

NBN Embedded Phenalene as a New Class of Zigzag Type Polycyclic Aromatic Hydrocarbons for Explosive Detection

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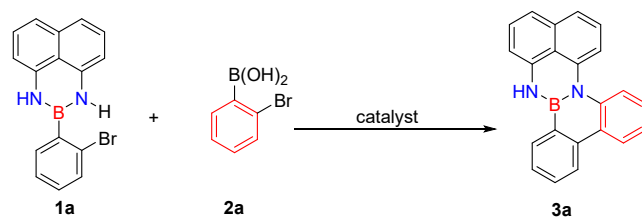
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General Information. All operations involving air- and moisture-sensitive compounds were carried out under an atmosphere of dry argon by using a modified Schlenk line. All solvents were freshly distilled from Na or CaH₂. The ¹H, ¹³C, ¹¹B spectra were recorded on a 400 MHz NMR spectrometer or 500 MHz NMR spectrometer. Chemical shifts are referenced against external BF₃·Et₂O (¹¹B) and tetramethylsilane (TMS). High-resolution mass spectra (HRMS) were obtained on a Varian QFT-ESI spectrometer. The UV-vis spectra were recorded on a RAYLEIGH UV-2100 spectrometer. Fluorescence spectra and quantum yield were performed on Edinburgh Instruments FS5 fluorescence spectrophotometer. Single crystals of 3a. A suitable crystal was selected and test on a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. The crystal was kept at 149.99(10) K during data collection. CCDC numbers: 2215352, 2247939 (for compounds 3a and 3f). Refinements were performed on *F*² anisotropically for all the non-hydrogen atoms by the full-matrix least-squares method. The commercially available catalysts and reagents were purchased from bidepharm.

Computational Details

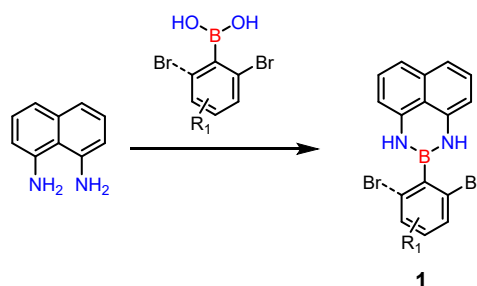
The theoretical calculations were performed via the Gaussian 16 suite of programs [16]. The structures of the complexes between 3a and TNT were fully optimized at the B3LYP-D3/6-31+G(d) level of theory. The vibrational frequencies of the optimized structure were carried out at the same level. Frequency analysis was performed to confirm that we have obtained stable structures on the potential energy surfaces. Different models were built and optimized including several hydrogen-bonded and π - π stacking structures. The interaction energies of the optimized structures between 3a and TNT were calculated at the B3LYP-D3/6-311+G(d) level of theory and the basis set superposition error (BSSE) correction was also included. Natural transitional orbital (NTO) [17] analysis was performed to assess the charge transfer character of the electronic transition respect to the fluorescence quenching. NTO analysis gives two new states, the “hole” and “electron” states, correspond to the detachment and attachment of charge densities upon the electronic excitation. A quantitative scheme that evaluates the amount of transferred charge upon excitation (χ) and the overlap between the ground and excited charge distributions (φ_s) was also used to ensuring the charge transfer character of the transitions in all the models [18]. Both χ index and φ_s takes the value in the range of 0 to 1, with greater χ values and less φ_s values indicating more significant charge transfer character. The NTO analysis was performed with Multiwfn software [19]. The Visual Molecular Dynamics (VMD) program [20] was used to plot the color-filled isosurfaces graphs to visualize the natural transitional orbitals.

Table S1: Optimization of Cyclization Conditions

entry	solvent	cat	ligand	bas	yield ^a
1	dioxane	PdCl ₂ (PPh ₃) ₂	X-Phos	NaOAc	16%
2	dioxane	Pd(dba) ₂	X-Phos	NaOAc	38%
3	dioxane	Pd(O ₂ CCF ₃) ₂	X-Phos	NaOAc	15%
4	dioxane	Pd(dppf)Cl ₂	X-Phos	NaOAc	13%
5	dioxane	Pd(PPh ₃) ₄	X-Phos	NaOAc	21%
6	dioxane	Pd(OAc) ₂	X-Phos	NaOAc	24%
7	dioxane	Pd(dba) ₂	P(Ph) ₃	NaOAc	29%
8	dioxane	Pd(dba) ₂	P(Py) ₃	NaOAc	32%
9	dioxane	Pd(dba) ₂	X-Phos	K ₂ CO ₃	29%
10	dioxane	Pd(dba) ₂	X-Phos	Na ₂ CO ₃	31%
11	dioxane:H ₂ O = 4:1	Pd(dba) ₂	X-Phos	NaOAc	46%
12	dioxane:H ₂ O:EtOH = 4:1:1	Pd(dba) ₂	X-Phos	NaOAc	73%
13	dioxane:H ₂ O:EtOH = 4:1:1	Pd(PPh ₃) ₄	X-Phos	NaOAc	52%
14	dioxane:H ₂ O:EtOH = 4:1:1	Pd(OAc) ₂	X-Phos	NaOAc	48%

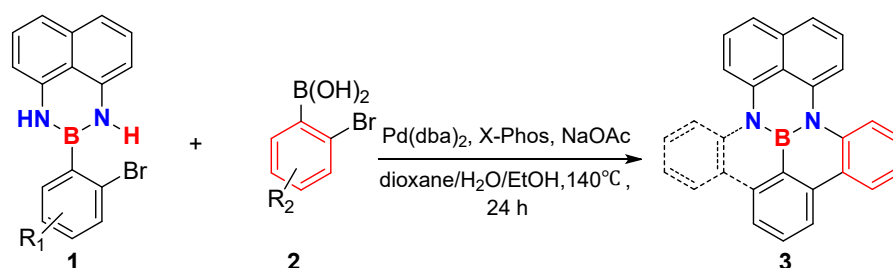
General procedure: 1a/2a = 1/3, 1a, 0.3 mmol, 10 mol % catalyst, 20 mol % ligand, 3 equivalents base, solvent 3 mL, 140 °C , 24 h. ^a Yields.

General Procedure for the Synthesis of compounds 1a-1f



The known compounds 1a-1f were synthesized according to the literatures^[21-22]. The synthesis process as follows : Under nitrogen atmosphere, a mixture of 2-bromophenylboronic acid derivatives (1 equiv.) or 2,6-dibromophenylboronic acid (1 equiv.) and 1,8-diaminonaphthalene (1.02 equiv.) in toluene (25 mL) were heated for 2 h under reflux with azeotropic removal of water. After evaporation of volatile material under reduced pressure, the residual solid was dissolved in CH₂Cl₂ and subjected to silica gel column chromatography, giving the title materials 1a-1f.

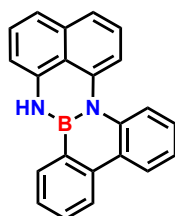
General Procedure for the Synthesis of 3a-3f



To an oven-dried schlenk tube with a stir bar was added compound 1 (0.2 mmol, 1 equiv) and compound 2 (0.6 mmol, 3 equiv), Pd(dba)₂ (0.02 mmol, 10 mol %), X-Phos (0.04 mmol, 20 mol %), and NaOAc (0.6 mmol, 3 equiv). The tube was sealed with schlenk system, evacuated under vacuum, and purged with Ar three times. Dioxane-H₂O-EtOH (total mix solvent 2 mL, dioxane: H₂O: EtOH = 4:1:1) was added, the resulting mixture was heated to 140 °C and stirred 24 h. The reaction mixture was cooled to rt, and filtered over Celite. The solvent was removed in vacuo, and the product was purified by flash column chromatography on silica gel with hexanes and dichloromethane as the eluent. The polarity of the eluent was respectively as follow: 3a, petroleum ether : dichloromethane = 5:1; 3b, petroleum ether : dichloromethane = 5:1; 3c, petroleum ether : dichloromethane = 4:1; 3d, petroleum ether : dichloromethane = 4:1; 3e, petroleum ether : dichloromethane = 4:1; 3f, petroleum ether : dichloromethane = 5:1. The reactions were set up with 0.2 mmol compound 1, and the final product masses were: 3a: 31 mg, 3b: 24 mg, 3c: 22.4 mg, 3d: 23 mg, 3f: 20 mg, 3g: 17 mg.

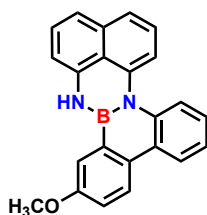
Characterization Data for the New Compounds

The carbon attached to the boron atom is no signal response in the NMR spectrum.



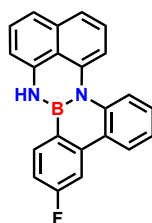
7H-dibenzo[3,4:5,6][1,2]azaborinino[1,2-a]naphtho[1,8-de][1,3,2]diazaborinine (3a)

¹H NMR (500 MHz, CDCl₃): δ 8.37 (1H, dd, *J* = 8.4, 1.3 Hz), 8.20 (1H, d, *J* = 7.9 Hz), 8.13 (1H, dd, *J* = 8.0, 1.7 Hz), 7.78 (1H, dd, *J* = 7.5, 1.4 Hz), 7.67-7.58 (2H, m), 7.41 (1H, t, *J* = 7.4, 1.0 Hz), 7.29-7.13 (6H, m), 6.54 (1H, dd, *J* = 7.0, 1.3 Hz), 6.35 (1H, s). ¹¹B NMR (CDCl₃, 160 MHz): δ 27.83. ¹³C NMR (126 MHz, CDCl₃): δ 139.50, 139.20, 138.30, 136.40, 131.41, 130.16, 127.22, 126.71, 126.68, 126.52, 126.23, 125.75, 122.72, 122.44, 122.30, 120.75, 118.40, 117.01, 111.68, 106.79. The carbon attaching to boron were not observed. HR-MS (ESI): calcd. for [M+H]⁺: Calcd. for C₂₂H₁₅BN₂: 319.1407; Found: 319.1408.



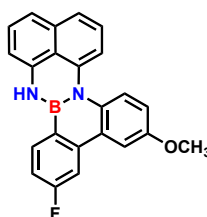
10-methoxy-7H-dibenzo[3,4:5,6][1,2]azaborinino[1,2-a]naphtho[1,8-de][1,3,2]diazaborinine (3b)

^1H NMR (400 MHz, CDCl_3): δ 8.38 (1H, d, $J = 9.6$ Hz), 8.17 (1H, d, $J = 9.6$ Hz), 8.08 (d, $J = 7.5$ Hz, 1H), 7.64 (1H, dd, $J = 5.8, 3.0$ Hz), 7.40-7.07 (8H, m), 6.59 (1H, d, $J = 7.0$ Hz), 6.36 (s, 1H), 3.94 (s, 3H). ^{11}B NMR (CDCl_3 , 160 MHz): δ 28.32. ^{13}C NMR (101 MHz, CDCl_3): δ 158.31, 139.14, 138.34, 137.43, 136.37, 132.79, 127.17, 126.61, 126.24, 125.68, 125.13, 124.48, 122.45, 122.30, 120.66, 118.70, 118.42, 116.94, 113.18, 111.76, 106.71, 55.51. The carbon attaching to boron were not observed. HR-MS (ESI): calcd. for $[\text{M}]^+$: Calcd. For $\text{C}_{23}\text{H}_{17}\text{BN}_2\text{O}$: 348.1434; Found: 348.1436.



11-fluoro-7H-dibenzo[3,4:5,6][1,2]azaborinino[1,2-a]naphtho[1,8-de][1,3,2]diazaborinine (3c)

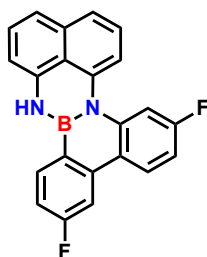
^1H NMR (400 MHz, CDCl_3): δ 8.39 (1H, d, $J = 8.5$ Hz), 8.05 (d, $J = 8.0$ Hz, 1H), 7.94-7.73 (m, 2H), 7.62 (d, $J = 7.1$ Hz, 1H), 7.42-7.07 (m, 7H), 6.58 (d, $J = 6.9$ Hz, 1H), 6.33 (1H, s). ^{11}B NMR (CDCl_3 , 160 MHz): δ 28.10. ^{13}C NMR (101 MHz, CDCl_3): δ 166.57 ($J_{\text{C-F}} = 257.55$ Hz, CF), 142.12, 138.97, 138.67, 138.03, 136.34, 132.59 ($J_{\text{C-F}} = 9.09$ Hz, CH), 127.36, 127.22, 126.19, 125.81, 125.74, 122.50, 122.16, 120.93, 118.51, 117.10, 114.44 ($J_{\text{C-F}} = 21.21$ Hz, CH), 111.72, 109.24 ($J_{\text{C-F}} = 21.21$ Hz, CH), 106.85. The carbon attaching to boron were not observed. HR-MS (ESI): calcd. for $[\text{M}+\text{H}]^+$: Calcd. For $\text{C}_{24}\text{H}_{14}\text{BFN}_2$: 337.1312; Found: 337.1303.



11-fluoro-14-methoxy-7H-dibenzo[3,4:5,6][1,2]azaborinino[1,2-a]naphtho[1,8-de][1,3,2]diazaborinine (3d)

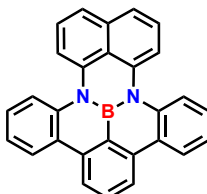
^1H NMR (400 MHz, CDCl_3): δ 8.31 (1H, d, $J = 9.2$ Hz), 7.88-7.73 (2H, m), 7.55 (1H, t, $J = 4.4$ Hz), 7.50 (1H, d, $J = 2.9$ Hz), 7.35-7.10 (5H, m), 6.88 (1H, dd, $J = 9.2, 2.9$ Hz), 6.55 (1H, d, $J = 7.0$ Hz), 6.30 (1H, s), 3.91 (3H, s). ^{11}B NMR (CDCl_3 , 160 MHz): δ 28.67. ^{13}C NMR (101 MHz, CDCl_3): δ 166.49 ($J_{\text{C-F}} = 249.47$ Hz, CF), 154.79, 141.97 ($J_{\text{C-F}} = 8.08$ Hz, CH), 139.15, 138.47, 136.40, 132.67 ($J_{\text{C-F}} = 9.09$ Hz, CH), 132.44, 127.22, 126.81, 126.27, 122.10, 120.48, 118.38, 118.35, 114.57 ($J_{\text{C-F}} = 21.21$ Hz, CH), 113.93, 111.02, 109.67, 109.32 ($J_{\text{C-F}} = 22.22$ Hz, CH), 106.67, 55.70. The carbon attaching to

boron were not observed. HR-MS (ESI): calcd. for $[M+H]^+$: Calcd. for $C_{23}H_{16}BFN_2O$: 367.1418; Found: 367.1411.



11,15-difluoro-7H-dibenzo[3,4:5,6][1,2]azaborinino[1,2-a]naphtho[1,8-de][1,3,2]diazaborinine (3e)

1H NMR (400 MHz, $CDCl_3$): δ 8.10 (1H, dd, $J = 12.2, 2.6$ Hz), 7.99 (1H, dd, $J = 8.9, 6.5$ Hz), 7.86-7.73 (2H, m), 7.59 (1H, d, $J = 7.3$ Hz), 7.36-7.21 (4H, m), 7.15 (1H, td, $J = 8.4, 2.3$ Hz), 6.92 (1H, ddd, $J = 9.4, 7.3, 2.6$ Hz), 6.66-6.53 (m, 1H), 6.33 (s, 1H). ^{11}B NMR ($CDCl_3$, 160 MHz): δ 28.73. ^{13}C NMR (101 MHz, $CDCl_3$): δ 166.63 ($J_{C-F} = 250.48$ Hz, CF), 163.26 ($J_{C-F} = 246.44$ Hz, CF), 141.69 ($J_{C-F} = 8.08$ Hz), 140.29 ($J_{C-F} = 10.1$ Hz), 138.56, 137.49, 136.27, 132.66 ($J_{C-F} = 9.09$ Hz), 127.55 ($J_{C-F} = 10.1$ Hz), 127.28, 126.21, 122.20, 121.98, 121.49, 118.74, 114.29 ($J_{C-F} = 22.22$ Hz), 111.89, 110.02 ($J_{C-F} = 22.22$ Hz), 109.07 ($J_{C-F} = 22.22$ Hz), 107.14, 103.98 ($J_{C-F} = 27.27$ Hz). The carbon attaching to boron were not observed. HR-MS (ESI): calcd. for $[M+H]^+$: Calcd. for $C_{22}H_{12}BF_2N_2$: 354.1140; Found: 354.1144.



3b,14b-diaza-3b1-boratribenzo[a,cd,f]perylene (3f)

1H NMR (500 MHz, $CDCl_3$): δ 8.37-8.33 (4H, m), 8.23 (2H, d, $J = 7.9$ Hz), 7.89-7.85 (1H, m), 7.75 (2H, d, $J = 7.0$ Hz), 7.45-7.33 (4H, m), 7.30-7.28 (2H, m). ^{11}B NMR (160 MHz, $CDCl_3$): δ 28.02. ^{13}C NMR (126 MHz, $CDCl_3$): δ 138.60, 138.54, 135.92, 135.77, 131.93, 127.19, 126.22, 125.64, 125.48, 125.33, 122.47, 120.87, 119.64, 115.91, 113.26. The carbon attaching to boron were not observed. HR-MS (ESI): calcd. for $[M+H]^+$: Calcd. for $C_{28}H_{17}BN_2$: 392.1485; Found: 392.1485.

X-ray Crystallographic Studies of 3a

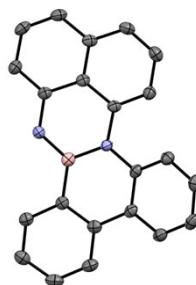


Table S2 Crystal data and structure refinement for Compound 3a.

Identification code	3a
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Empirical formula	C ₂₂ H ₁₅ BN ₂
Formula weight	318.17
Temperature/K	149.99(10)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	12.5564(11)
b/Å	11.0122(7)
c/Å	12.4231(12)
α/°	90
β/°	117.687(11)
γ/°	90
Volume/Å³	1521.1(3)
Z	4
ρ_{calc}/cm³	1.389
μ/mm⁻¹	0.081
F(000)	664.0
Crystal size/mm³	0.13 × 0.11 × 0.09
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	5.206 to 49.994
Index ranges	-14 ≤ h ≤ 12, -13 ≤ k ≤ 13, -14 ≤ l ≤ 14
Reflections collected	6200
Independent reflections	2677 [R _{int} = 0.0301, R _{sigma} = 0.0440]
Data/restraints/parameters	2677/0/230
Goodness-of-fit on F²	1.045
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0441, wR ₂ = 0.0991
Final R indexes [all data]	R ₁ = 0.0577, wR ₂ = 0.1081
Largest diff. peak/hole / e Å⁻³	0.17/-0.22

X-ray Crystallographic Studies of 3f

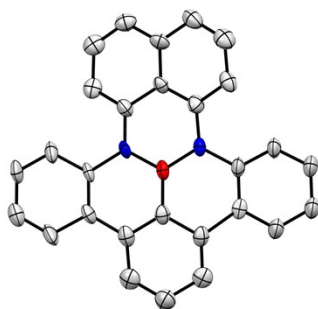


Table S3 Crystal data and structure refinement for Compound 3f.

Identification code	3f
Empirical formula	C ₂₈ H ₁₇ BN ₂
Formula weight	392.25
Temperature/K	169.99(10)
Crystal system	monoclinic
Space group	P2 ₁
a/Å	32.664(3)
b/Å	7.5997(4)
c/Å	23.6427(19)
α/°	90
β/°	108.644(9)
γ/°	90
Volume/Å³	5561.0(8)
Z	12
ρ_{calc}/cm³	1.406
μ/mm⁻¹	0.629
F(000)	2448.0
Crystal size/mm³	0.15 × 0.13 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	5.71 to 133.198
Index ranges	-38 ≤ h ≤ 38, -9 ≤ k ≤ 9, -28 ≤ l ≤ 28
Reflections collected	11539
Independent reflections	11539 [R _{int} = ?, R _{sigma} = 0.1599]
Data/restraints/parameters	11539/1765/1676
Goodness-of-fit on F²	0.928
Final R indexes [I ≥ 2σ(I)]	R ₁ = 0.0951, wR ₂ = 0.2391
Final R indexes [all data]	R ₁ = 0.1686, wR ₂ = 0.2793
Largest diff. peak/hole / e Å⁻³	0.62/-0.40
Flack parameter	1.6(10)

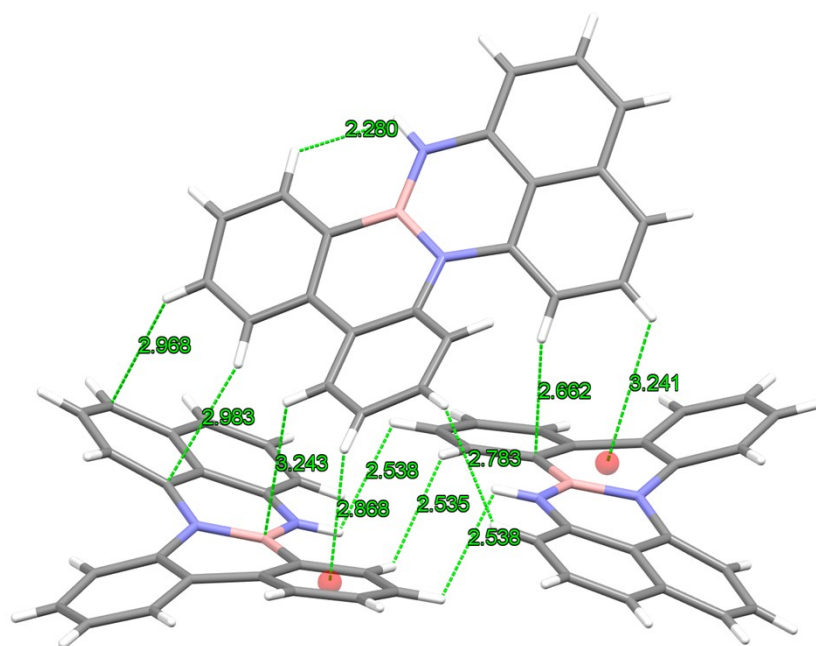


Figure S1. Intermolecular interactions for 3a.

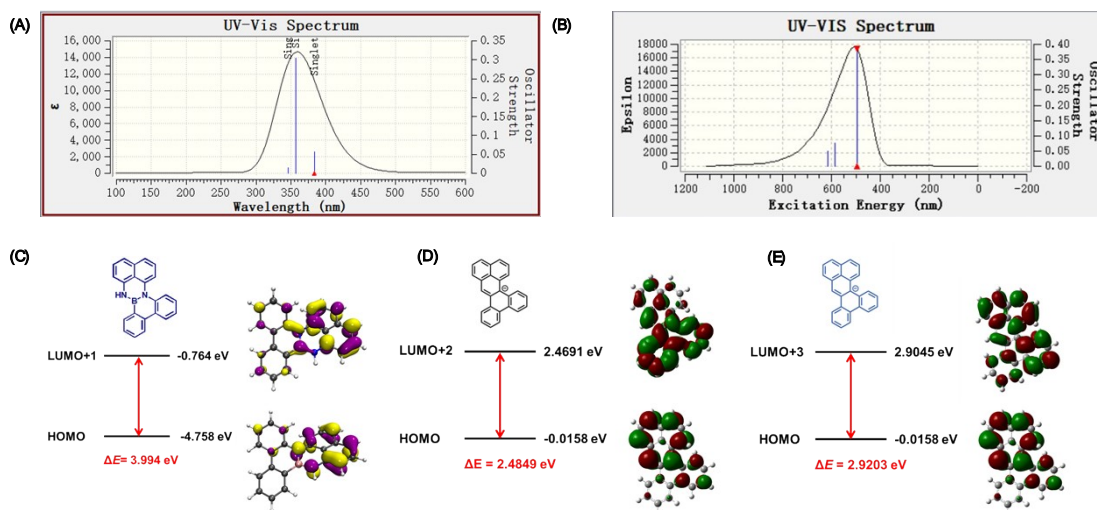


Figure S2. Calculated UV-vis absorption for 3a (A), 3a' (B), (C-D) Frontier orbitals energies and diagrams for 3a (C), 3a' (D).

Table S4. Cartesian coordinates for 3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.479829	-1.927591	0.666653
2	6	0	3.140115	-2.349452	0.785703
3	6	0	2.108016	-1.493159	0.437664
4	6	0	2.385313	-0.164712	-0.008322
5	6	0	3.750947	0.224254	-0.195658
6	6	0	4.784825	-0.678613	0.174837

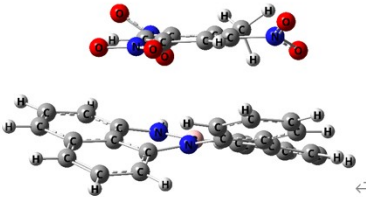
7	6	0	1.330745	0.754066	-0.325183
8	6	0	1.653163	1.939143	-0.973792
9	6	0	2.999051	2.298835	-1.191390
10	6	0	4.030348	1.487337	-0.778645
11	7	0	0.775493	-1.898585	0.433913
12	7	0	-0.007552	0.379376	-0.007102
13	5	0	-0.312490	-1.022901	0.177100
14	6	0	-1.774675	-1.485574	0.001734
15	6	0	-2.132512	-2.837995	-0.144964
16	6	0	-3.432659	-3.217481	-0.453361
17	6	0	-4.403834	-2.227436	-0.643564
18	6	0	-4.076852	-0.884733	-0.502203
19	6	0	-2.768823	-0.489848	-0.157659
20	6	0	-1.047479	1.325988	0.194215
21	6	0	-2.408434	0.918372	0.092024
22	6	0	-3.407040	1.883818	0.326172
23	6	0	-3.111711	3.194242	0.670607
24	6	0	-1.775303	3.565875	0.831029
25	6	0	-0.763958	2.642620	0.604342
26	1	0	5.276085	-2.612993	0.944837
27	1	0	2.911176	-3.356402	1.126798
28	1	0	5.818529	-0.370275	0.044823
29	1	0	0.868554	2.604121	-1.311503
30	1	0	3.212376	3.243352	-1.685047
31	1	0	5.065735	1.785020	-0.920447
32	1	0	0.621844	-2.882565	0.609682
33	1	0	-1.373864	-3.611259	-0.038229
34	1	0	-3.689753	-4.267339	-0.564052
35	1	0	-5.419744	-2.506517	-0.911143
36	1	0	-4.846234	-0.140610	-0.679010
37	1	0	-4.447781	1.583233	0.276565
38	1	0	-3.912305	3.906751	0.846422
39	1	0	-1.516067	4.570879	1.152836
40	1	0	0.263868	2.935851	0.772842
41	0	0	-2.107764	1.988773	1.416679
42	0	0	-3.324474	-1.906315	0.656160
43	0	0	-1.444652	-0.101393	1.047604
44	0	0	1.048657	-0.316161	1.084112
45	0	0	2.719333	1.522260	0.322405
46	0	0	3.431144	-0.711334	1.245506

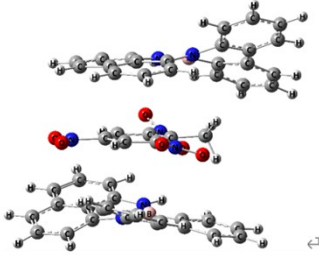
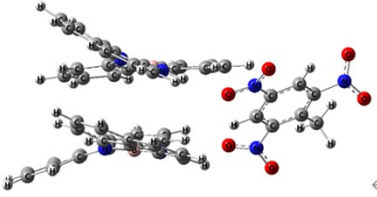
Table S5. Cartesian coordinates for 3a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.484227	-1.976131	-0.584566
2	6	0	-3.153541	-2.381104	-0.670865
3	6	0	-2.101594	-1.482141	-0.370385
4	6	0	-2.412748	-0.137055	0.003949
5	6	0	-3.784192	0.250184	0.145500
6	6	0	-4.802797	-0.686776	-0.174135
7	6	0	-1.358150	0.794755	0.260592
8	6	0	-1.722648	2.046014	0.814761
9	6	0	-3.060290	2.409055	0.986076
10	6	0	-4.084940	1.548029	0.623052
11	6	0	-0.751370	-1.887891	-0.354856
12	6	0	0.017397	0.394104	0.020617
13	6	0	0.301445	-0.994239	-0.115115
14	6	0	1.685300	-1.466786	0.029853
15	6	0	1.984609	-2.841037	0.151548
16	6	0	3.274736	-3.287044	0.383984
17	6	0	4.315899	-2.359694	0.520493
18	6	0	4.047424	-1.006598	0.404416
19	6	0	2.745075	-0.529517	0.141903
20	6	0	1.113212	1.342575	-0.148495
21	6	0	2.465211	0.892426	-0.065126
22	6	0	3.505795	1.825687	-0.249258
23	6	0	3.253654	3.155636	-0.543563
24	6	0	1.930637	3.584723	-0.707323
25	6	0	0.889250	2.692033	-0.522120

26	1	0	-5.278165	-2.679001	-0.822580
27	1	0	-2.907651	-3.400111	-0.958612
28	1	0	-5.841687	-0.380660	-0.082161
29	1	0	-0.951743	2.723761	1.158768
30	1	0	-3.294469	3.379572	1.415591
31	1	0	-5.124694	1.843963	0.736442
32	1	0	-0.541756	-2.931566	-0.560548
33	1	0	1.187486	-3.573572	0.099025
34	1	0	3.470550	-4.351356	0.481100
35	1	0	5.328330	-2.696277	0.726067
36	1	0	4.862099	-0.303319	0.535410
37	1	0	4.536929	1.494692	-0.200708
38	1	0	4.079872	3.846443	-0.687004
39	1	0	1.717220	4.607823	-1.004809
40	1	0	-0.121184	3.024362	-0.721597

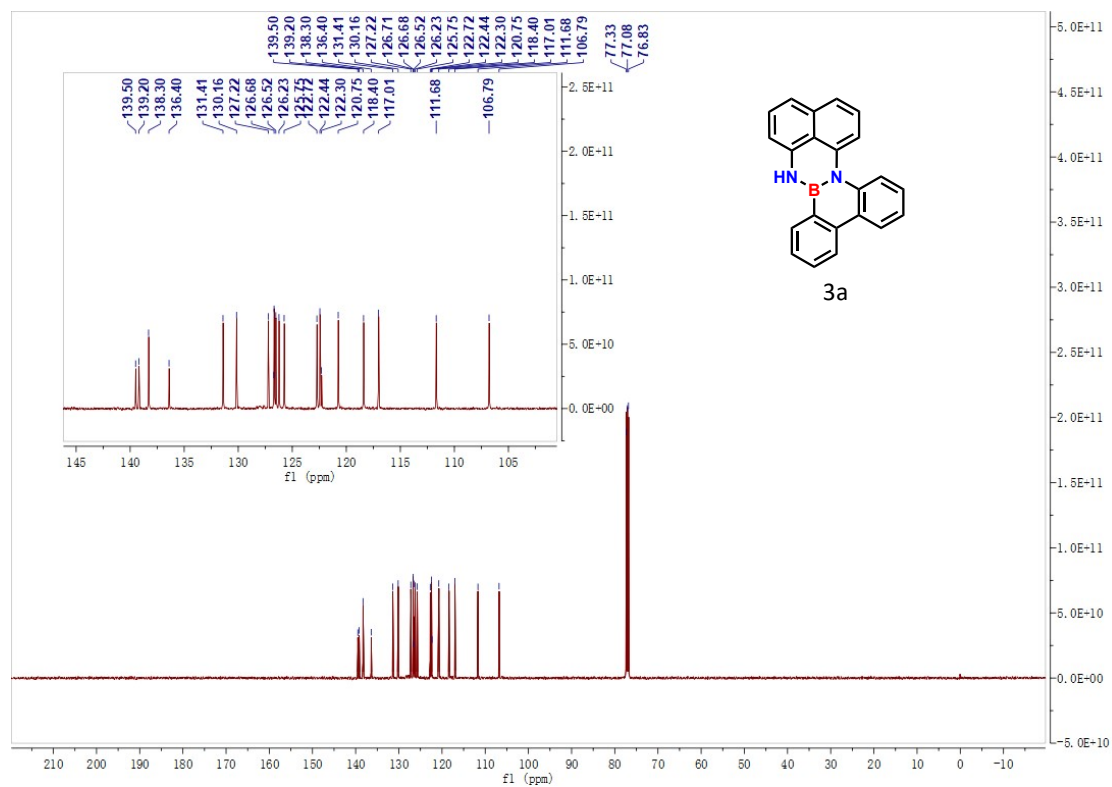
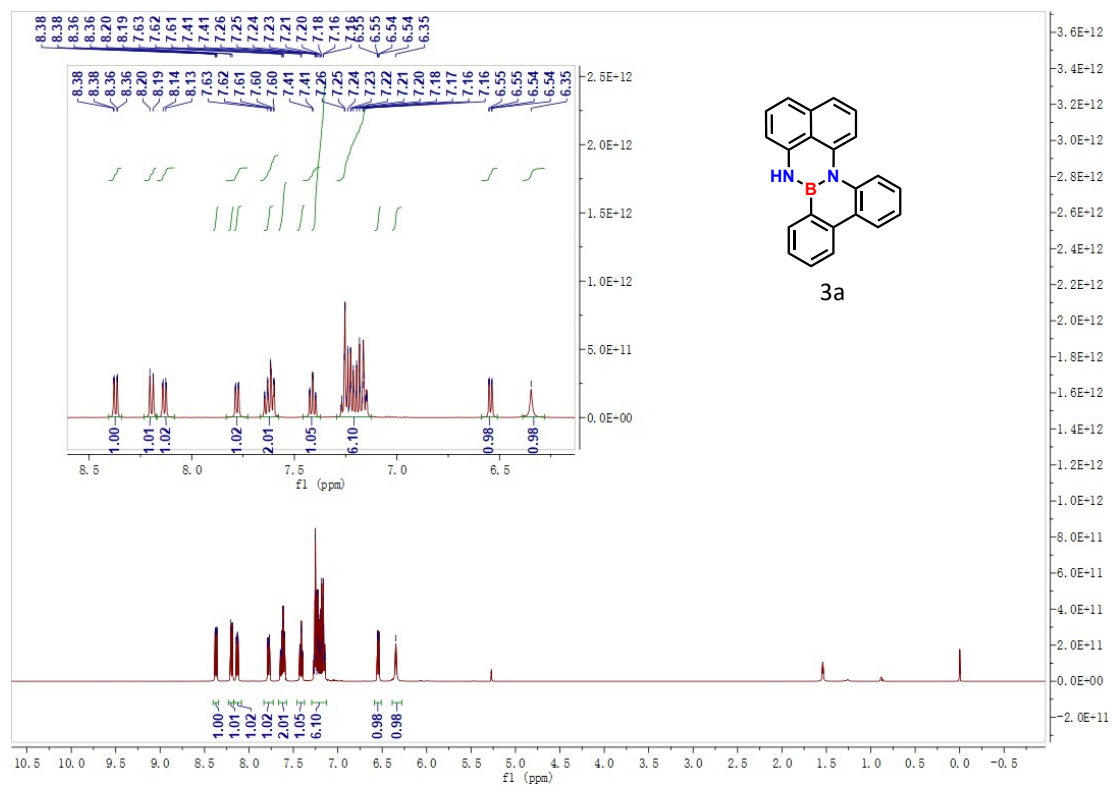
Table S6. The amount of transferred charge (χ) and the overlap (φ_s) between the hole and electron states for the first electronic transitions of the four models.

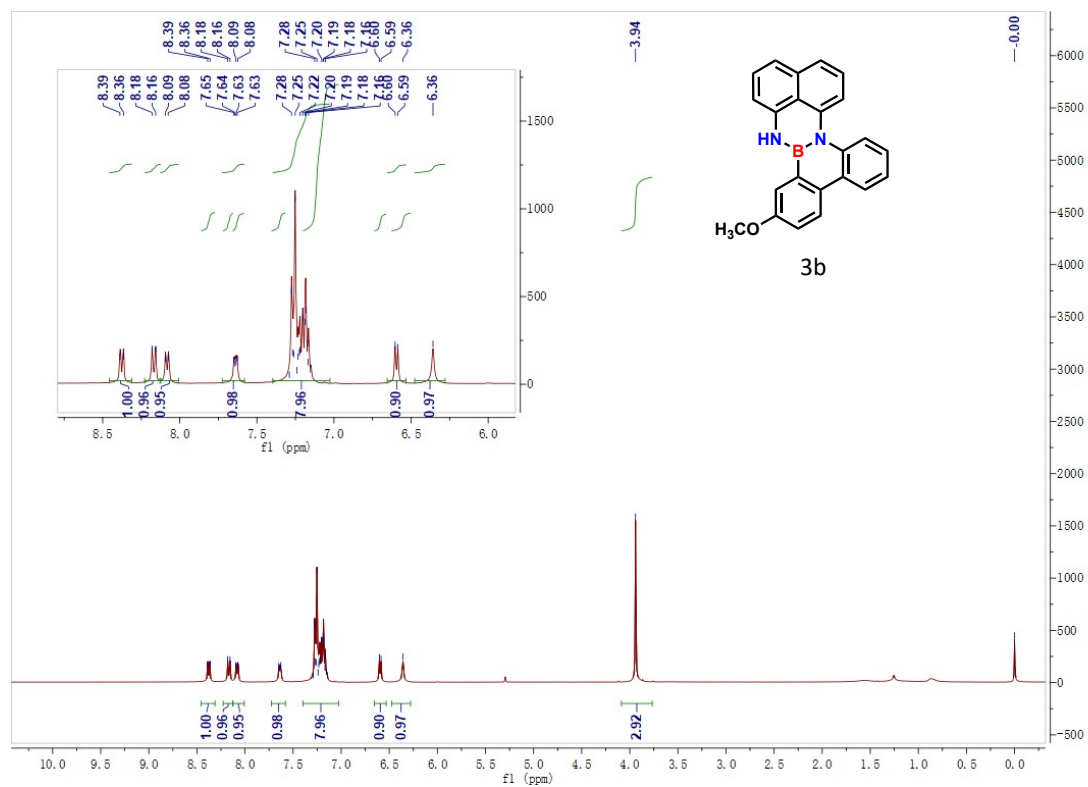
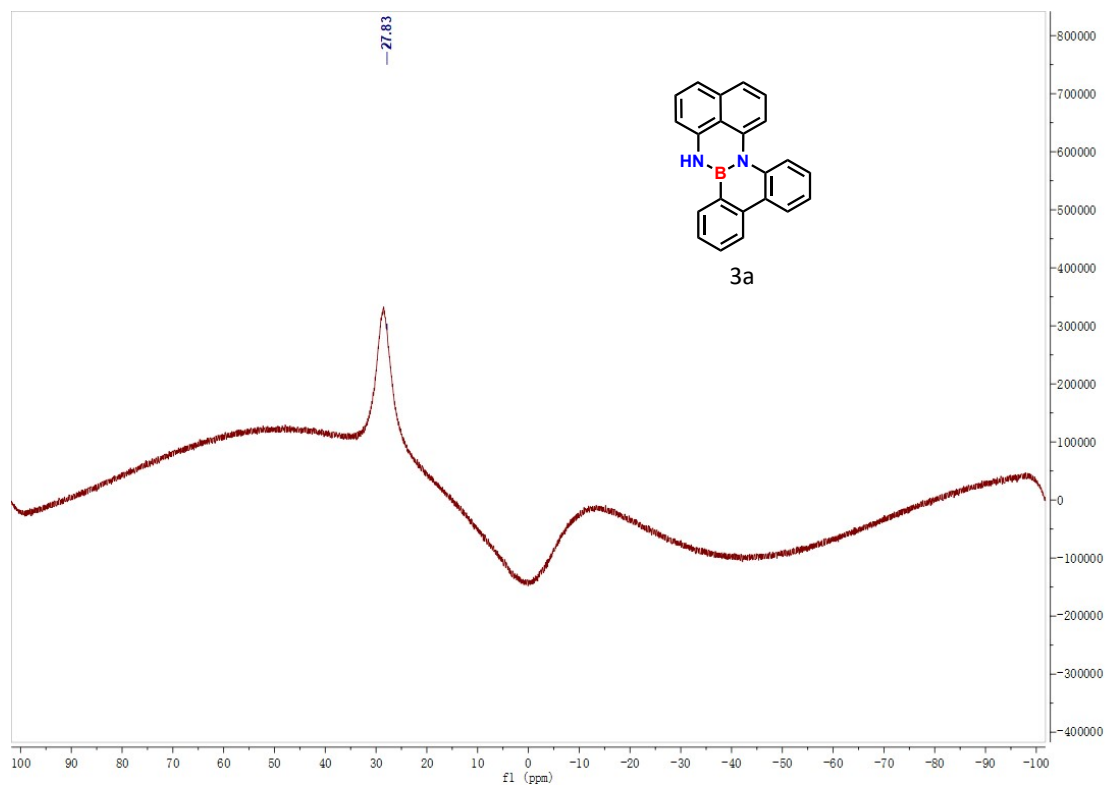
\leftarrow	(a) π - π stacking (dimer) \leftarrow	(b) hydrogen-bonding (dimer) \leftarrow
χ^{\leftarrow}	0.97392 \leftarrow	— \leftarrow
φ_s^{\leftarrow}	0.02773 \leftarrow	— \leftarrow
Geometry \leftarrow		The dimer hydrogen bond configuration could not be obtained \leftarrow
Binding Energy \leftarrow	-20.85 kcal/mol \leftarrow	— \leftarrow

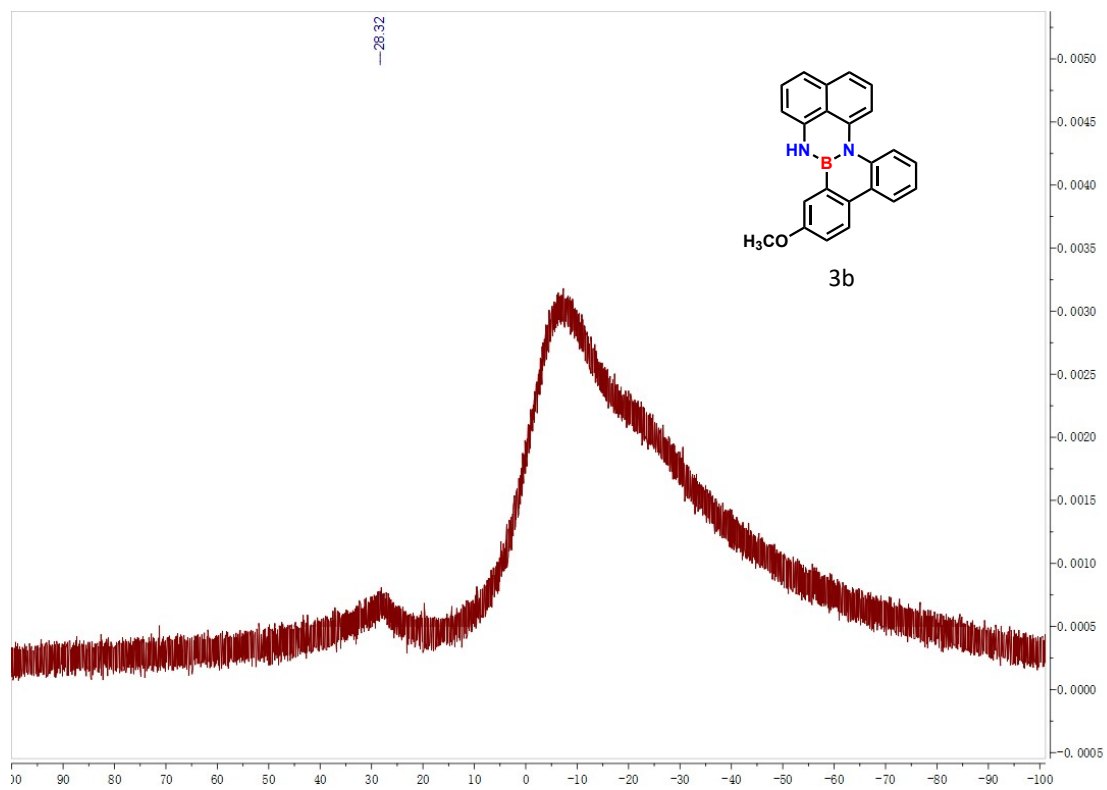
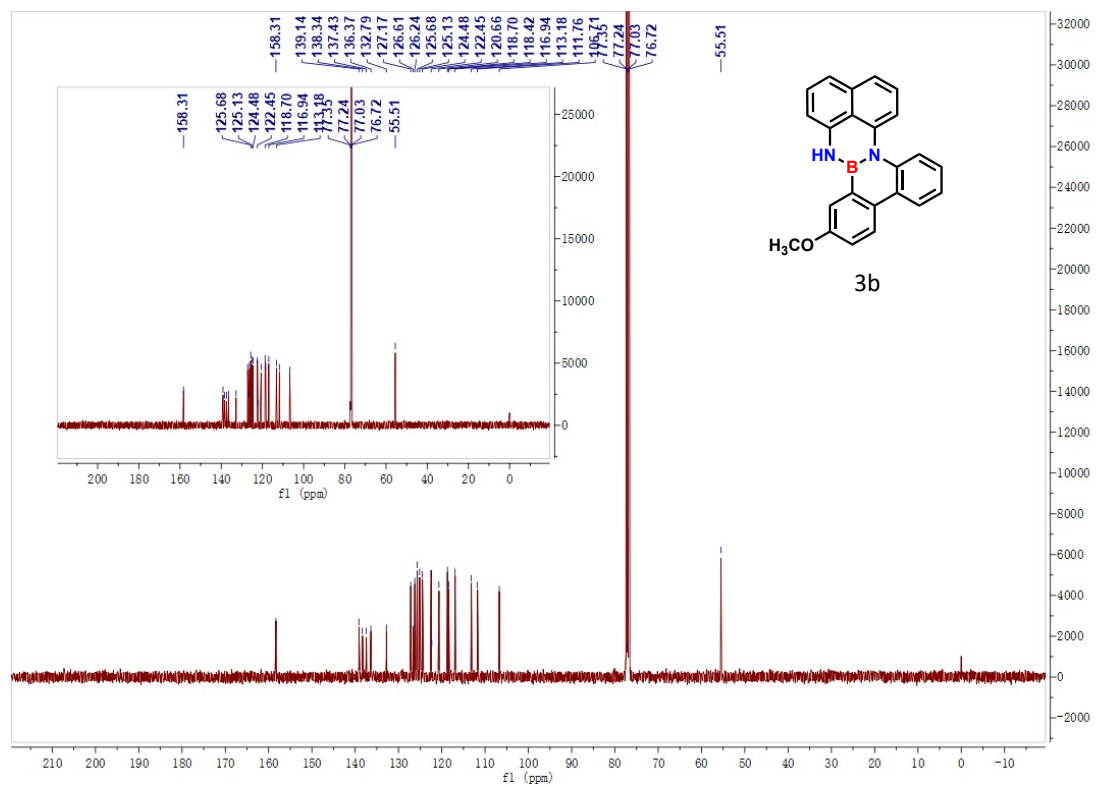
	(a) π - π stacking (trimer)	(b) hydrogen-bonding (trimer)
χ	0.95129	0.98625
φ_s	0.02853	0.00833
Geometry		
Binding Energy	-42.59 kcal/mol	-31.15 kcal/mol

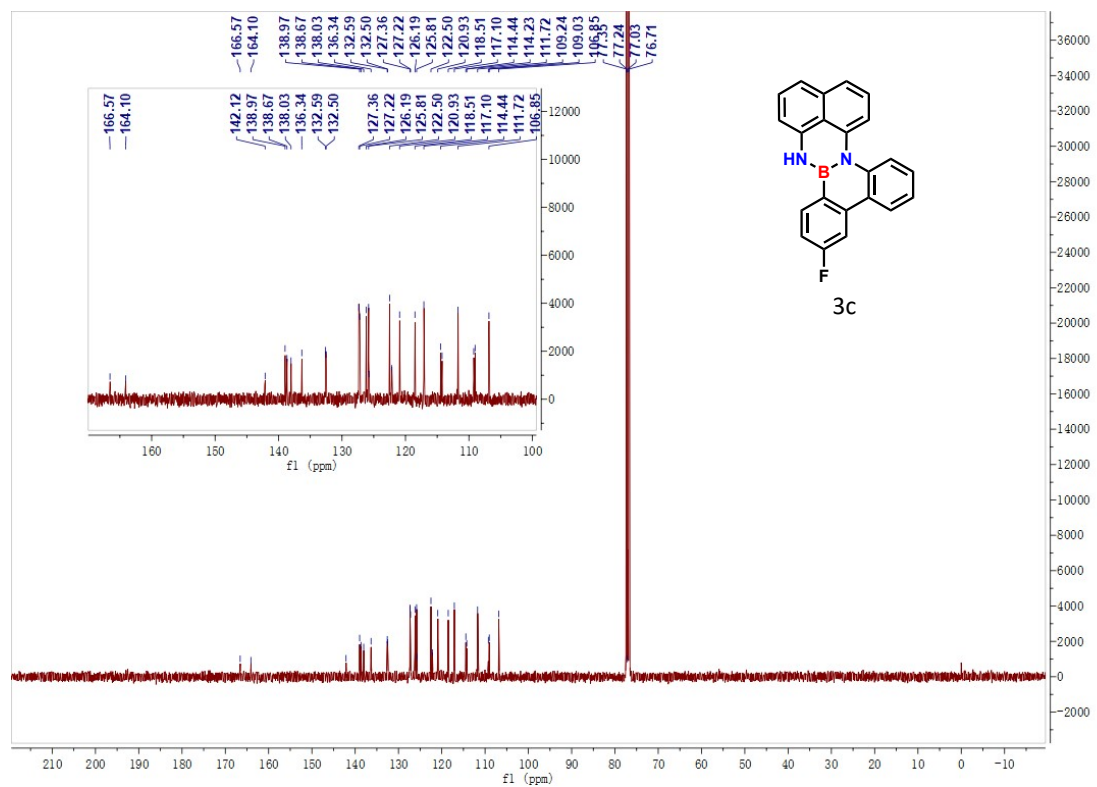
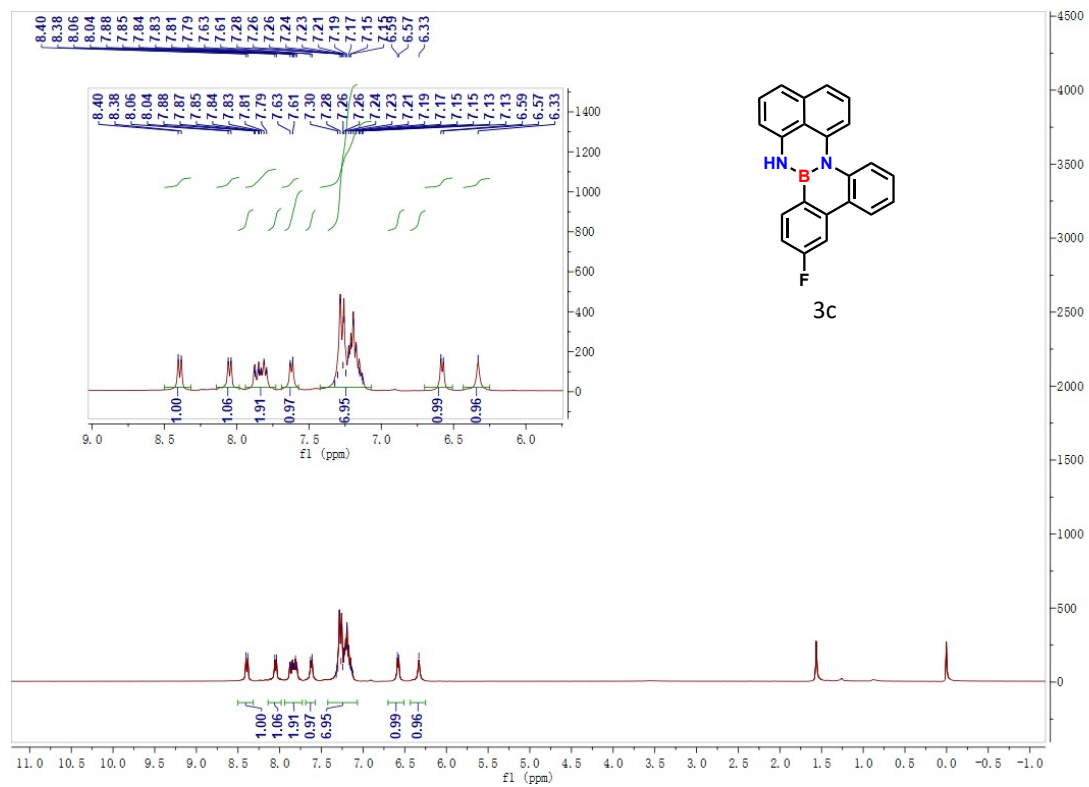
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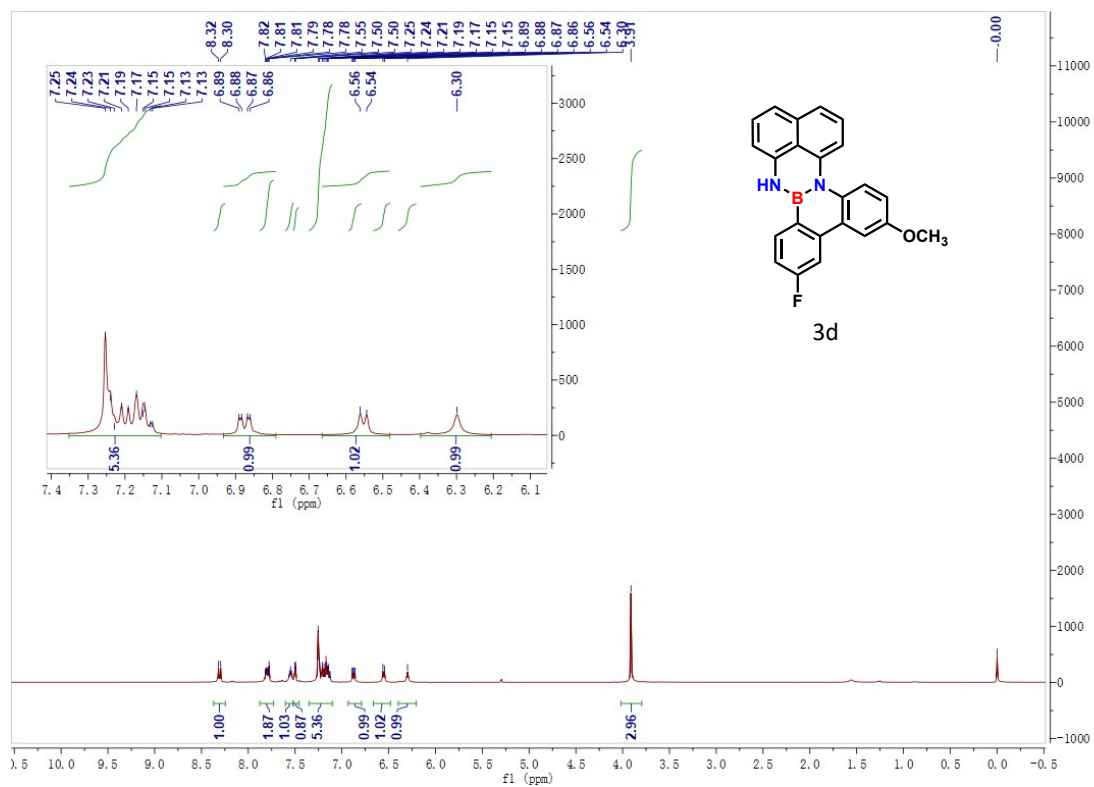
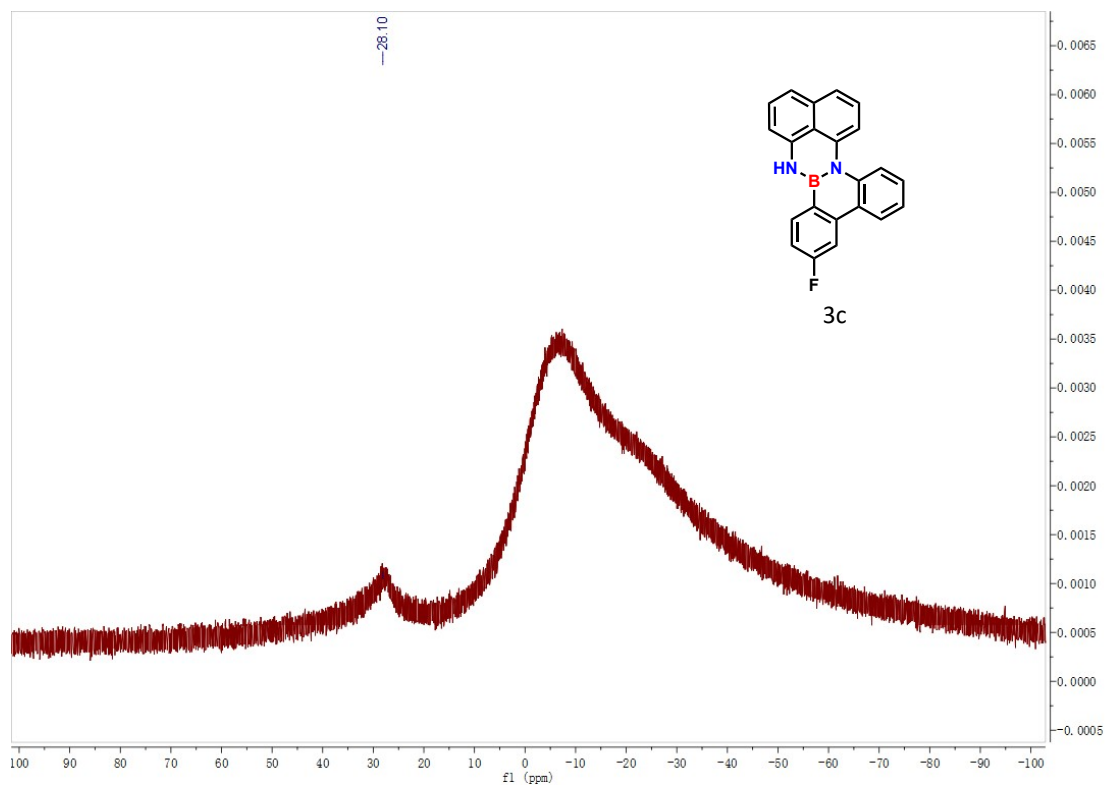
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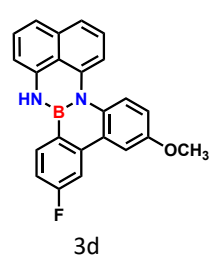
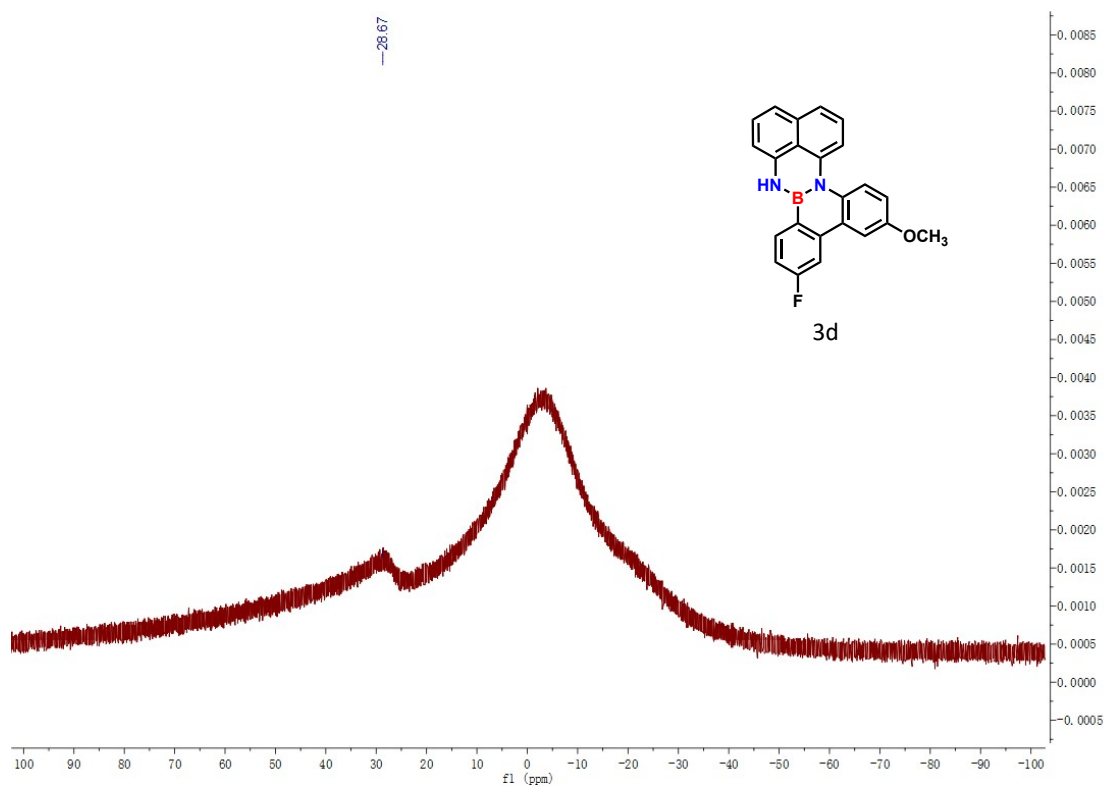
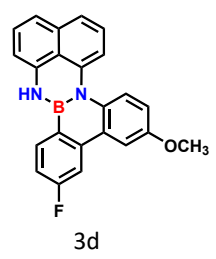
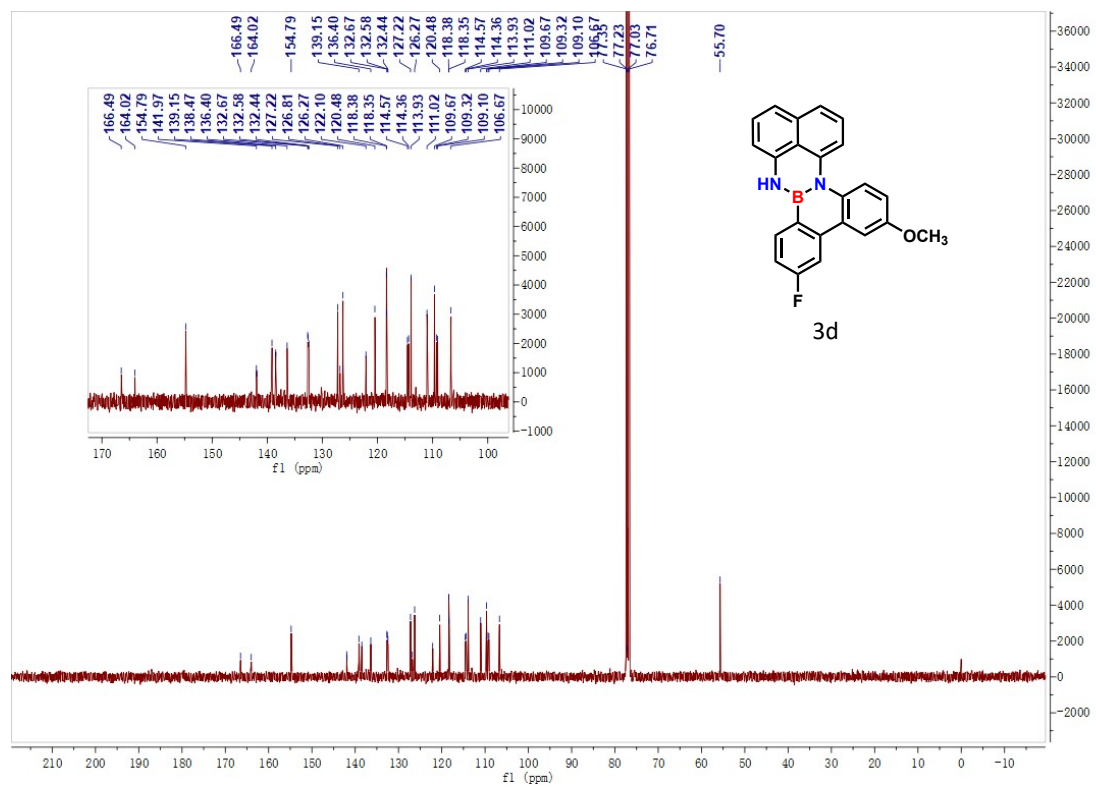


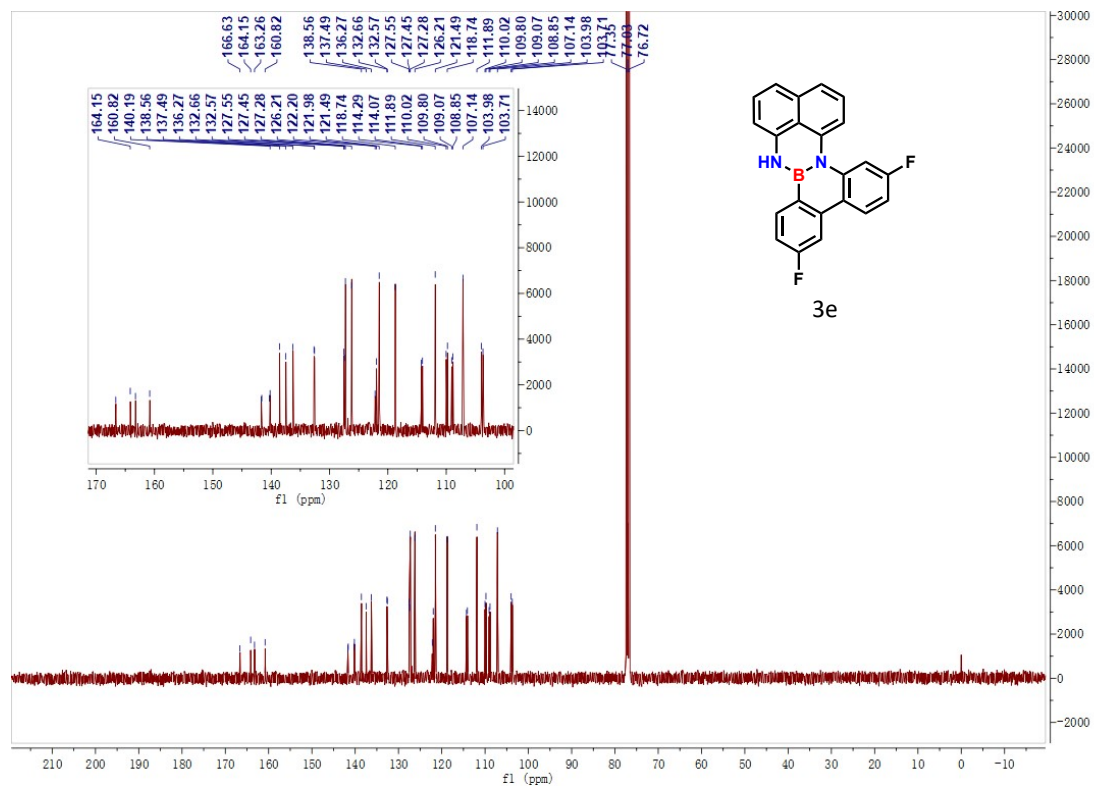
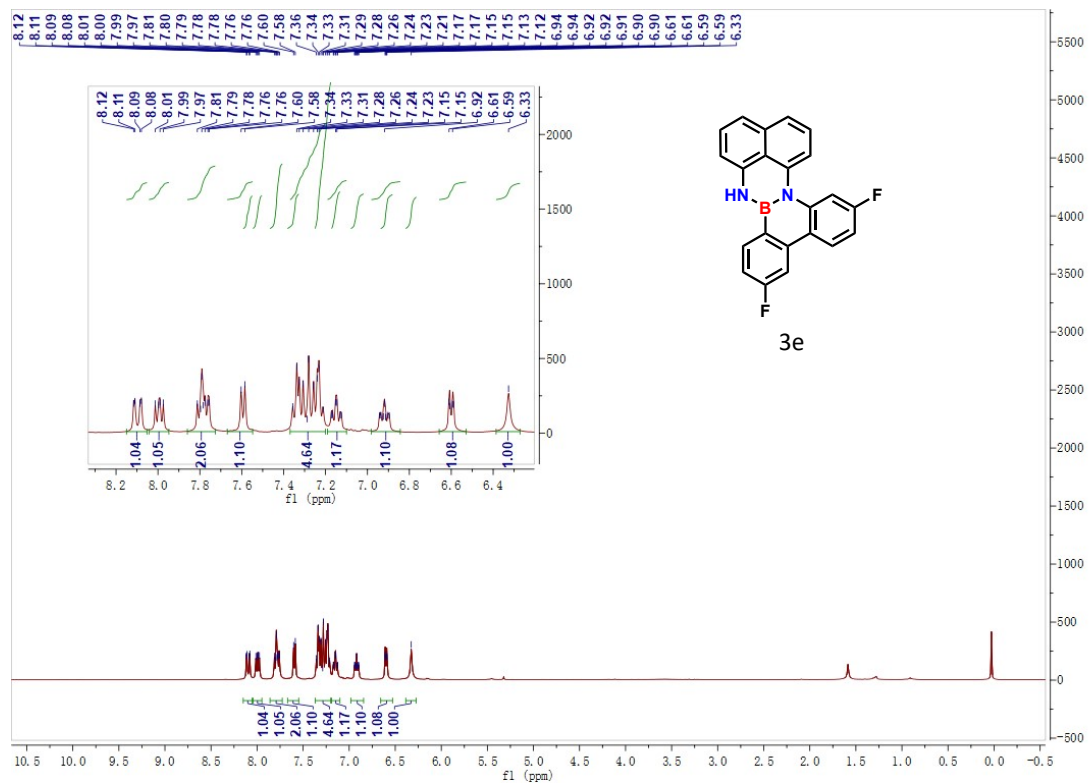


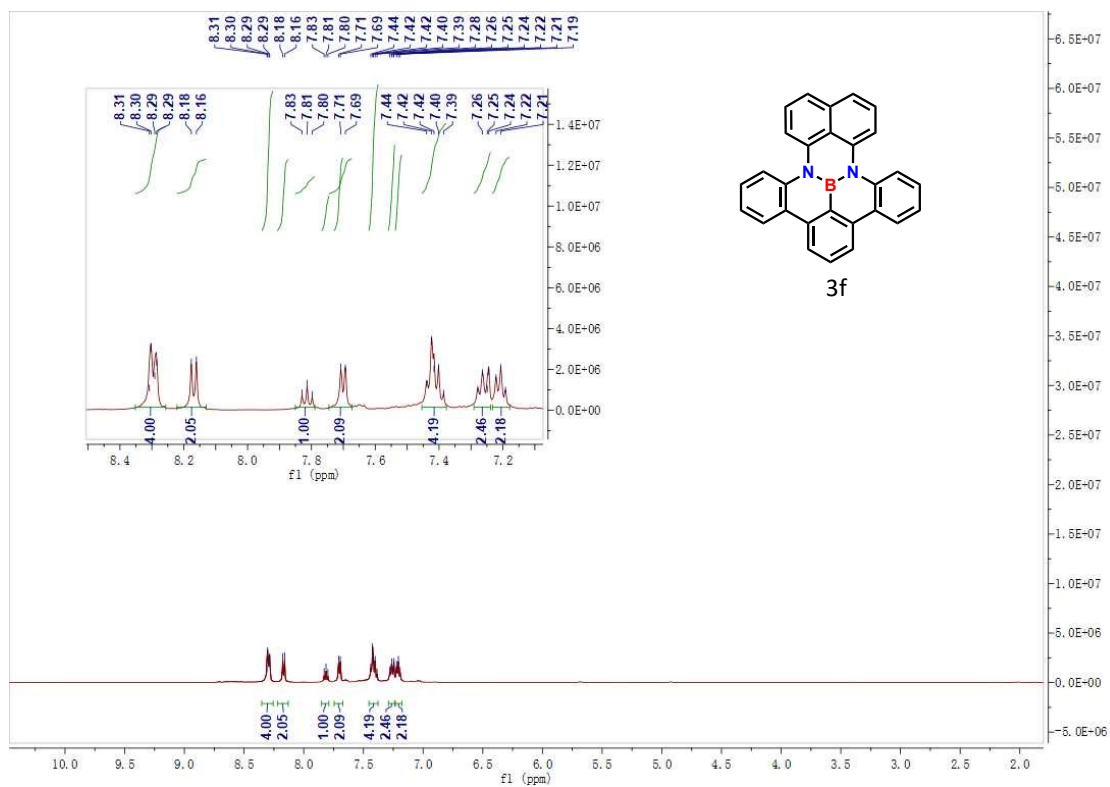
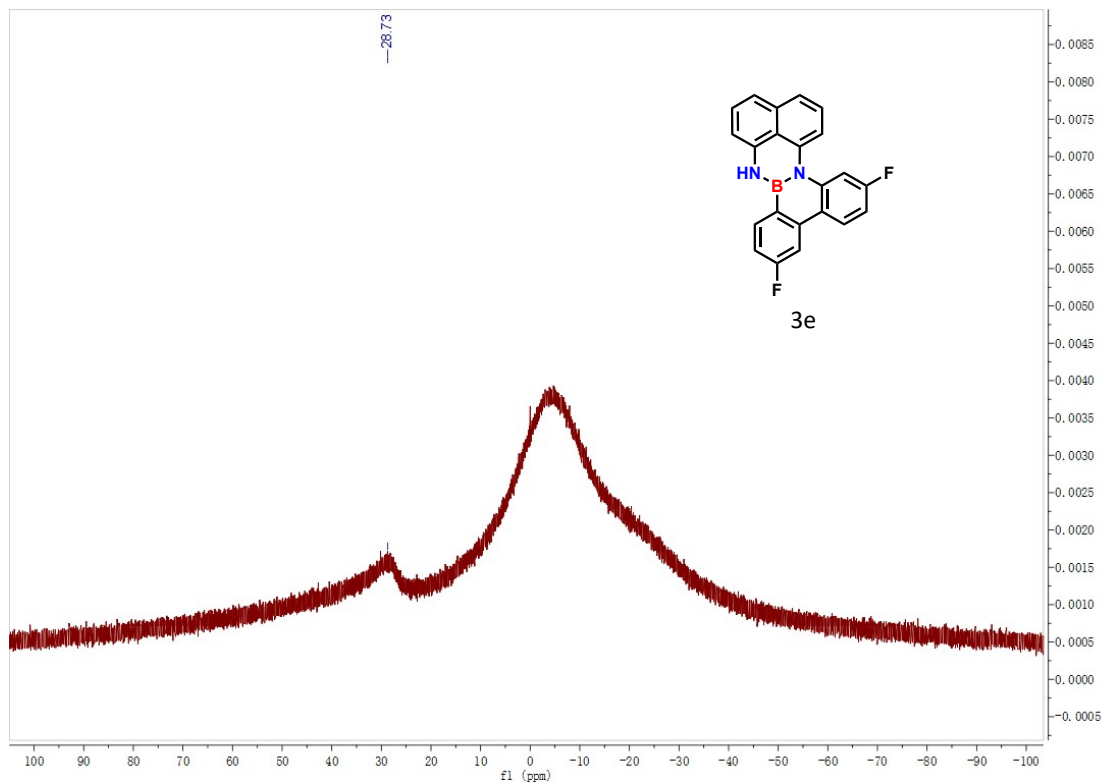


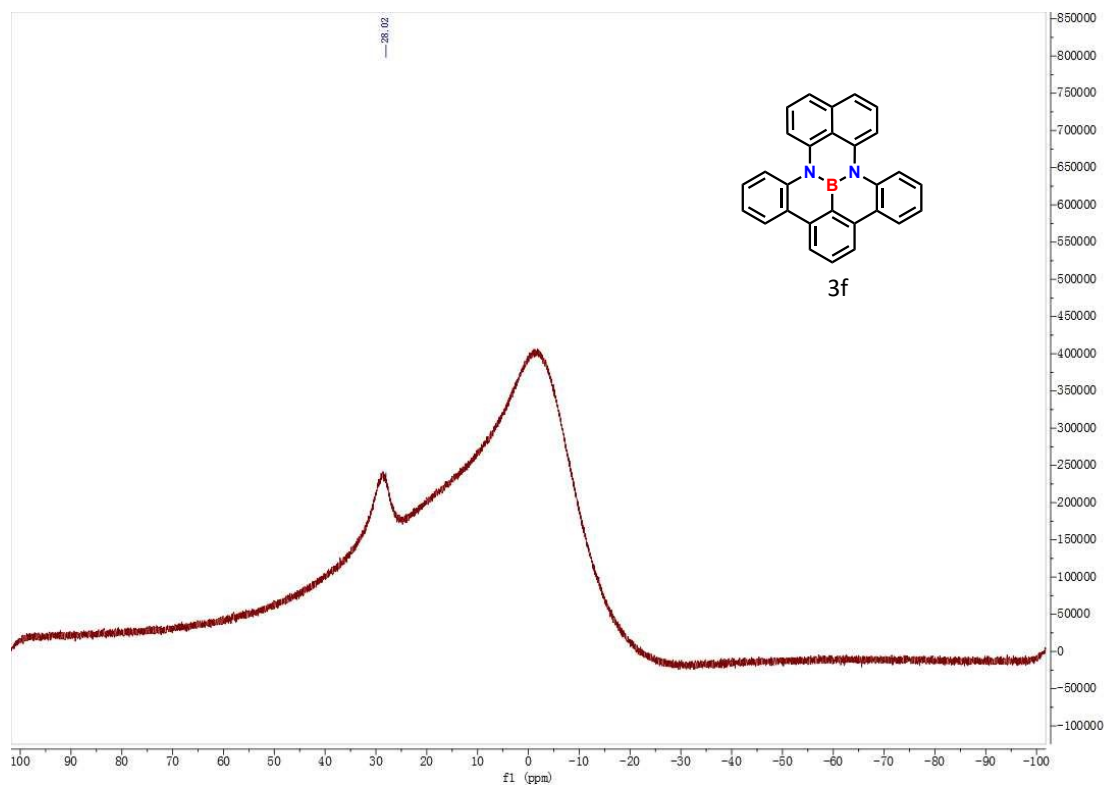
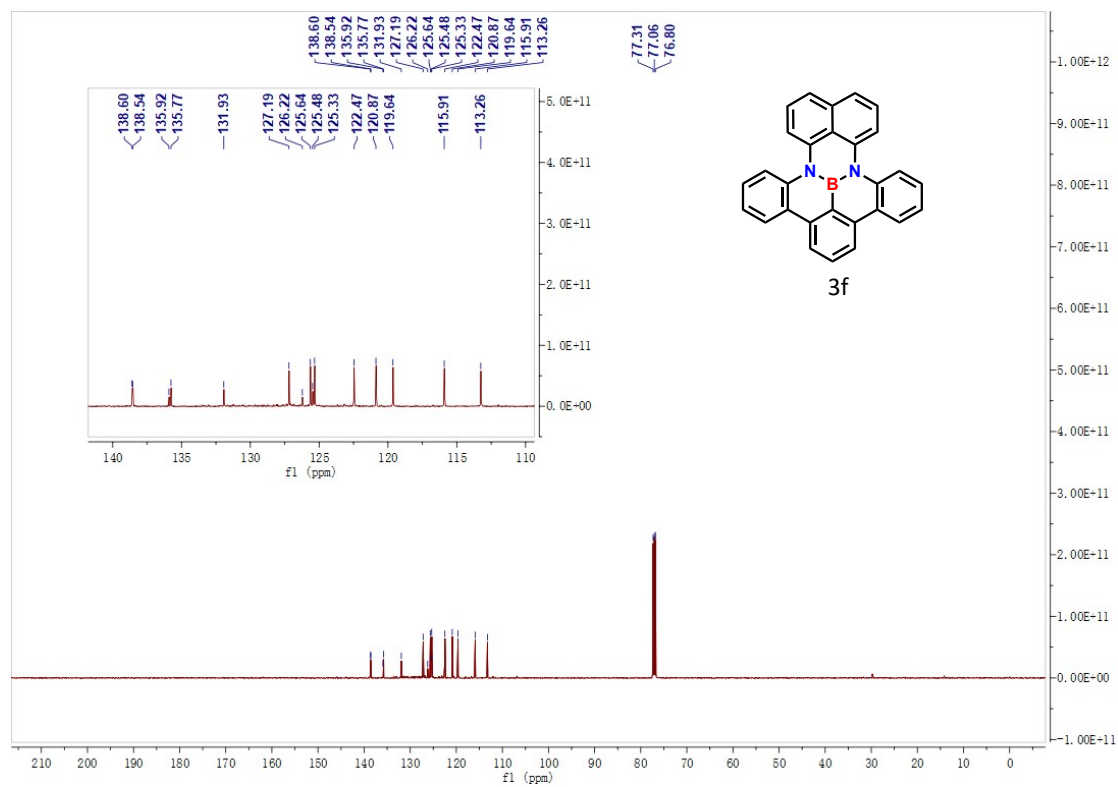












Scanned mass spectrum for the New Compounds

