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Supplementary Information

Aza boron-pyridyl-isoindoline analogues: synthesis and photophysical properties

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I. Experimental section

II. Supplementary Figure

I. Experimental Section

I.1 Materials and instrumentations

All reagents were obtained from commercial suppliers and used without further purification unless otherwise indicated. All air and moisture-sensitive reactions were carried out under nitrogen atmosphere in oven-dried glassware. Glassware was dried in an oven at 120 °C and cooled under a stream of inert gas before use. Both dichloromethane and triethylamine were distilled over calcium hydride and toluene was distilled over sodium. ^{1}H NMR spectra were recorded on a Bruker DRX400 spectrometer, and referenced to the residual proton signals of deuterated solvents. HR-MS were recorded on a Bruker Daltonics microTOF-Q II spectrometer. All the solvents employed for the spectroscopic measurements were of UV spectroscopic grade (Aldrich).

II. Supplementary Figure

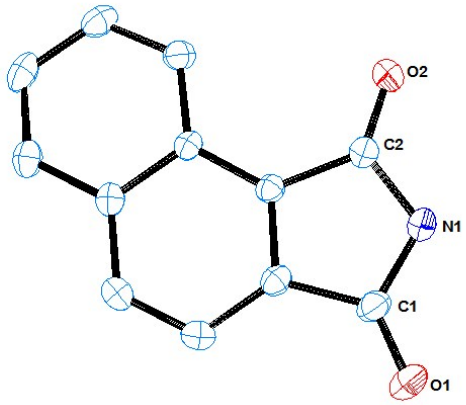


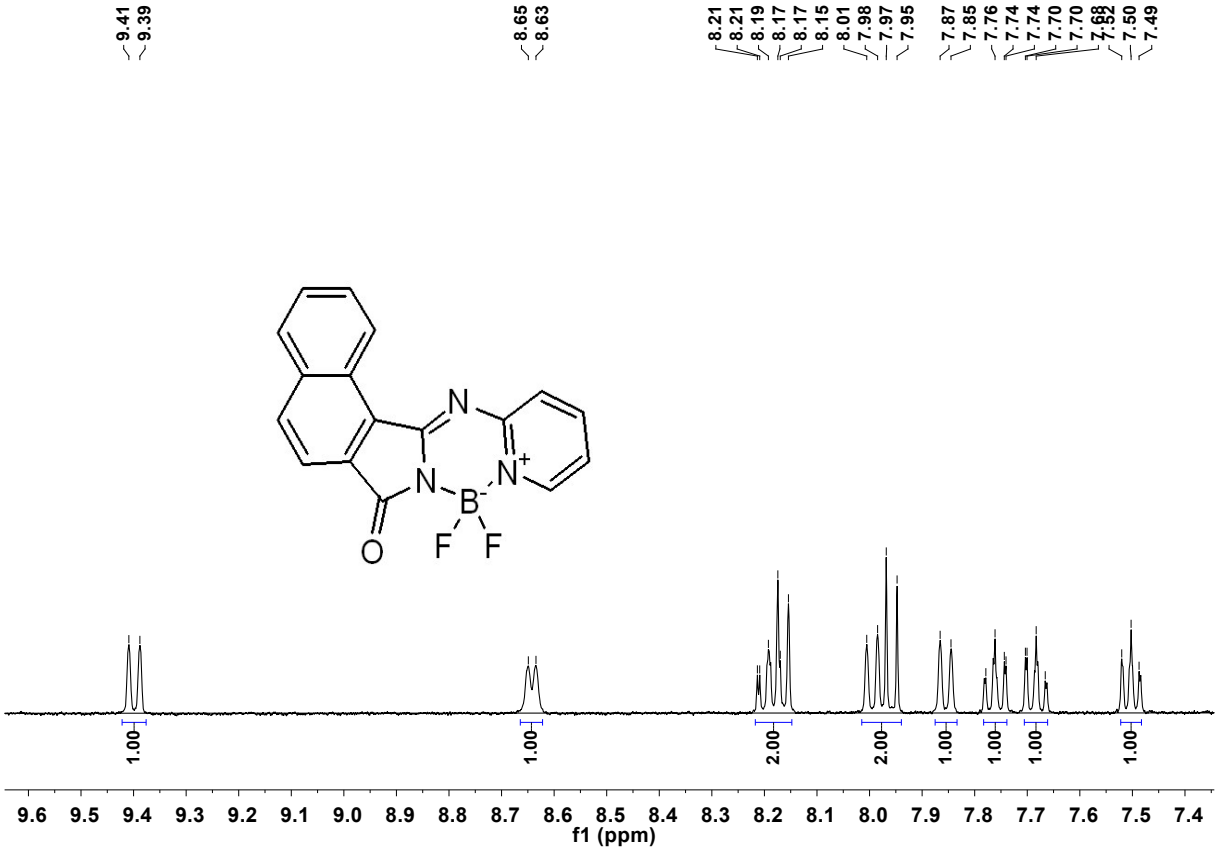
Fig. S1 Front views of the molecular structures of **d** with the thermal ellipsoids set at 50% probability. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å], for 1: C1–N1 1.386(3), C2–N1 1.375(3), O1–C1 1.202 (3), O2–C2 1.215 (3).

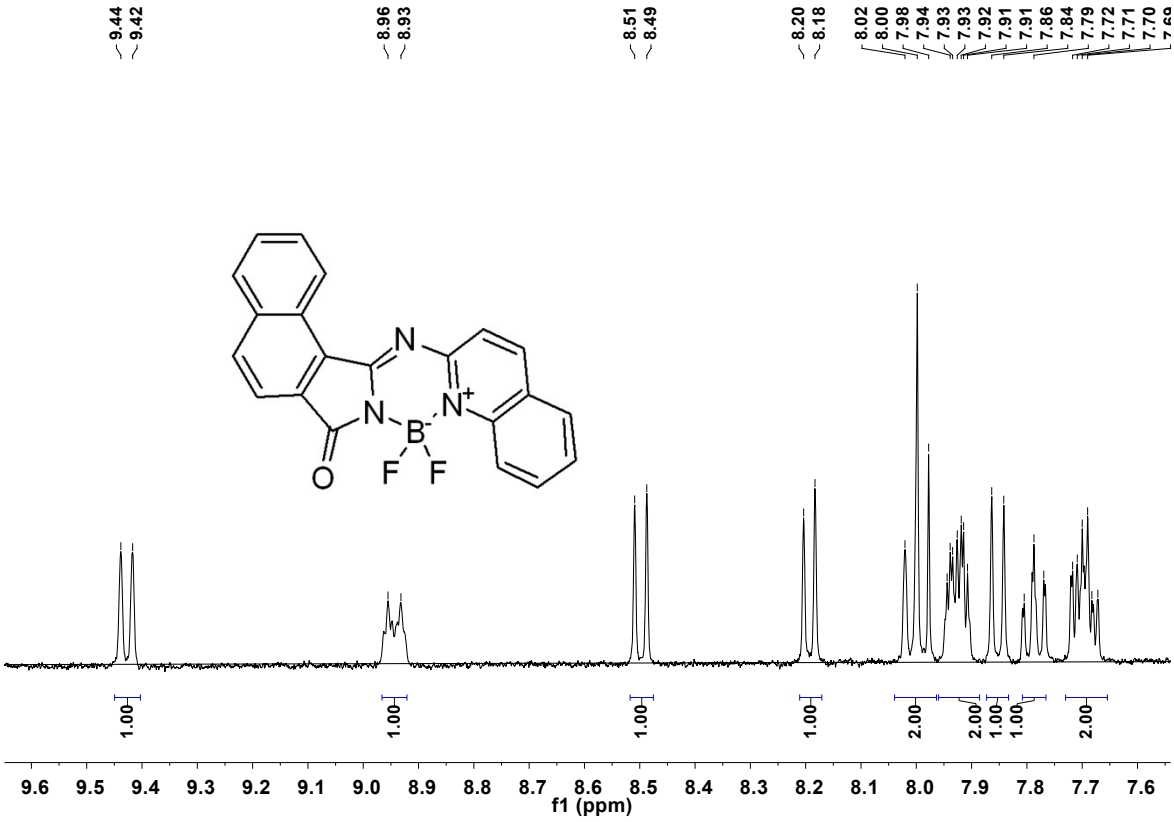
Table S1. Details of the TD-DFT calculations carried out for B3LYP optimized geometries of the **aza-BDY**, **1_noNP** and **1_Bz** model complexes and **1-4** in CH_2Cl_2 at the CAM-B3LYP level of theory.

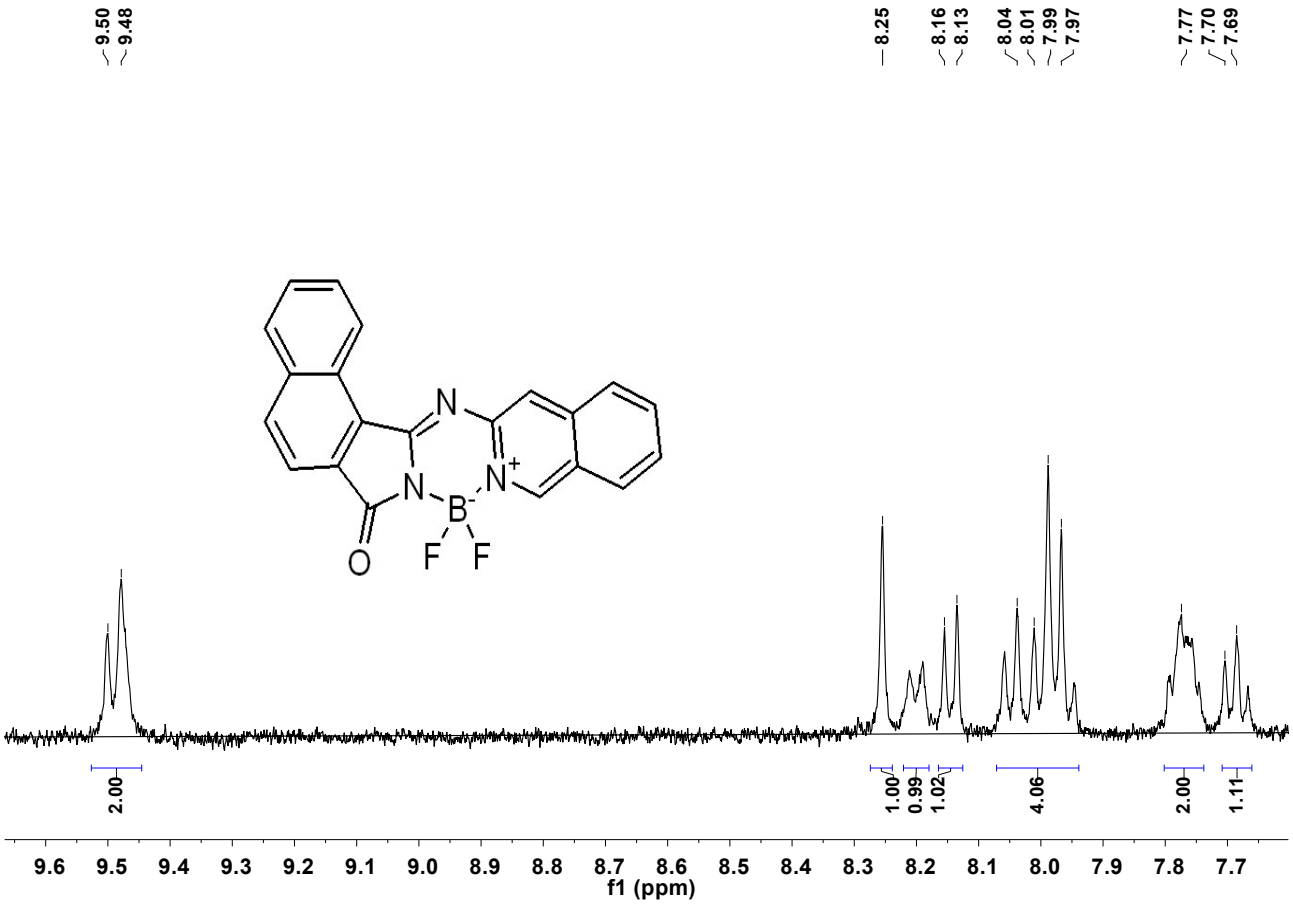
# [a]	E [b] [eV]	$\lambda_{(calc)}$ [nm]	f [c]	$\lambda_{(obs)}$ [nm]	Wavefunction = [d]
			aza-BDY		
S_1	2.71	458	0.56	–––	**96% H → L; ...**
S_2	3.64	341	0.15	–––	95% H−1 → L; ...
S_3	3.86	321	0.05	–––	99% H−2 → L; ....
S_4	3.88	320	0.00	–––	98% H−3 → L ; ...
			1_noNP		
S_1	3.81	325	0.00	–––	90% H−1 → L; ...
S_2	3.84	323	0.46	–––	**85% H → L;**...
S_3	4.44	279	0.16	–––	84% H−2 →L; ...
S_4	4.73	262	0.00	–––	92% H−3 → L; ...
			1_Bz		
S_1	3.92	316	0.68	361[e]	**88% H → L;** ...
S_2	4.11	302	0.00	–––	85% H−3 → L; ...
S_3	4.30	289	0.08	–––	82% H−1 → L; ...
S_4	4.70	264	0.03	–––	70% H−2 → L; ...
			1		
S_1	3.39	367	0.16	396	89% H → L; ...
S_2	3.79	327	0.52	378	**85% H−1 → L;** ...
S_3	3.97	312	0.00	–––	87% H−3 → L; ...
S_4	4.20	295	0.12	–––	66% H−2 → L; 19% H → L+3; ...
			2		
S_1	3.30	376	0.25	423	88% H → L; ...
S_2	3.57	347	0.62	402	8**4% H−1 → L;** ...
S_3	3.90	318	0.00	–––	85% H−4 → L; ...
S_4	4.10	302	0.04	–––	67% H−3 → L; ...
			3		
S_1	3.45	359	0.62	430	82% H → L; ...
S_2	3.59	345	0.23	407	**71% H−1 → L;** ...
S_3	3.93	315	0.18	–––	52% H → L+1; 23% H−1 → L+1; ...
S_4	4.05	306	0.00	–––	86% H−4→ L; ...
			4		
S_1	3.28	379	0.31	437	85% H → L; ...
S_2	3.51	353	0.37	415	**74% H−1→ L;** ...
S_3	3.89	319	0.00	–––	86% H−4→ L; ...
S_4	4.06	305	0.03	–––	71% H−2→ L; ...

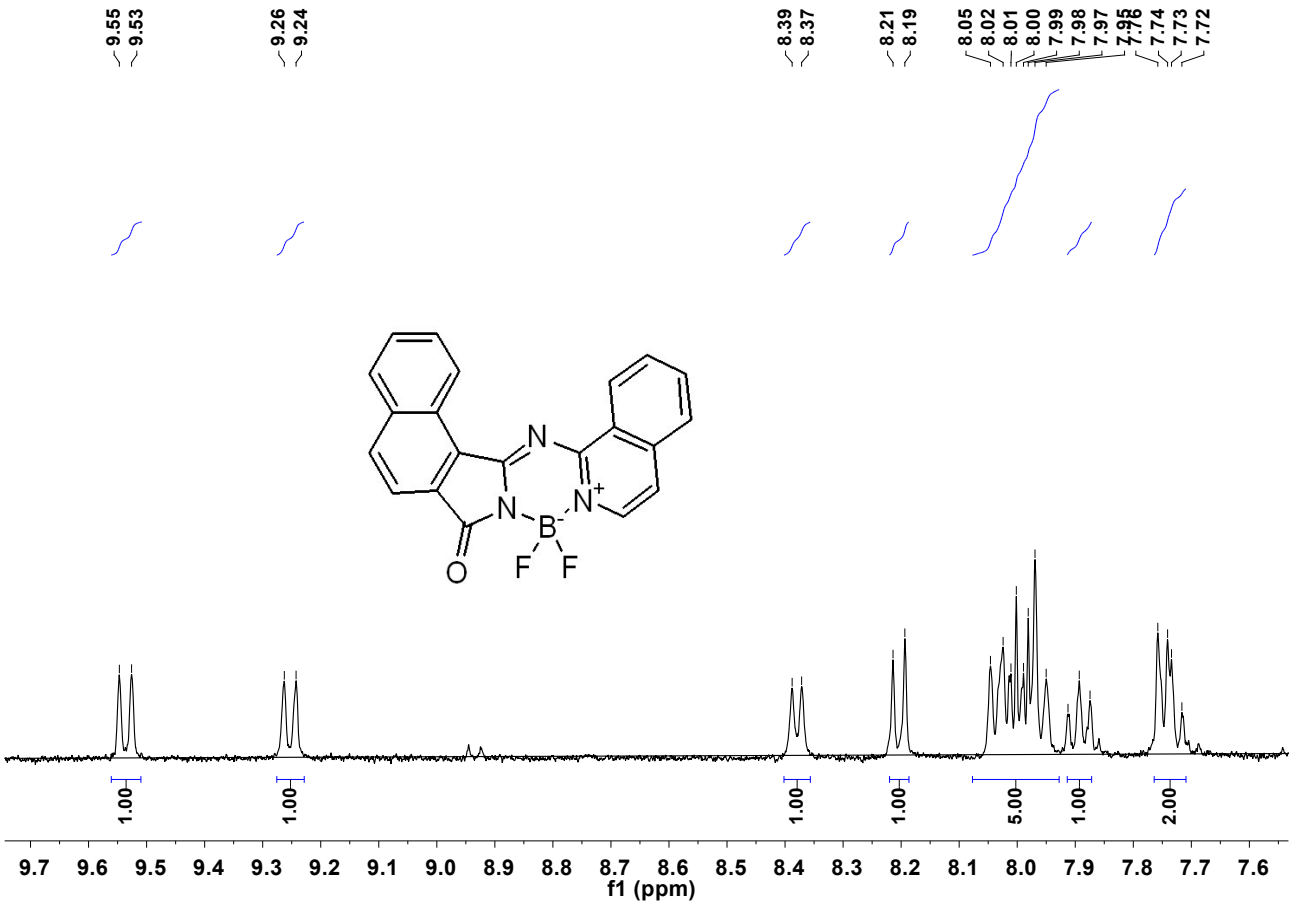
[a] Excited state, [b] Energy of excited state, [c] Oscillator strength, [d] One-electron transitions between MOs derived from the HOMO and LUMO of the **aza-BDY** model complex are highlighted in bold. Only one-electron transitions that provide a contribution of greater than 10% are included. H and L denote the HOMO and LUMO, respectively, [e] experimental value is from reference 5(a).

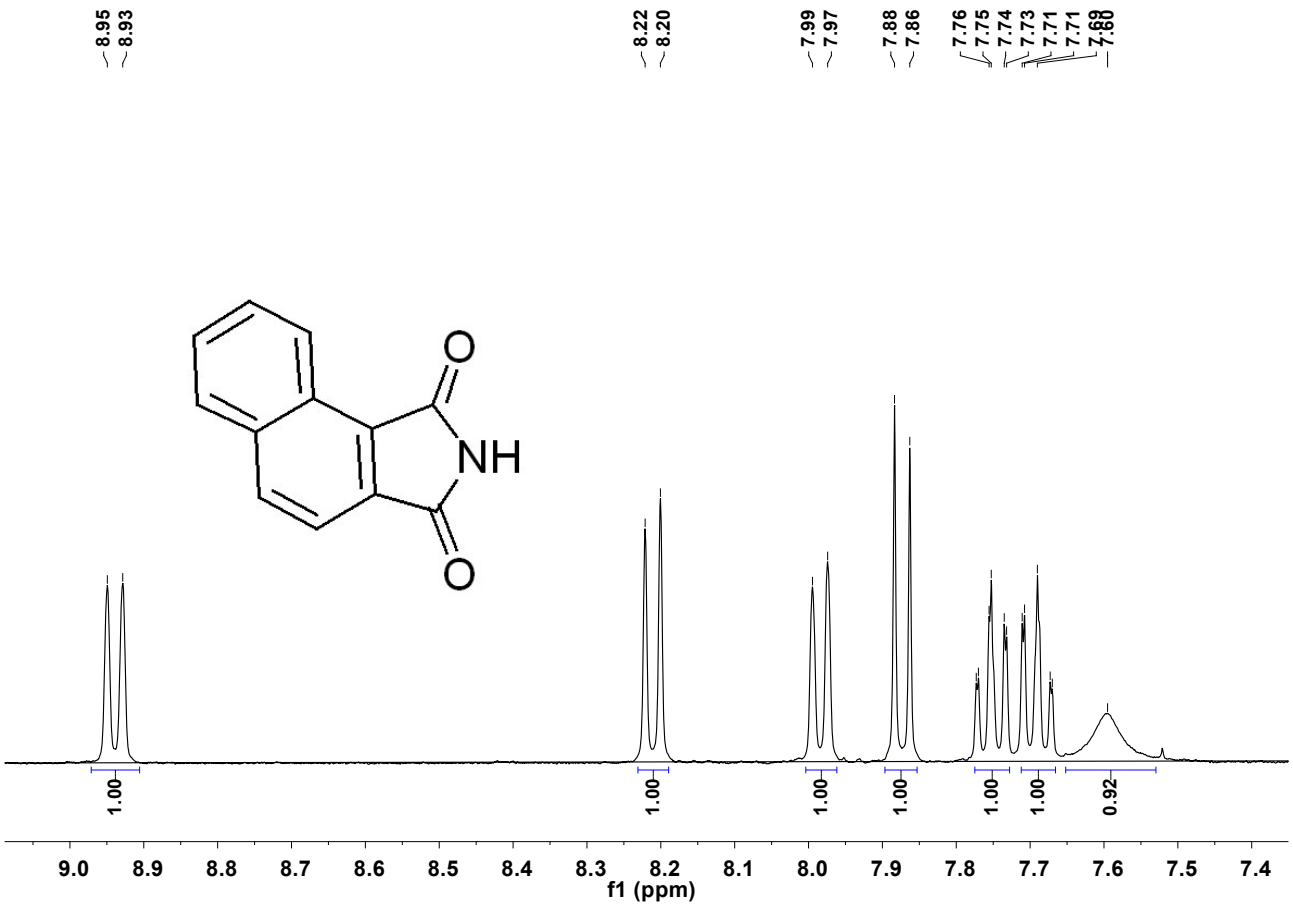
III. ^{1}H NMR Spectroscopy






9.50
9.48
8.25
8.16
8.13
8.04
8.01
7.99
7.97
7.77
7.70
7.69
N
N
N+
B-
O
F
F
2.00
1.00
0.99
1.02
4.06
2.00
1.11
9.6 9.5 9.4 9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7
f1 (ppm)


9.55
9.53
9.26
9.24
8.39
8.37
8.21
8.19
8.05
8.02
8.01
8.00
7.99
7.98
7.97
7.74
7.73
7.72
N
N
N+
B-
O
F
F
1.00
1.00
1.00
1.00
5.00
1.00
2.00
9.7 9.6 9.5 9.4 9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6
f1 (ppm)


8.95
8.93
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8.20
7.99
7.97
7.88
7.86
7.76
7.75
7.74
7.73
7.71
7.71
7.69
7.68
O
NH
O
1.00
1.00
1.00
1.00
1.00
1.00
0.92
9.0
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
f1 (ppm)