440500	-0.32184900
C	-2.38601000	-1.02493800	-0.24737900
C	-4.89840100	-2.20728500	-0.36147600
H	-3.82833400	-4.06170500	-0.32097100
C	-3.52695500	-0.20518400	-0.34084300
C	-4.78271600	-0.80805100	-0.39471500
C	-3.01464300	1.14944600	-0.35130800
C	-1.59568200	1.05617200	-0.24174600
H	-5.66846600	-0.18958600	-0.45431700
C	-3.65121800	2.38501600	-0.45738600
C	-0.78093700	2.21479700	-0.22731000
C	-2.88608400	3.54682100	-0.46489900
H	-4.72920700	2.42051700	-0.54290700
C	-1.48893300	3.42087000	-0.35782000
H	-0.91842400	4.33579300	-0.40468000
N	1.21070300	-0.26201400	-0.28703500
N	-1.24688300	-0.29010700	-0.17363500
C	3.41174200	5.00492600	0.08909900
C	2.89228800	5.92033100	-1.04391700
C	3.01048900	5.60440000	1.45696500
C	4.94967300	4.98459500	0.01336700

H	3.16592500	5.51970100	-2.02376500
H	1.80499100	6.02250000	-1.01848700
H	3.32253200	6.92278300	-0.95265300
H	3.37366400	4.97890700	2.27680100
H	3.43818000	6.60516000	1.57514000
H	1.92657100	5.69164300	1.56129100
H	5.33624900	6.00122400	0.12530200
H	5.38719700	4.37557300	0.80908900
H	5.30431000	4.60129400	-0.94738500
C	6.26622500	-2.78864200	-0.79545100
C	6.48216800	-3.73823300	0.40600500
C	6.33061000	-3.60191300	-2.10935100
C	7.42520600	-1.77463600	-0.81064400
H	6.44577700	-3.18661200	1.34913100
H	5.72088700	-4.52088700	0.44929200
H	7.45825600	-4.22827600	0.33448900
H	6.18489000	-2.95235500	-2.97662500
H	7.30502600	-4.09031700	-2.20886400
H	5.56506600	-4.38083200	-2.14450300
H	8.37583200	-2.30744000	-0.89784300
H	7.35437400	-1.08736700	-1.65806400
H	7.46204100	-1.18452500	0.10897600
C	-6.26654900	-2.92027000	-0.38160700
C	-6.36486200	-3.83192300	-1.62705600
C	-6.42234400	-3.77856300	0.89540400
C	-7.44207200	-1.92656800	-0.42998000
H	-6.26036000	-3.24851800	-2.54579900
H	-5.58940400	-4.60174200	-1.63119900
H	-7.33444300	-4.33897800	-1.65347100

H	-6.36263200	-3.15611700	1.79208400
H	-7.39114400	-4.28792900	0.89709800
H	-5.64527500	-4.54304800	0.97005300
H	-8.38630600	-2.47748300	-0.43703400
H	-7.45266700	-1.26612400	0.44122900
H	-7.41607600	-1.30756700	-1.33093800
C	-3.50571900	4.95146500	-0.60118900
C	-3.13276300	5.80878800	0.63061000
C	-2.97301700	5.63530700	-1.88184100
C	-5.04196800	4.90074200	-0.69445100
H	-3.50407100	5.34945400	1.55073700
H	-2.05160200	5.92770300	0.73154400
H	-3.57110900	6.80837200	0.54715700
H	-3.23143500	5.05204900	-2.76978600
H	-3.40822700	6.63388200	-1.99066200
H	-1.88648700	5.74659200	-1.86251300
H	-5.43817400	5.91592500	-0.78336900
H	-5.37771800	4.33831200	-1.56996700
H	-5.48805400	4.44918700	0.19595500
N	0.00545400	-2.49708500	-0.32122900
B	0.01145700	-0.97630500	0.31997100
C	0.07339800	-1.11626500	1.94332200
C	-0.49063100	-0.11931300	2.75788500
C	0.71477600	-2.17678800	2.60484900
C	-0.41204000	-0.17025400	4.14793700
H	-1.00818300	0.71745500	2.30239100
C	0.79785100	-2.23893400	3.99498900
H	1.16281200	-2.98347900	2.03486300
C	0.23491000	-1.23240800	4.77463100

H	-0.86056800	0.61948800	4.74167300
H	1.30077100	-3.07602300	4.46835200
H	0.29573100	-1.27730500	5.85669900
NBNN-2f			
Atom	X	Y	Z
C	-0.04431000	-5.30801900	-0.51468200
C	-1.23292600	-4.61994000	-0.34701600
C	-1.22022800	-3.24907700	-0.07710700
C	1.17215500	-3.25644600	-0.16727400
C	1.15764700	-4.62523900	-0.44334600
H	-0.05538900	-6.37123500	-0.72529000
H	-2.17853700	-5.13089900	-0.44474400
H	2.09052600	-5.13954700	-0.61715000
C	2.42539900	-2.49780900	-0.12780900
C	3.71073600	-3.05811300	-0.17391000
C	2.36456800	-1.10249000	-0.12362900
C	4.87968200	-2.27759800	-0.22467200
H	3.81534700	-4.13498700	-0.15743800
C	3.50406400	-0.27897300	-0.17474600
C	4.76157400	-0.87827600	-0.23168200
C	2.99225400	1.07598100	-0.10922900
C	1.57376000	0.97819800	-0.03554800
H	5.64675800	-0.25713100	-0.26571800
C	3.63104500	2.31458000	-0.08121200
C	0.75505600	2.12957500	0.03289600
C	2.86682300	3.46993300	0.05103500
H	4.71027600	2.35761200	-0.14361200
C	1.46734500	3.33802900	0.10698700
H	0.90257400	4.25105600	0.21671200

C	-2.46281300	-2.48042500	0.03067100
C	-3.75485900	-3.02770500	0.01503600
C	-2.38923300	-1.08499300	0.02804900
C	-4.91662700	-2.23658800	-0.03071000
H	-3.87033800	-4.10320000	0.04230200
C	-3.52056700	-0.25168000	-0.05520600
C	-4.78418000	-0.83929500	-0.08405100
C	-2.99217000	1.09740100	-0.08344300
C	-1.57382500	0.98919300	0.00194600
H	-5.66299200	-0.21059300	-0.13856700
C	-3.61596500	2.33925500	-0.18935100
C	-0.74297300	2.13507600	-0.01560900
C	-2.83649100	3.49110100	-0.21804700
H	-4.69473100	2.38754400	-0.25636000
C	-1.43922900	3.34880000	-0.13817800
H	-0.86080400	4.25766200	-0.19925700
N	1.21988500	-0.37004400	-0.05257600
N	-1.24072500	-0.36120500	0.06751200
C	3.49242700	4.87624200	0.13447200
C	2.98012900	5.74848600	-1.03526000
C	3.10458100	5.53918000	1.47665000
C	5.02963300	4.83268000	0.05406500
H	3.24569400	5.30294500	-1.99778500
H	1.89422700	5.86467300	-1.01131100
H	3.42273900	6.74859900	-0.98825700
H	3.46289400	4.94469100	2.32133800
H	3.54591000	6.53828200	1.55024200
H	2.02240600	5.64529300	1.58116500
H	5.42957300	5.84825900	0.11854200

H	5.46299100	4.25474000	0.87487500
H	5.37507900	4.40172900	-0.88968200
C	6.24912600	-2.98741000	-0.26487000
C	6.42329800	-3.85495500	1.00352000
C	6.33298300	-3.88948100	-1.51830500
C	7.42201500	-1.99101400	-0.32095700
H	6.37217700	-3.23955600	1.90560200
H	5.65049500	-4.62341300	1.08168300
H	7.39397300	-4.36052700	0.98960900
H	6.21729300	-3.29906300	-2.43119200
H	7.30232900	-4.39597900	-1.56020900
H	5.55726400	-4.65903900	-1.51901000
H	8.36690800	-2.54008000	-0.35020800
H	7.37947900	-1.36144200	-1.21388900
H	7.44650100	-1.34088600	0.55770300
C	-6.29373300	-2.93258500	-0.02934100
C	-6.41225100	-3.86158500	-1.26010600
C	-6.45119600	-3.76957600	1.26155900
C	-7.45723000	-1.92515100	-0.08434700
H	-6.30796100	-3.29323600	-2.18824400
H	-5.64559400	-4.64017700	-1.25847200
H	-7.38784200	-4.35757300	-1.27167700
H	-6.37655600	-3.13453800	2.14826200
H	-7.42664000	-4.26582100	1.27807700
H	-5.68402100	-4.54343100	1.34201100
H	-8.40820500	-2.46436200	-0.07765900
H	-7.45416900	-1.25237400	0.77743600
H	-7.42932700	-1.31927200	-0.99409900
C	-3.44131100	4.90276000	-0.34894800

C	-3.03373800	5.76046400	0.87156000
C	-2.92556000	5.57442500	-1.64291300
C	-4.97961600	4.87076500	-0.41196400
H	-3.39202800	5.30925800	1.80075800
H	-1.94944400	5.86653400	0.95072800
H	-3.46158200	6.76494800	0.79233100
H	-3.20828200	4.99045500	-2.52296400
H	-3.35073700	6.57773100	-1.74785300
H	-1.83759600	5.67264800	-1.64531000
H	-5.36487700	5.89043000	-0.49778500
H	-5.33947800	4.30878200	-1.27816100
H	-5.41358100	4.42868600	0.48909500
N	-0.01648500	-2.59068700	0.02712700
B	0.01275600	-1.03552200	0.56727000
C	0.08799500	-1.11544900	2.14728800
C	0.14500500	-1.16883800	3.35251200
H	0.19516700	-1.20351200	4.41396800

5. Photophysical Properties

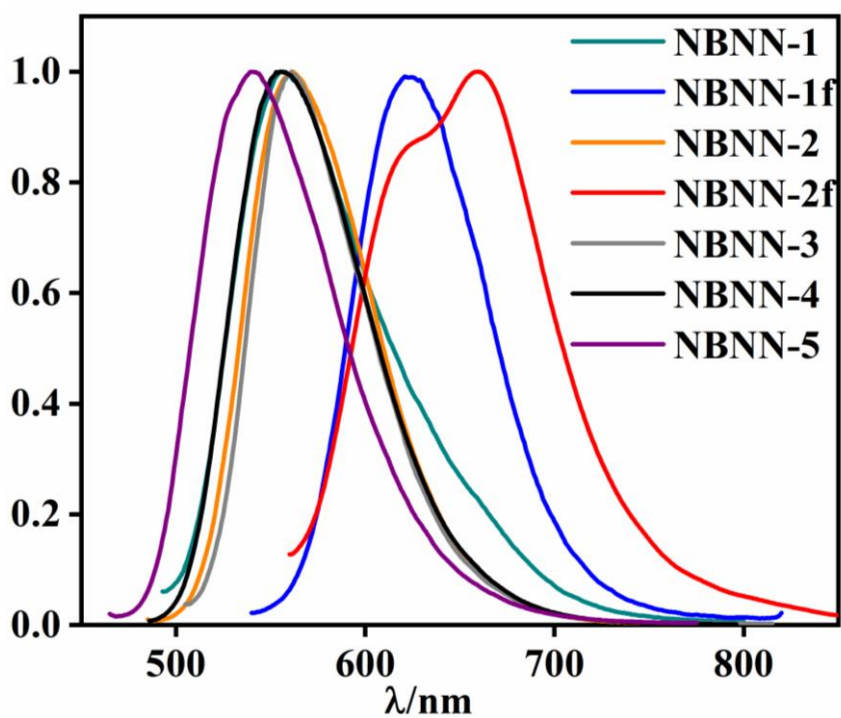


Figure S5.1 Fluorescence spectra in PMMA(10 wt%) film

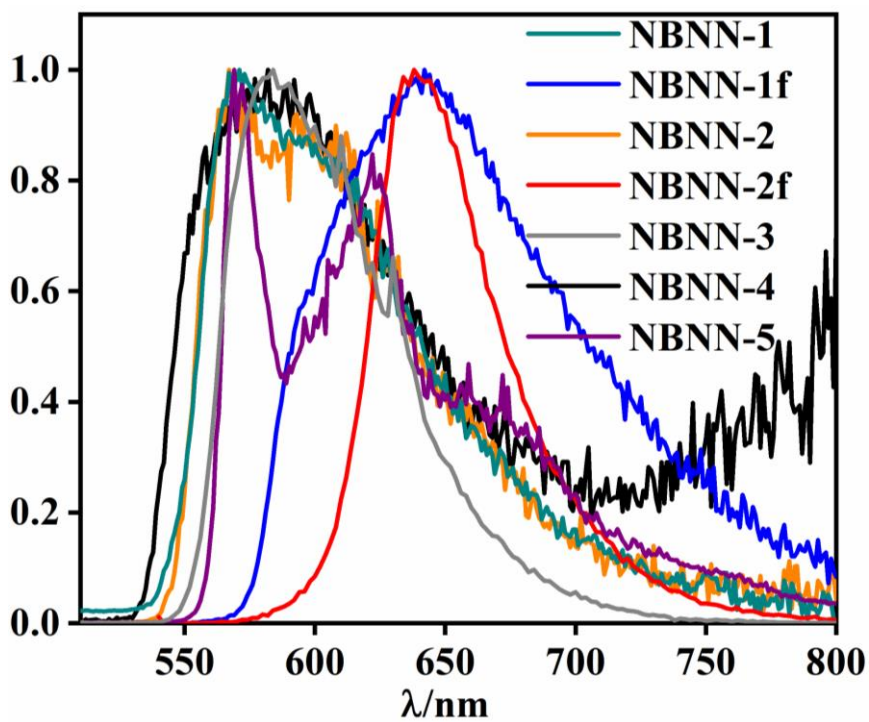


Figure S5.2 Phosphorescence spectra in PMMA(10 wt%) film at 77K

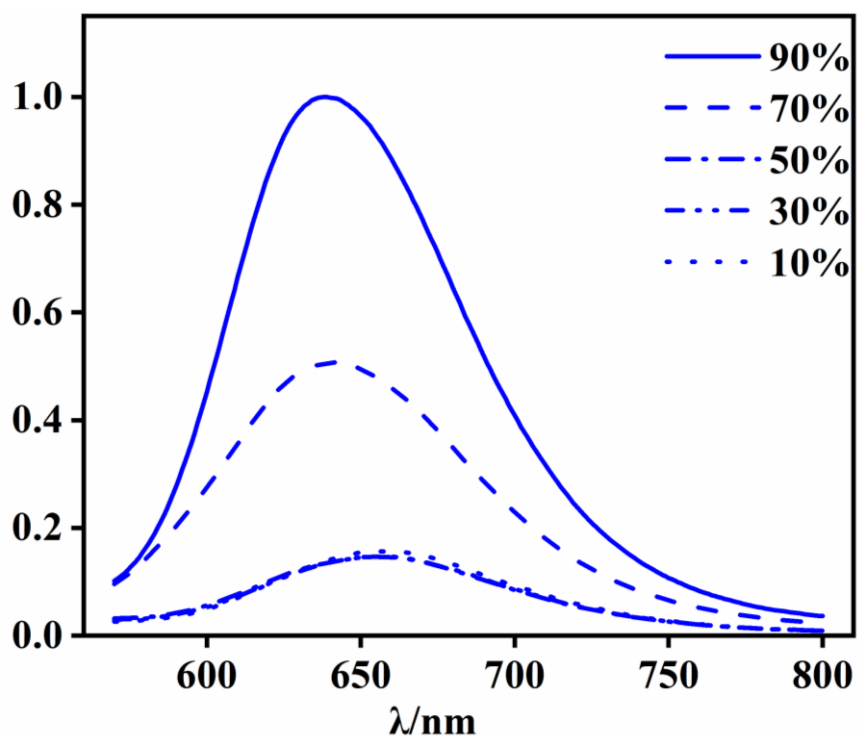


Figure S5.3 Fluorescence spectra of NBNN-1f in THF (10^{-5} M) with different H₂O fractions (vol%).

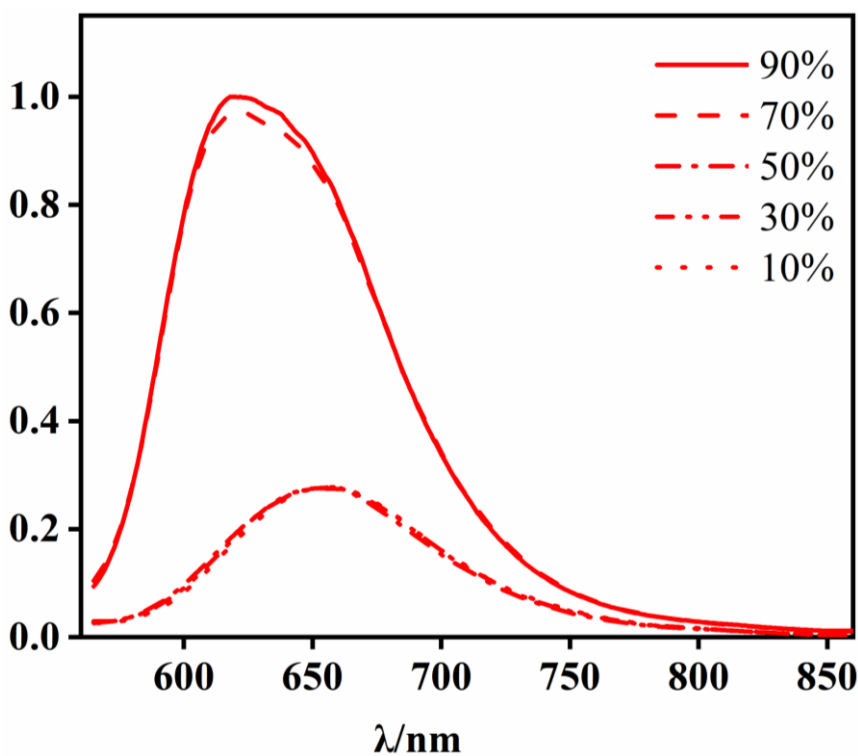


Figure S5.4 Fluorescence spectra of NBNN-2f in THF (10^{-5} M) with different H₂O fractions (vol%).

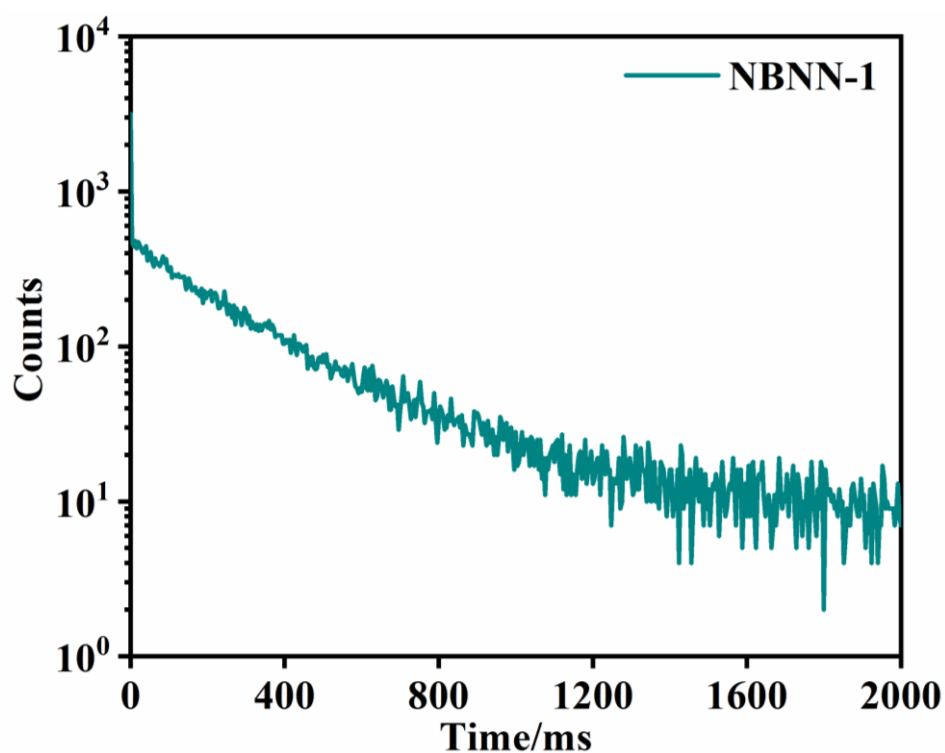


Figure S5.5 Phosphorescence decay curve of NBNN-1 in PMMA(10 wt%) film at 77K

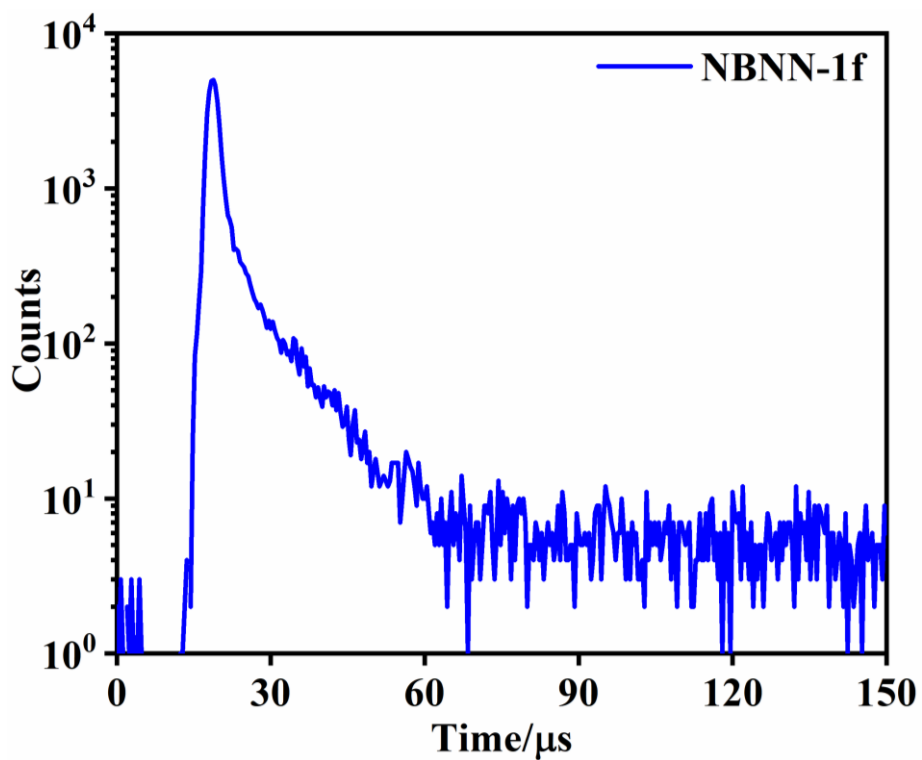


Figure S5.6 Phosphorescence decay curve of NBNN-1f in PMMA(10 wt%) film at 77K

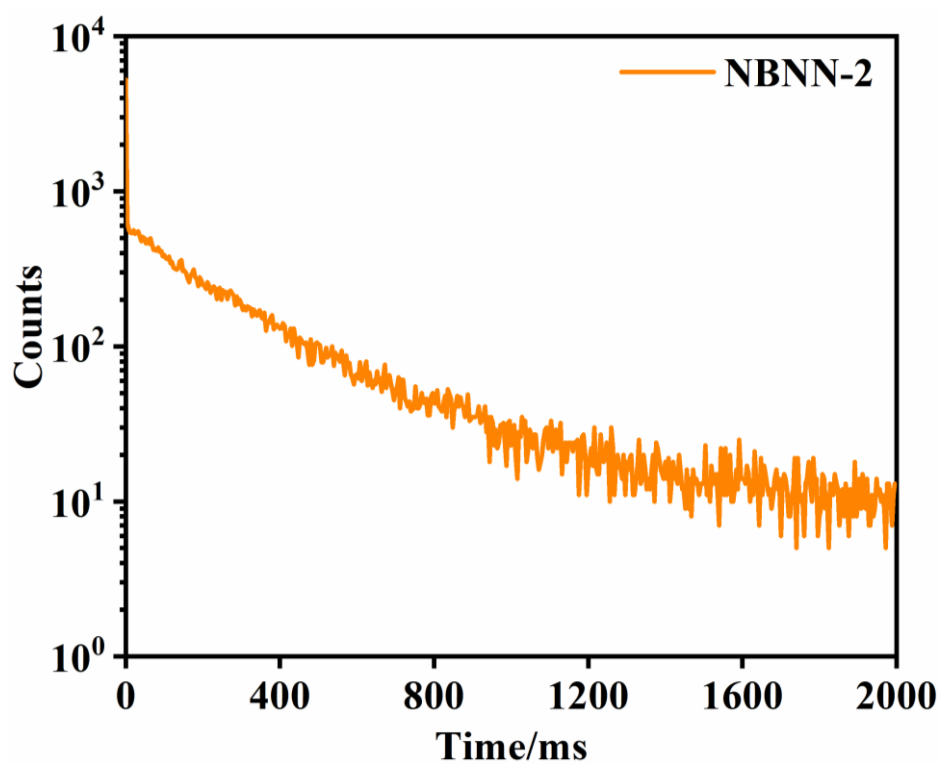


Figure S5.7 Phosphorescence decay curve of **NBNN-2** in PMMA(10 wt%) film at 77K

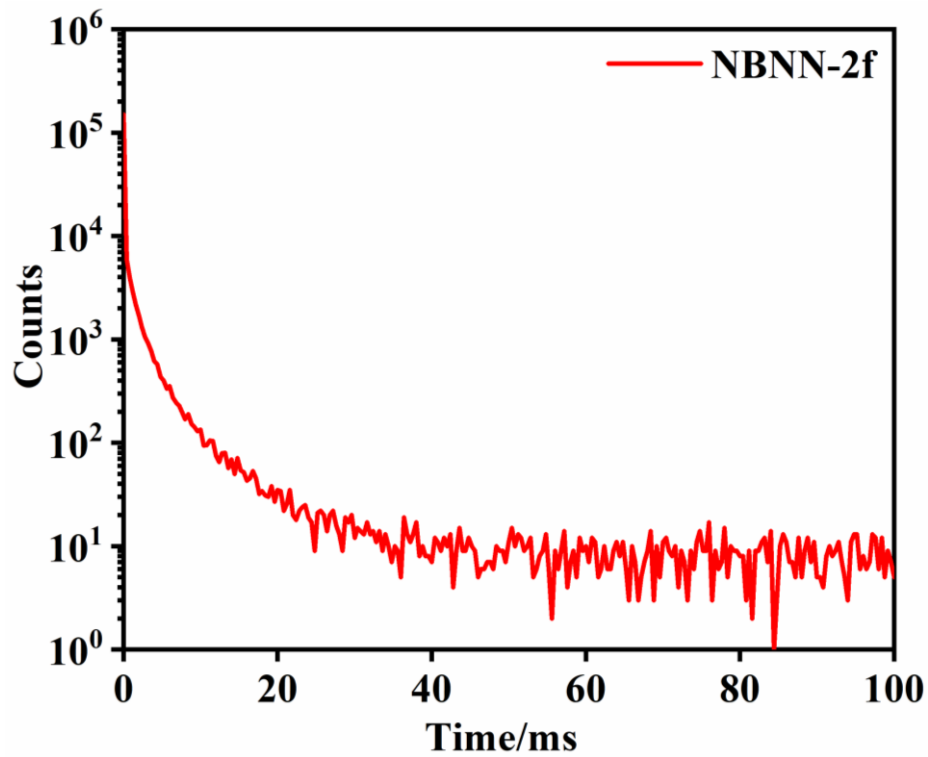


Figure S5.8 Phosphorescence decay curve of **NBNN-2f** in PMMA(10 wt%) film at 77K

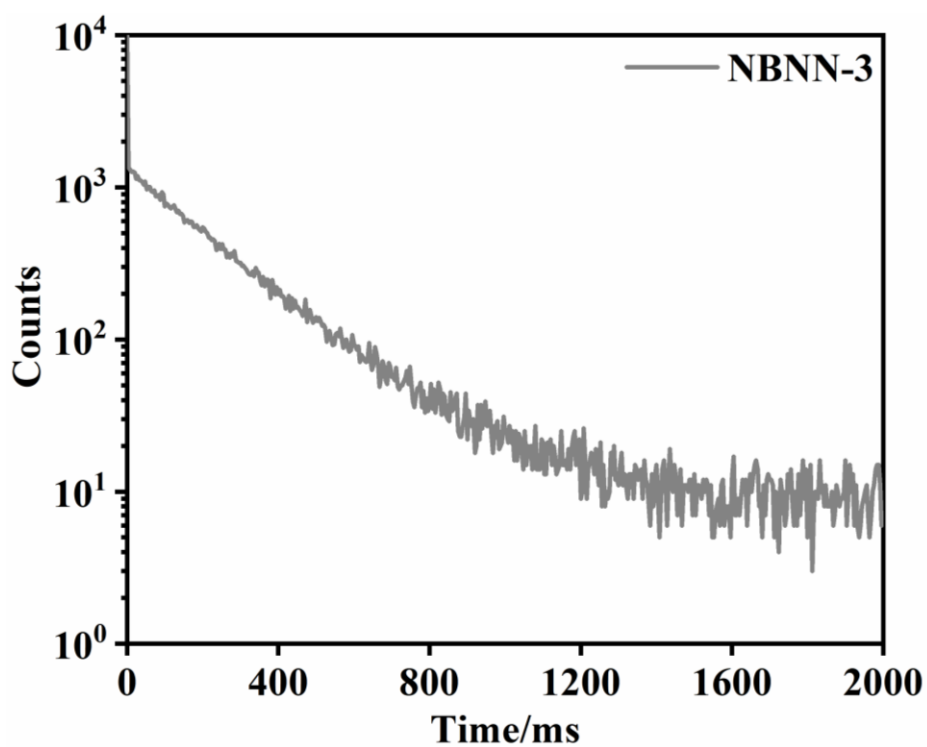


Figure S5.9 Phosphorescence decay curve of NBNN-3 in PMMA(10 wt%) film at 77K

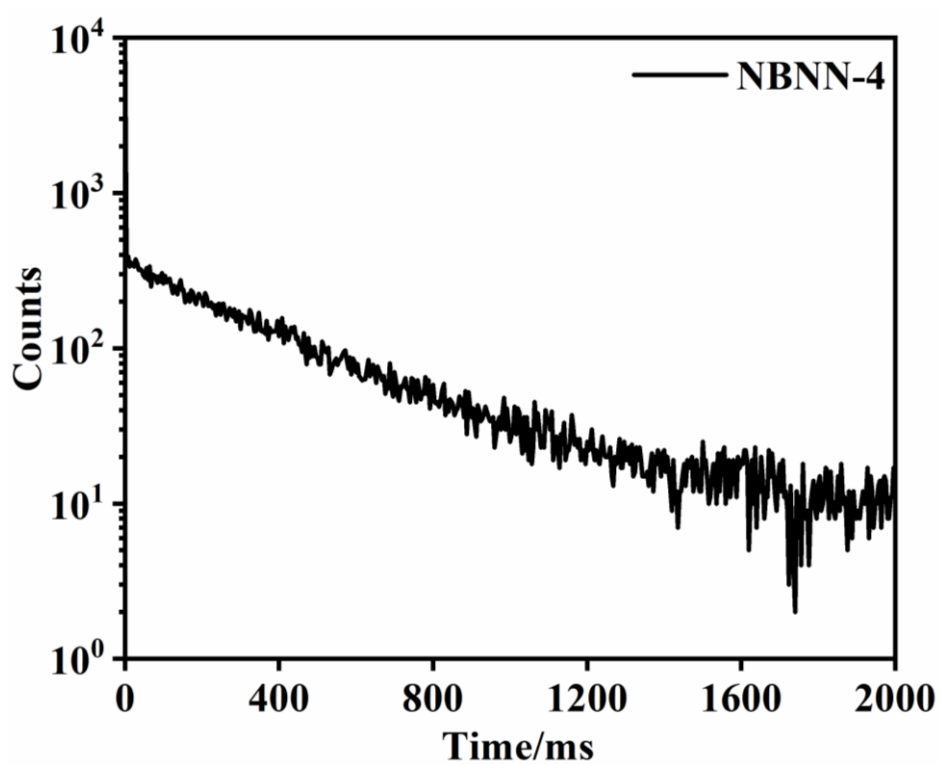


Figure S5.10 Phosphorescence decay curve of NBNN-4 in PMMA(10 wt%) film at 77K

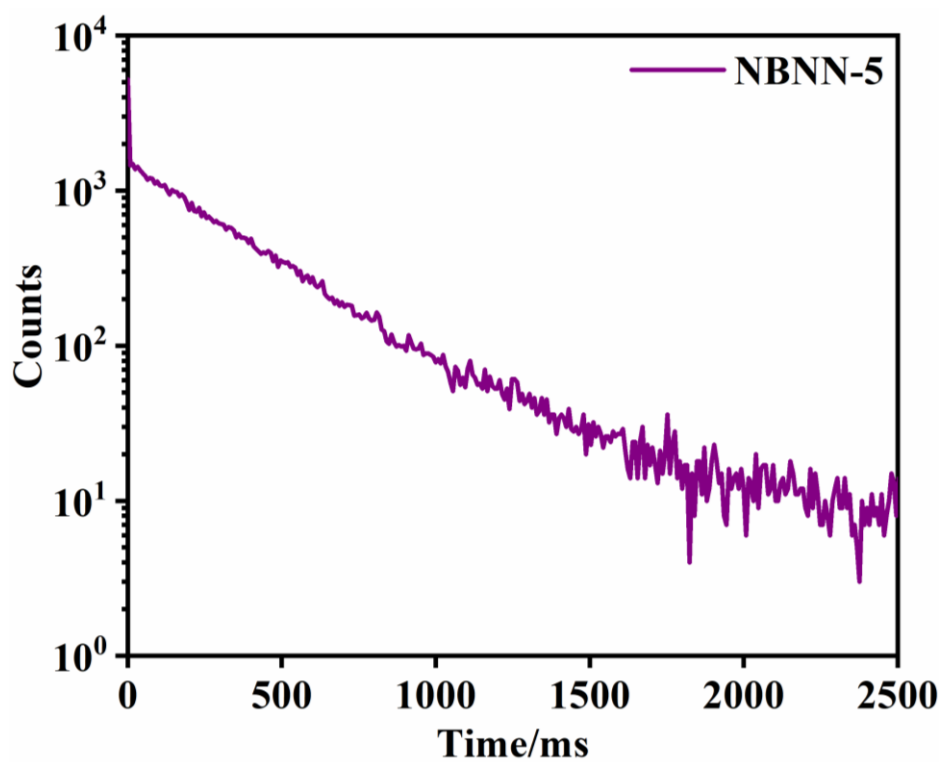


Figure S5.11 Phosphorescence decay curve of **NBNN-5** in PMMA(10 wt%) film at 77K

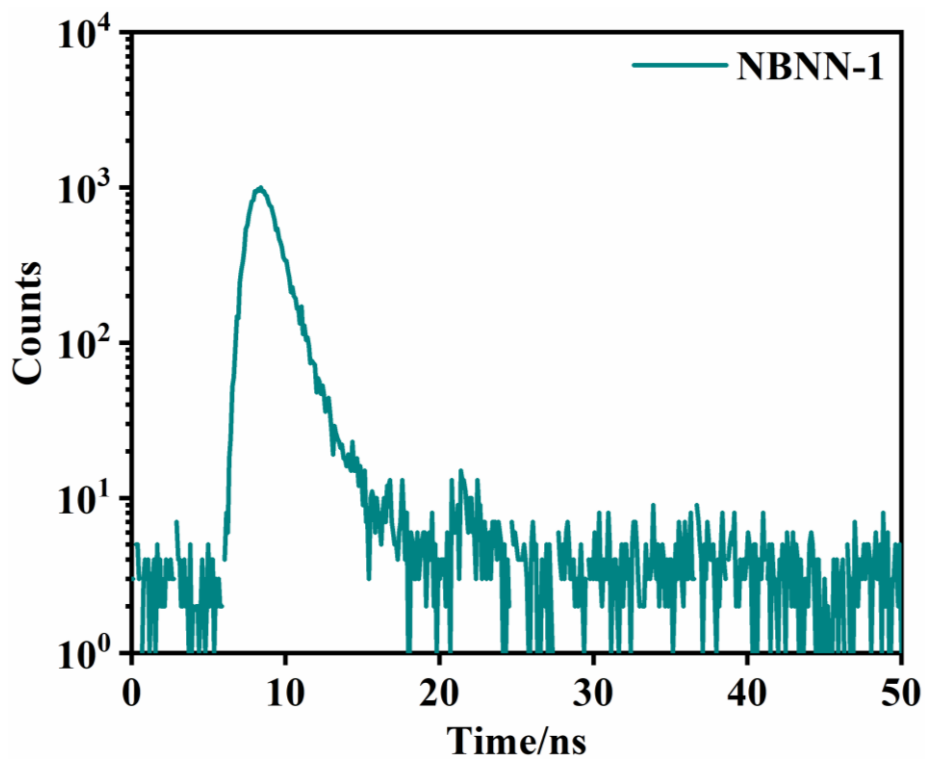


Figure S5.12 Transient fluorescence decay curve of **NBNN-1** in THF (10^{-5} M)

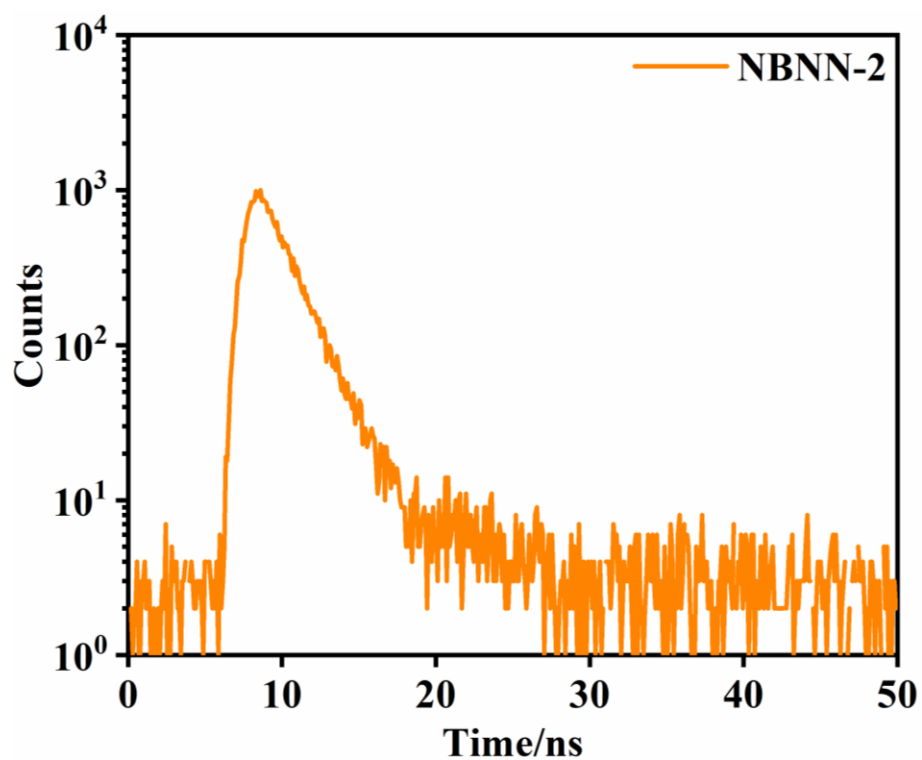


Figure S5.13 Transient fluorescence decay curve of **NBNN-2** in THF (10^{-5} M)

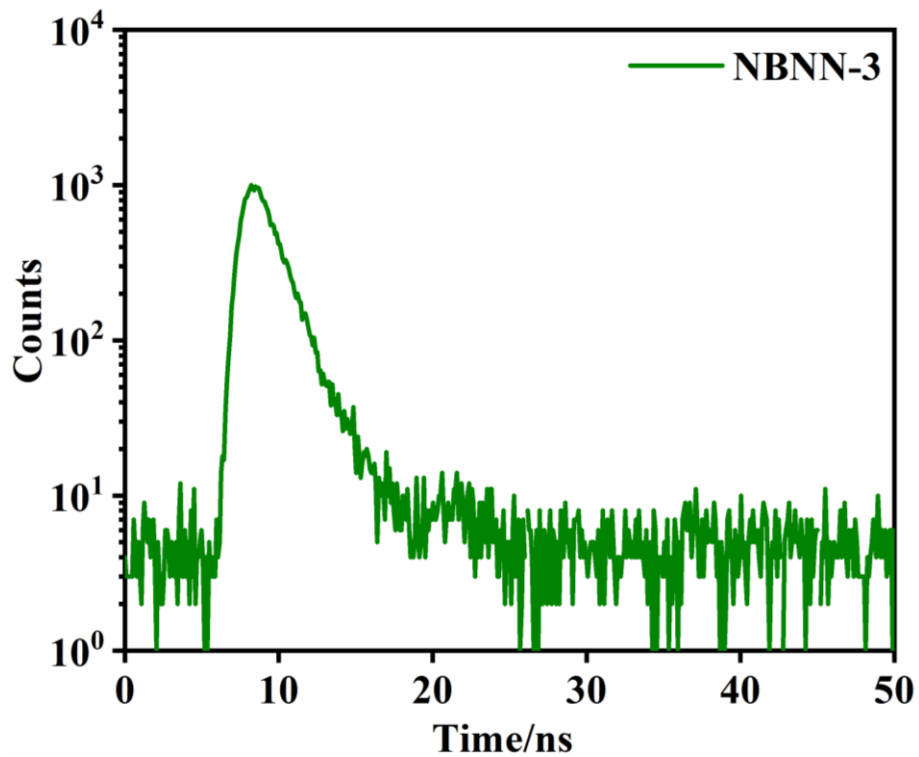


Figure S5.14 Transient fluorescence decay curve of **NBNN-3** in THF (10^{-5} M)

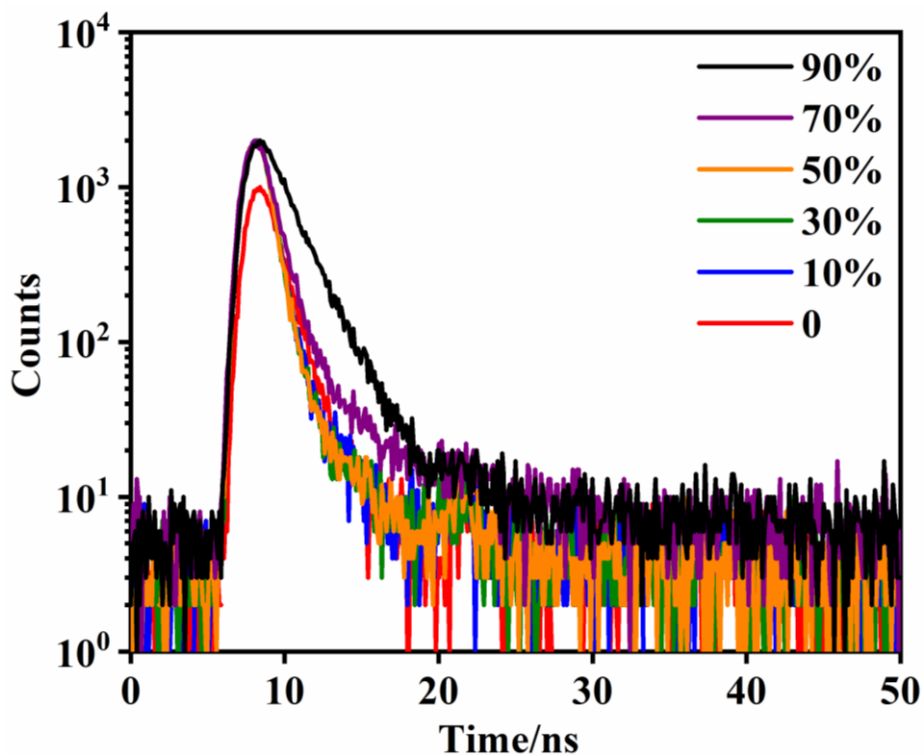


Figure S5.15 Transient fluorescence decay curves of **NBNN-1f** in THF (10^{-5} M) with different H₂O fractions (vol%).

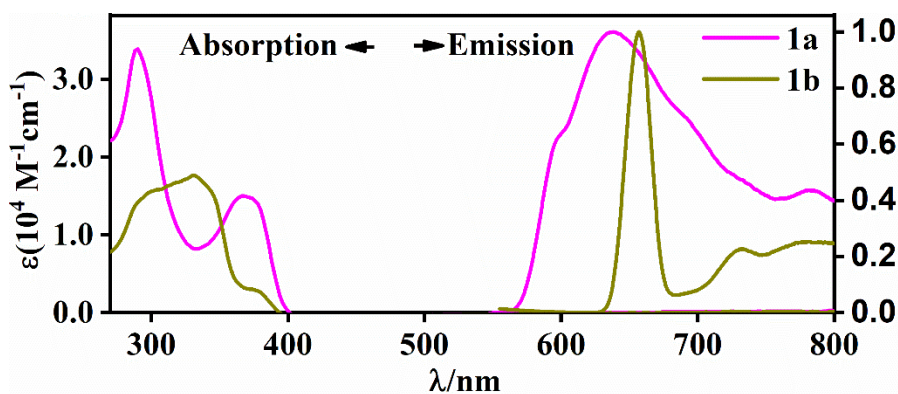


Figure S5.16 UV/vis and emission spectra of **1a** and **1b** in THF (10^{-5} M).

Table S5.1 Photophysical data of **NBNN-1f** and **NBNN-2f**

H ₂ O(%)		10	30	50	70	90
NBNN-1f	λ_{em} (nm)	657	659	656	641	638
	ϕ^d (%)	0.6	0.7	0.5	1.2	2.0
	τ_{PF} (ns)	1.28	1.19	1.29	1.87	1.88
NBNN-2f	λ_{em} (nm)	653	658	657	622	618
	ϕ^d (%)	0.8	0.8	0.8	1.9	1.9

6. X-ray Crystallographic Analysis

Crystals of **NBNN-1** and **NBNN-1f** were grown by mixed solution of CH_2Cl_2 and petroleum ether. The crystal data were collected on a Bruker SMART APEX-II diffractometer at 296.15 K. Crystal of **NBNN-3** was grown by mixed solution of ethyl acetate and petroleum ether. The crystal data were collected on a Bruker SMART APEX-II diffractometer at 180.00 K. The crystal data of **NBNN-1**, **NBNN-1f** and **NBNN-3** have been deposited at the Cambridge Crystallographic Data Center (CCDC). No. 2128933 (**NBNN-1**), 2128995 (**NBNN-1f**), and 2129008 (**NBNN-3**).

Table 6.1 Crystal data and structure refinement for **NBNN-1**.

Identification code	nbnn-1
Empirical formula	C ₅₁ H ₅₄ B N ₃
Formula weight	719.78
Temperature	296.15 K
Crystal system	monoclinic
Space group	C2/c
Unit cell dimensions	
	$a = 15.582(3) \text{ \AA}$ $\alpha = 90^\circ$
	$b = 33.295(6) \text{ \AA}$ $\beta = 90.452(3)^\circ$
	$c = 18.241(3) \text{ \AA}$ $\gamma = 90^\circ$
Volume	$9463(3) \text{ \AA}^3$
Z	8
ρ_{calc}	1.010 g/cm^3
μ	0.058 mm^{-1}
F(000)	3088.0
Crystal size	$0.21 \times 0.19 \times 0.18 \text{ mm}^3$
Radiation	MoK α ($\lambda = 0.71073$)
2 Θ range for data collection	3.312° to 49.998°
Index ranges	$-18 \leq h \leq 14$, $-37 \leq k \leq 39$, $-21 \leq l \leq 21$
Reflections collected	23691
Independent reflections	8337 [$R_{\text{int}} = 0.1065$, $R_{\text{sigma}} = 0.1328$]
Data/restraints/parameters	8337/138/571
Goodness-of-fit on F^2	0.906
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0897$, $wR_2 = 0.2024$
Final R indexes [all data]	$R_1 = 0.1804$, $wR_2 = 0.2425$
Largest diff. peak and hole	0.56 and $-0.60 \text{ e\AA}^{-3}$

Table 6.2 Crystal data and structure refinement for **NBNN-1f**.

Identification code	NBNN-1f
Empirical formula	C ₅₆ H ₆₂ B N ₃
Formula weight	787.89
Temperature	296.15 K
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	
	$a = 11.0795(12) \text{ \AA}$ $\alpha = 83.621(2)^\circ$
	$b = 14.2380(16) \text{ \AA}$ $\beta = 78.486(2)^\circ$
	$c = 15.3074(17) \text{ \AA}$ $\gamma = 77.897(2)^\circ$
Volume	$2307.5(4) \text{ \AA}^3$
Z	2
ρ_{calc}	1.134 g/cm^3
μ	0.065 mm^{-1}
F(000)	848.0
Crystal size	$0.20 \times 0.19 \times 0.18 \text{ mm}^3$
Radiation	MoK α ($\lambda = 0.71073$)
2 Θ range for data collection	2.722° to 55.32°
Index ranges	$-14 \leq h \leq 14$, $-14 \leq k \leq 18$, $-12 \leq l \leq 19$
Reflections collected	13990
Independent reflections	10109 [$R_{\text{int}} = 0.0257$, $R_{\text{sigma}} = 0.0686$]
Data/restraints/parameters	10109/52/554
Goodness-of-fit on F^2	1.020
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0949$, $wR_2 = 0.2608$
Final R indexes [all data]	$R_1 = 0.1631$, $wR_2 = 0.3179$
Largest diff. peak and hole	0.98 and $-0.60 \text{ e\AA}^{-3}$

Table 6.3 Crystal data and structure refinement for **NBNN-3**.

Identification code	nbnn-3
Empirical formula	C ₆₀ H ₇₂ B N ₃
Formula weight	846.01
Temperature	180.00 K
Crystal system	monoclinic
Space group	I2/a
Unit cell dimensions	
	$a = 21.747(2) \text{ \AA}$ $\alpha = 90^\circ$
	$b = 19.582(2) \text{ \AA}$ $\beta = 90.748(7)^\circ$
	$c = 23.834(3) \text{ \AA}$ $\gamma = 90^\circ$
Volume	10148.8(16) $\text{\AA}^3$
Z	8
ρ_{calc}	1.107 g/cm ³
μ	0.063 mm ⁻¹
F(000)	3664.0.0
Crystal size	0.28 × 0.20 × 0.14 mm ³
Radiation	MoK α ($\lambda = 0.71073$)
2 Θ range for data collection	4.4° to 55.272°
Index ranges	-28 ≤ h ≤ 24, -25 ≤ k ≤ 24, -30 ≤ l ≤ 31
Reflections collected	57572
Independent reflections	11749 [$R_{\text{int}} = 0.1938$, $R_{\text{sigma}} = 0.1567$]
Data/restraints/parameters	11749/42/592
Goodness-of-fit on F ²	0.986
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.1053$, $wR_2 = 0.2829$
Final R indexes [all data]	$R_1 = 0.2383$, $wR_2 = 0.3589$
Largest diff. peak and hole	1.04 and -0.50 e $\text{\AA}^{-3}$

7. References

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