Supporting Information for

The Opposite and Amplifying Effect of B←N Coordination on Photophysical Properties of Regioisomers with an Unsymmetrical Backbone

Chao Zeng, Kang Yuan, Nan Wang, Tai Peng,* Gang Wu, and Suning Wang*

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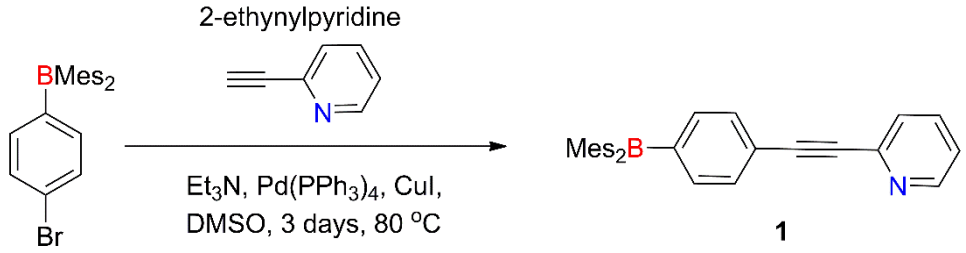
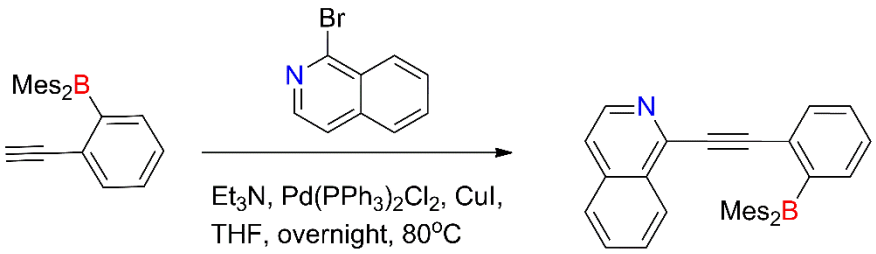
General Procedure: Solvents was freshly distilled over Na or CaH_2 and stored under nitrogen prior to use. Starting materials were purchased from Sun Chemical Technology Co., Ltd. and used without further purification. 2-(2'-(dimesitylboryl)phenylethynyl)pyridine (**2**)[1], (4-bromophenyl)dimesitylborane[2], 2-ethynylpyridine[3], pyrido[1,2-a]isoindole[4], 1-Dimesitylboryl-2-ethynylbenzene[5] were synthesized according to procedures reported in literature. All the reactions were performed under nitrogen and in dry solvent. ^{1}H, ^{13}C and ^{11}B NMR spectra were recorded on a Bruker Ascend 400 or 700 MHz spectrometer. Melting point (m.p.) determination was performed using a SGW X-4A microscopic melting point instrument. UV−vis spectra were obtained on an Agilent Cary 300 UV−vis spectrophotometer. Fluorescence spectra were recorded on an Edinburgh Instruments FLS980 spectrophotometer. High-resolution mass spectra (HRMS) were obtained from an Agilent Q-TOF 6520 LC-MS spectrometer. Fluorescent quantum efficiencies were determined using a Hamamatsu Quantaurus-QY spectrometer (C11347). DFT and TD-DFT calculations were performed using the Gaussian 09 suite of programs[6]. Geometry optimizations of all compounds were obtained at the M062X[7]/6-31g(d)[8]level of theory using Polarizable Continuum Models (PCMs) and the resulting structures were confirmed to be stationary points through vibrational frequency analysis. The Natural Bond Orbital (NBO)[9] analysis were performed at the same level of theory, ^{11}B-NMR of **2a/2a-open** was obtained at the B972[10]/def2TZVP[11] level of theory in $CHCl_3$ using SMD [12]. All the calculations were performed at 298 K. Orbital composition analysis with Ros-Schuit (C- squared Population Analysis, SCPA) method using Multiwfn software version 3.4 [13].

I. Synthetic Procedures for alkyne compounds 1, 3 – 5.



Synthesis of Compound 1: (4-Bromophenyl)dimesitylborane (291 mg, 0.72 mmol), 2-ethynylpyridine (0.42 mL, 0.864 mmol), $Pd_2(PPh_3)_4$ (50 mg, 0.043 mmol) and CuI (7 mg, 0.036 mmol) were added to an oven-dried Schlenk flask, the flask was evacuated and back-filled with N_2 three times, and then degassed DMSO (15.0 mL) and Et_3N (3.0 mL) was injected into the mixture. The resulting solution was stirred at 80 °C for 3 days under the N_2 atmosphere. After being cooled to room temperature, addition of water, the mixture was extracted with CH_2Cl_2. The extract was washed with brine, dried over anhydrous Na_2CO_3, the solvent was then removed under reduced pressure. The crude product was further purified by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1) as eluent to obtain the product **1** as white solid (200 mg, 65% yield).

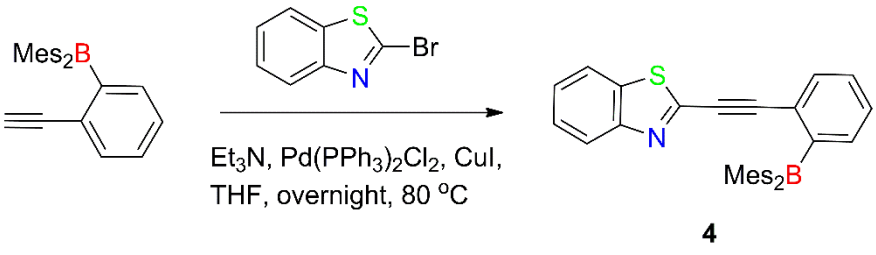
1:^{1}H NMR (400 MHz, $CDCl_3$): δ 8.63 (d, *J* = 4.7 Hz, 1H), 7.68 (td, *J* = 7.7, 1.7 Hz, 1H), 7.59-7.49 (m, 5H), 7.30-7.21 (m, 1H), 6.83 (s, 4H), 2.31 (s, 6H), 2.00 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.07, 146.55, 143.22, 141.40, 140.74, 138.84, 136.08, 135.89, 131.42, 128.19, 127.19, 125.37, 122.82, 90.37, 89.33, 23.36, 21.16. HR-ESIMS (m/z): $[M+H]^+$ calcd. for $C_{31}H_{31}BN$, 428.2550; found: 428.2558.



3

Synthesis of Compound 3: 1-Dimesitylboryl-2-ethynylbenzene (699 mg, 2.00 mmol), 1-bromoisoquinoline (479 mg, 2.30 mmol), $Pd(PPh_3)_2Cl_2$ (85 mg, 0.12 mmol) and CuI (19 mg, 0.10 mmol) were added to an oven-dried Schlenk flask, the flask was evacuated and back-filled with N_2 three times, and then THF (30.0 mL) and Et_3N (0.4 mL) was injected into the mixture. The resulting solution was stirred at 80 °C overnight under the N_2 atmosphere. After being cooled to room temperature, the solvent was then removed under reduced pressure. The crude product was further purified by column chromatography on silica gel using petroleum ether/ethyl acetate (20:1) as eluent to obtain the product **3** as yellow solid (600 mg, 63% yield).

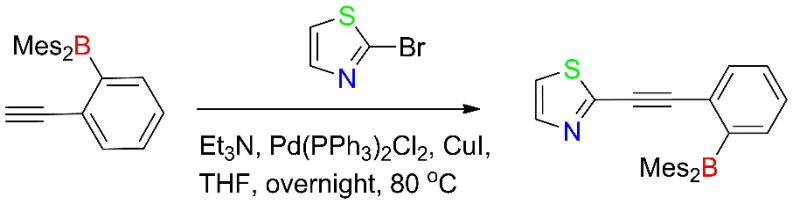
3:^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46 (d, J = 5.7 Hz, 1H), 7.76 (m, 1H), 7.72 (m, 1H), 7.69-7.62 (m, 2H), 7.55 (d, J = 5.7 Hz, 1H), 7.50 -7.41 (m, 2H), 7.35 (m, 2H), 6.61 (s, 4H), 2.02 (m, 18H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 150.58, 144.53, 142.57, 140.78, 139.10, 135.44, 134.31, 133.36, 130.18, 128.78, 128.56, 128.22, 127.55, 127.17, 126.27, 125.98, 120.01, 94.23, 89.62, 23.21, 21.05. HR-ESIMS (m/z): $[M+H]^+$ calcd. for $C_{35}H_{33}BN$, 478.2706; found: 478.2687.



4

Synthesis of Compound 4: 1-Dimesitylboryl-2-ethynylbenzene (500 mg, 1.43 mmol), 2-Bromobenzothiazole (367 mg, 1.72 mmol), $Pd(PPh_3)_2Cl_2$ (55 mg, 0.078 mmol) and CuI (14 mg, 0.073 mmol) were added to an oven-dried Schlenk flask, the flask was evacuated and back-filled with N_2 three times, and then THF (22.5 mL) and Et_3N (0.3 mL) was injected into the flask. The resulting solution was stirred at 80 °C overnight under the N_2 atmosphere. After being cooled to room temperature, the solvent was removed in *vacuo*. The crude product was further purified by column chromatography on silica gel using petroleum ether/ethyl acetate (50:1) as eluent to obtain the product **4** as yellow solid (502 mg, 75% yield).

4: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (d, J = 8.1 Hz, 1H), 7.82 (d, J = 7.9 Hz, 1H), 7.69 (d, J = 7.6 Hz, 1H), 7.51-7.38 (m, 3H), 7.36 (m, 2H), 6.78 (s, 4H), 2.24 (s, 6H), 2.04 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$): δ 152.85, 151.07, 148.83, 142.45, 140.77, 139.34, 135.60, 134.52, 133.80, 130.40, 129.30, 128.53, 126.40, 125.85, 124.96, 123.36, 121.09, 96.16, 85.40, 23.23, 21.28. HR-ESIMS (m/z): $[M+H]^+$ calcd. for $C_{33}H_{31}BNS$, 484.2270; found: 484.2251



5

Synthesis of Compound 5: 1-Dimesitylboryl-2-ethynylbenzene (508 mg, 1.45 mmol), 2-bromothiazole (287 mg, 1.75 mmol), $Pd(PPh_3)_2Cl_2$ (61 mg, 0.087 mmol) and CuI (14 mg, 0.073 mmol) were added to an oven-dried Schlenk flask, the flask was evacuated and back-filled with N_2 three times, and then THF (22.5 mL) and Et_3N (0.3 mL) was injected into the flask. The resulting solution was stirred at 80 °C overnight under the N_2 atmosphere. After being cooled to room temperature, the solvent was removed in *vacuo*. The crude product was further purified by column chromatography on silica gel using petroleum ether/ethyl acetate (50:1) as eluent to obtain the product **5** as yellow solid (309 mg, 50% yield).

5: ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.74 (s, 1H), 7.65 (d, J = 7.7 Hz, 1H), 7.46 (t, J = 7.5 Hz, 1H), 7.42-7.27 (m, 3H), 6.80 (s, 4H), 2.26 (s, 6H), 2.04 (s, 12H). ^{13}C NMR (101 MHz, CD_2Cl_2): δ 151.37, 148.86, 143.67, 142.91, 141.07, 139.77, 139.70, 134.77, 133.74, 130.83, 129.39, 128.88, 125.68, 121.23, 94.25, 85.47, 23.36, 21.47, 21.45, 21.42, 21.39. HR-ESIMS (m/z): $[M+H]^+$ calcd. for $C_{29}H_{29}BNS$,434.2114; found: 434.2105.

II. Characterization Data

Table S1. Melting point of 1a/1b-5a/5b

	1a	1b	2a	2b	3a	3b	4a	4b	5a	5b
M.P.(℃)	230	214	197	309	197	264	283	303	238	262

UV-vis and Fluorescence data of **1a/1b-5a/5b**

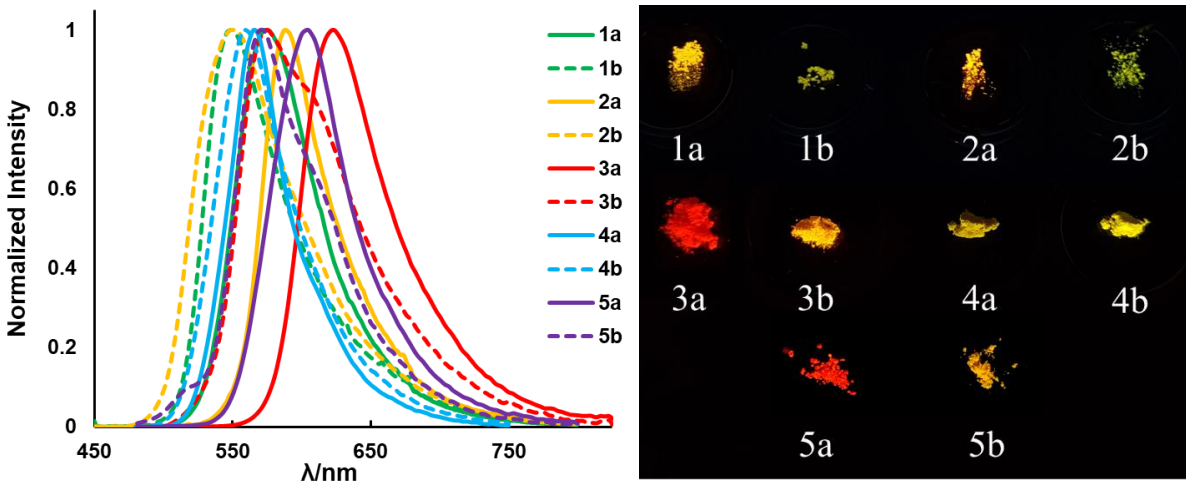


Figure S1 Fluorescent Spectra of Compounds **1a/1b-5a/5b** in the solid state.

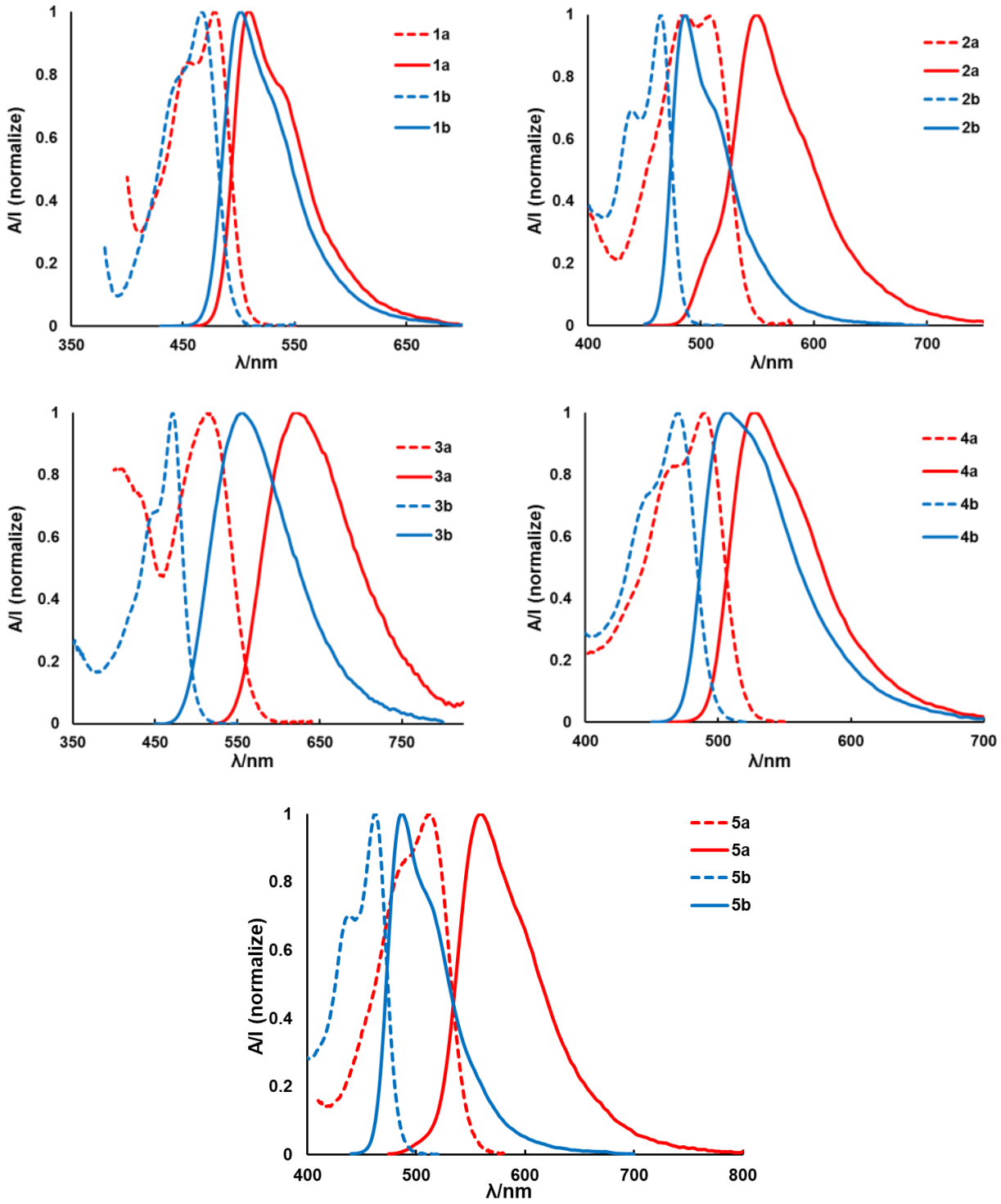


Figure S2: Absorption (dotted lines) and fluorescence spectra (solid line) of **1a/1b-5a/5b** in THF (C = 1×10^{-5} M).

UV-vis and Fluorescent Spectra in Different Solvents

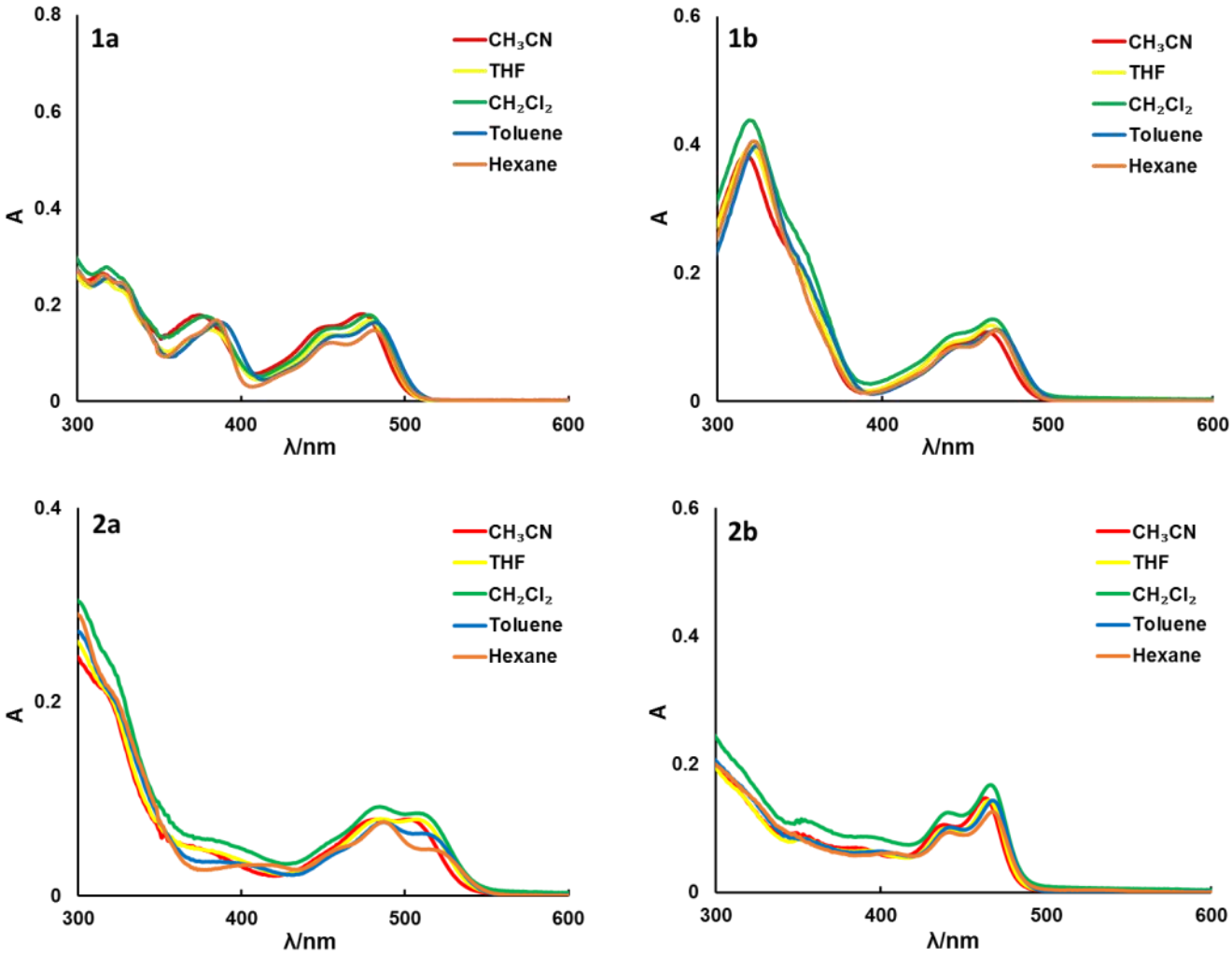


Figure S3: UV-vis Spectra of Compounds **1a/1b-2a/2b** in Different Solvents (c= 1×10^{-5} mol/L).

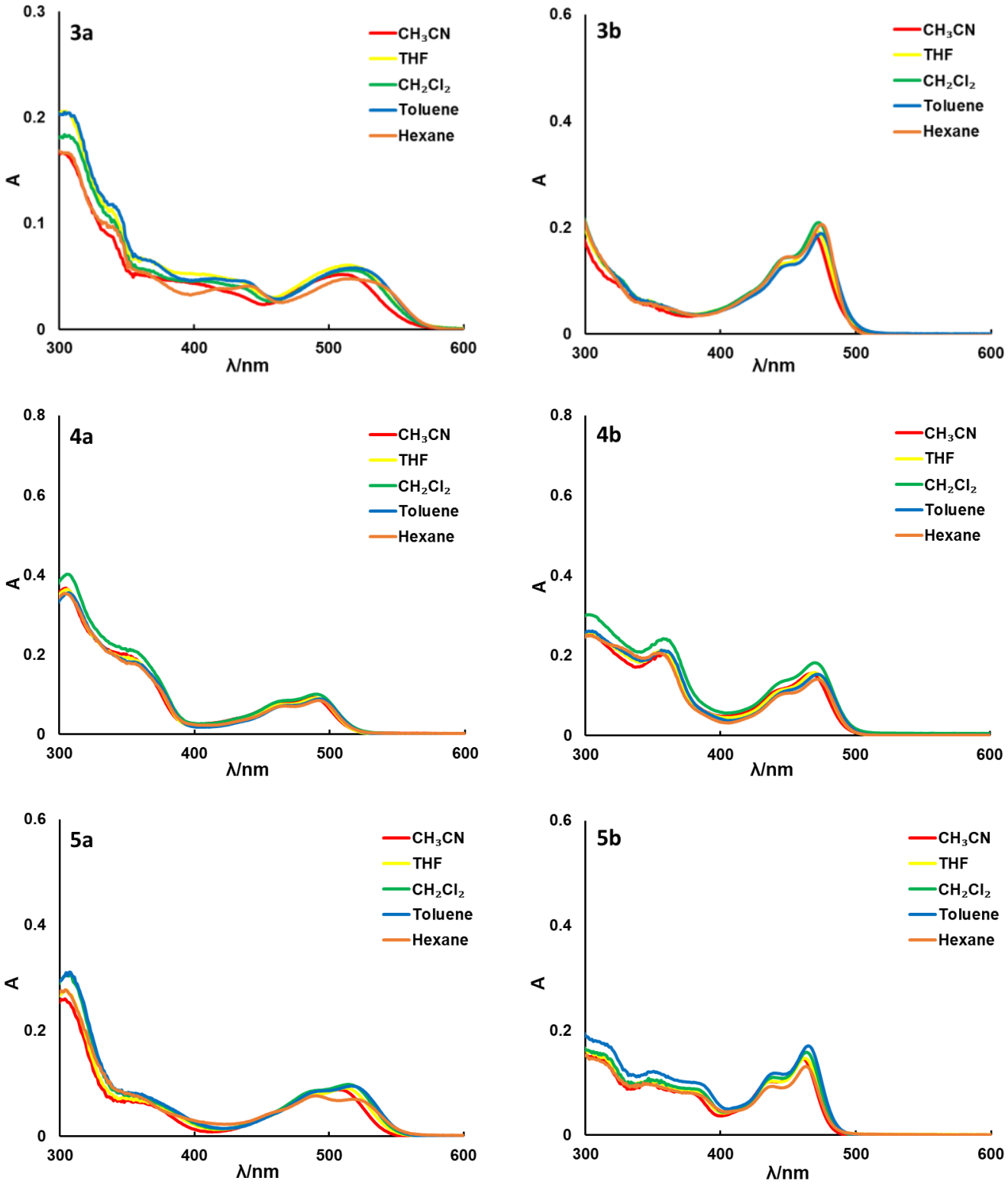


Figure S4: UV-vis Spectra of Compounds **3a/3b-5a/5b** in Different Solvents (c= 1×10^{-5} mol/L).

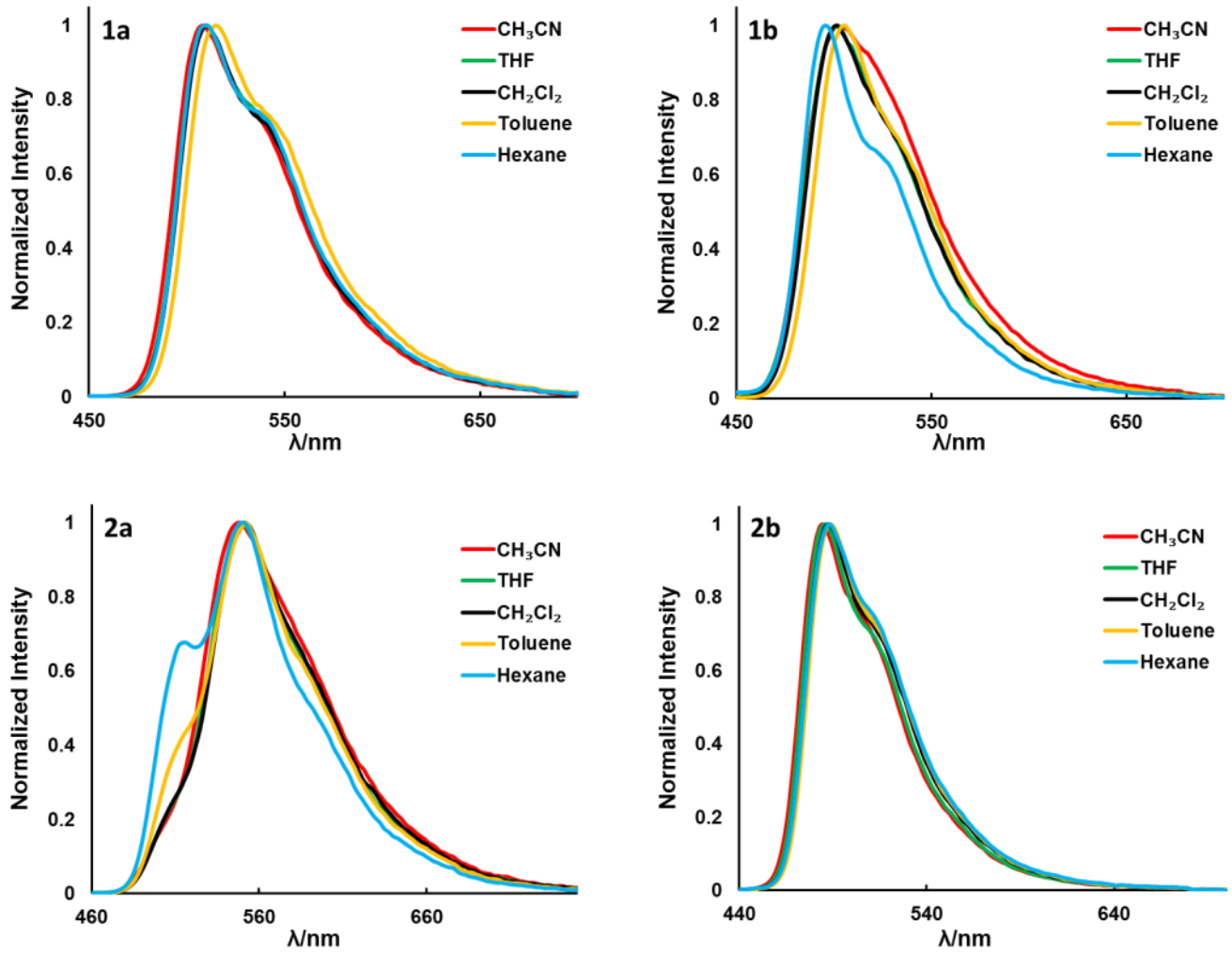


Figure S5: Fluorescence Spectra of Compounds **1a/1b-2a/2b** in Different Solvents (c= 1×10^{-5} mol/L).

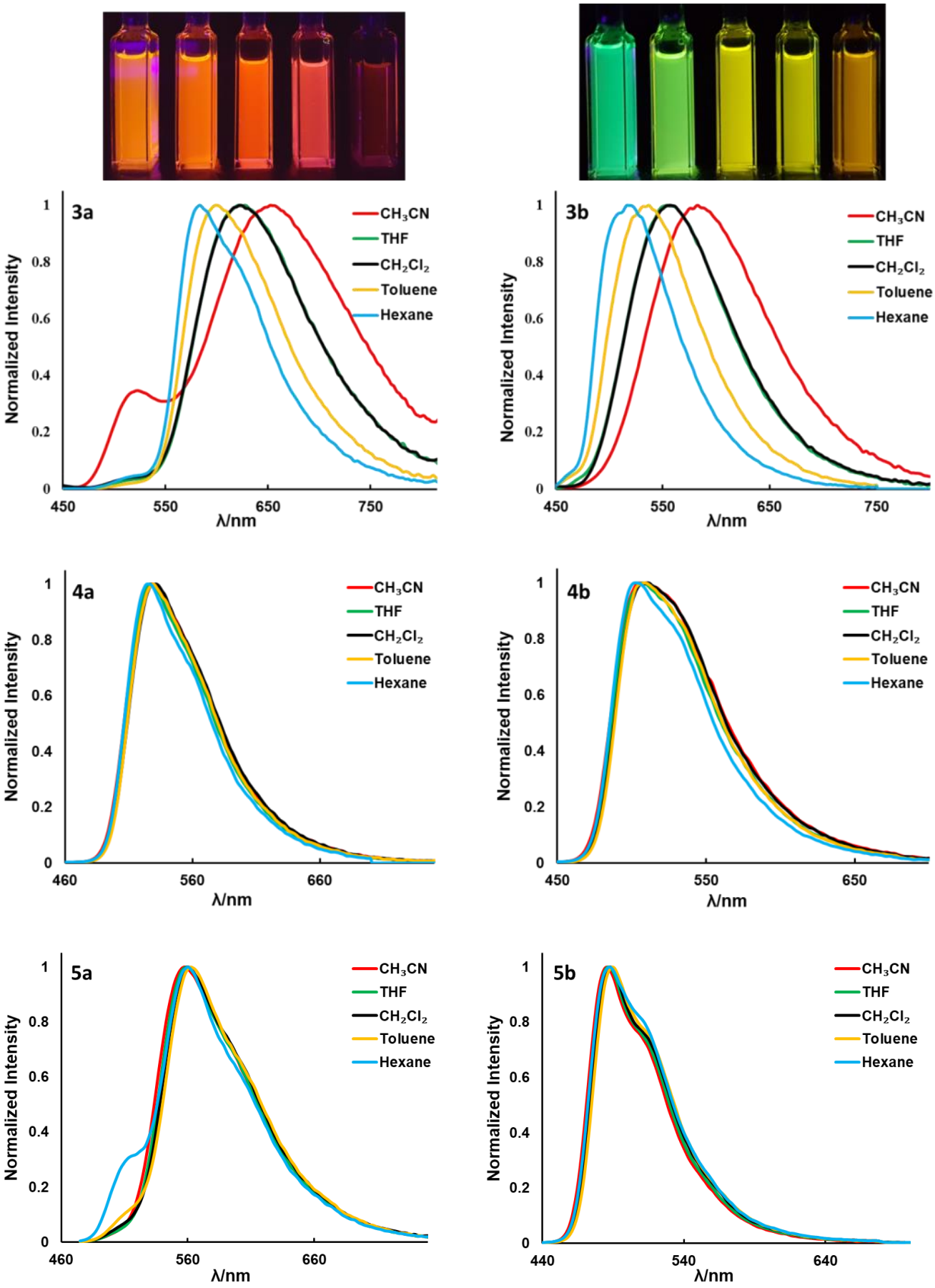


Figure S6: Fluorescence Spectra of Compounds **3a/3b-5a/5b** in Different Solvents (c= 1×10^{-5} mol/L).

Fluorescence Spectra at Different Concentrations in THF

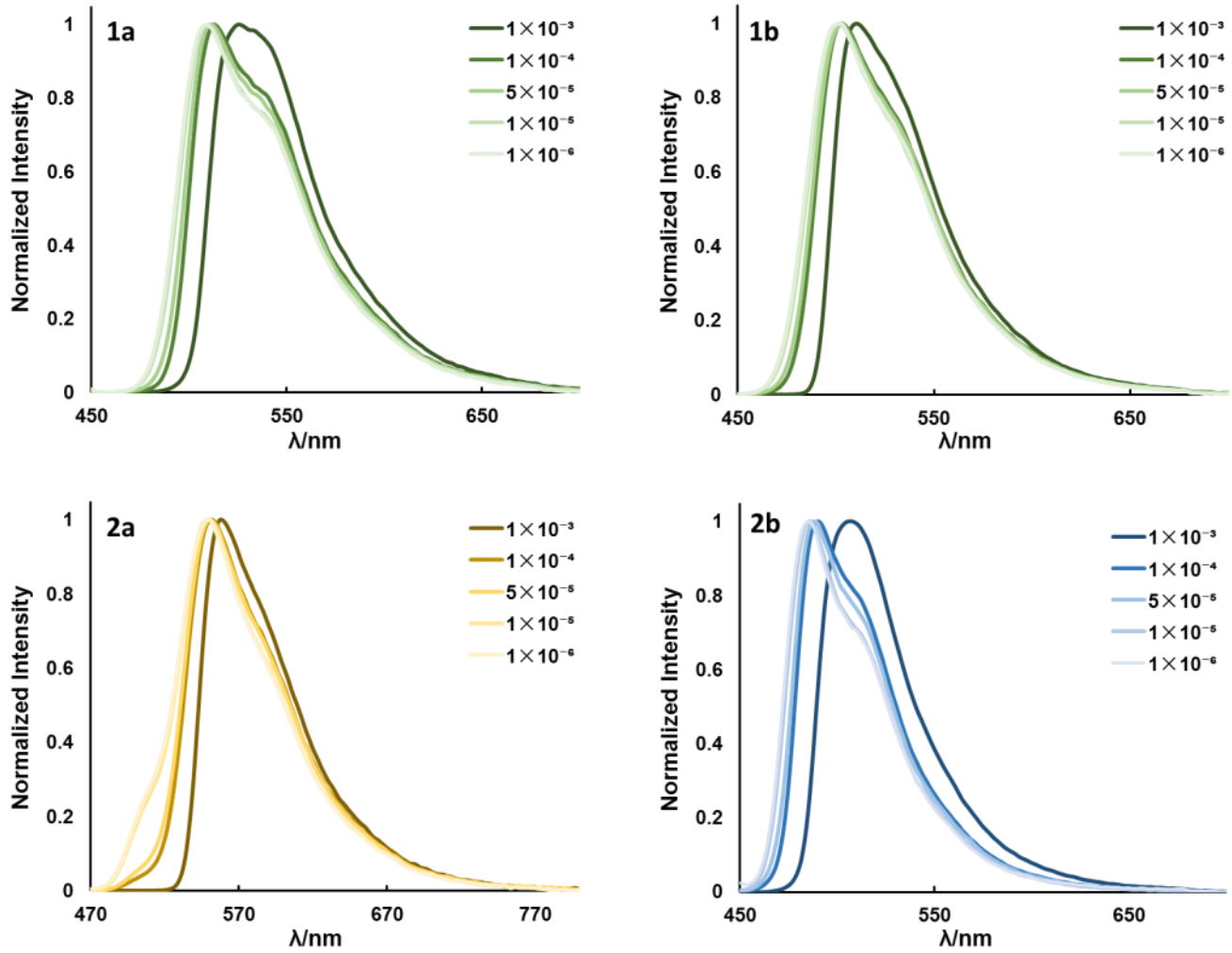


Figure S7: Fluorescence Spectra of Compounds **1a/1b-2a/2b** at different concentrations of THF solution.

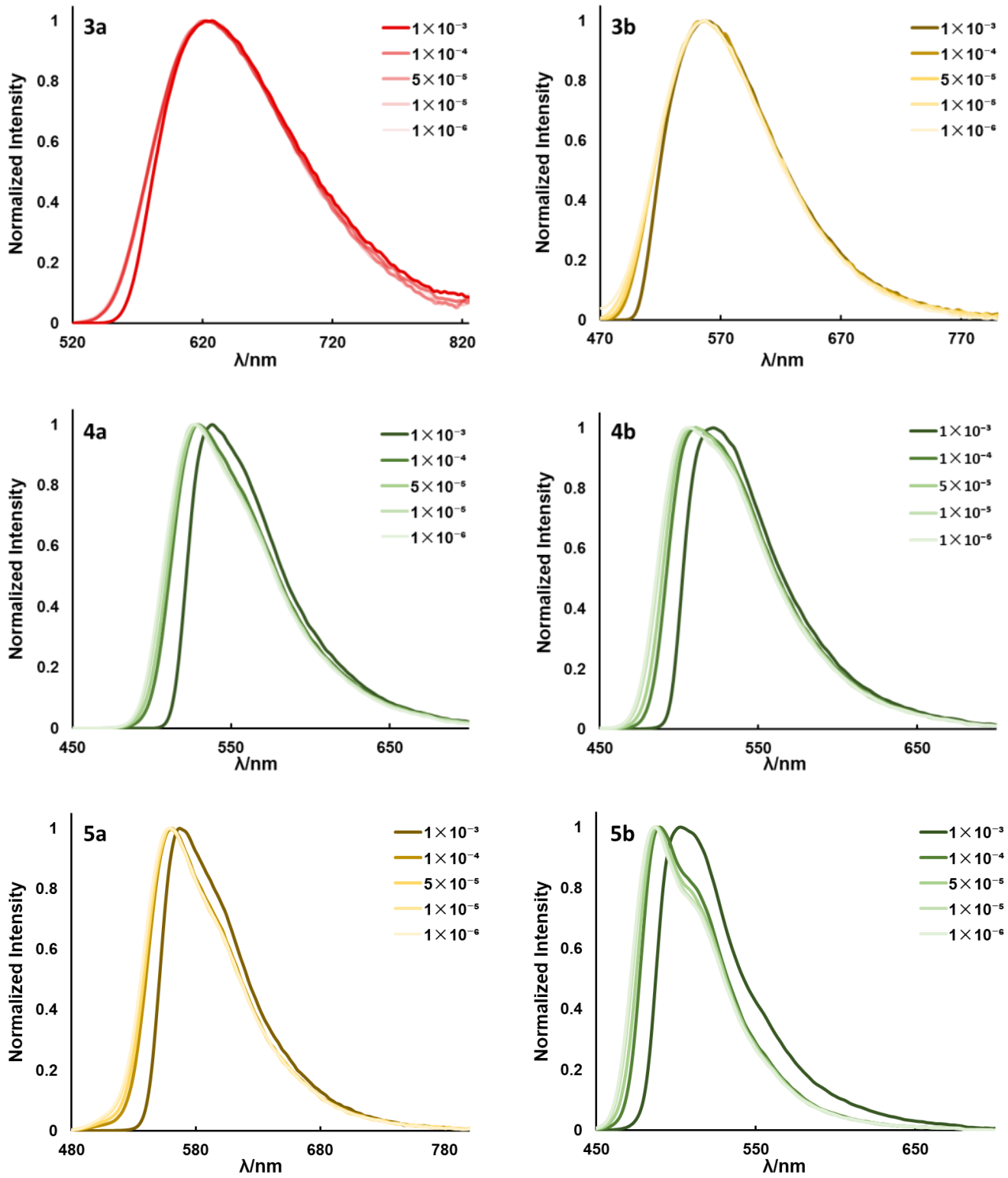


Figure S8: Fluorescence Spectra of Compounds **3a/3a-5a/5b** at different concentrations of THF solution.

Table S2: Fluorescence Data in different solvents and at different concentrations in THF.

	Different Solvents [a]					THF				
	solution	**λ_{em} (nm)**	**Φ^b**	**$\tau_{av.}$ (ns)**	**χ^2**	**con.(mol/L) [c]**	**λ_{em} (nm)[c]**	**Φ^b**	**$\tau_{av.}$ (ns)**	**χ^2**
1a	CH_3CN	508	96%	10.3	1.057	1×10^{-3}	526	93%	16.2	1.179
	THF	510	99%	9.7	1.148	1×10^{-4}	513	94%	10.4	1.048
	CH_2Cl_2	510	90%	9.6	1.011	5×10^{-5}	511	95%	10.0	1.048
	Toluene	515	94%	9.0	1.010	1×10^{-5}	509	98%	9.6	1.004
	Hexane	510	93%	10.1	1.051	1×10^{-6}	509	99%	9.5	0.992
1b	CH_3CN	501	84%	15.5	1.103	1×10^{-3}	511	75%	21.7	1.135
	THF	502	85%	13.5	1.107	1×10^{-4}	503	82%	14.1	1.094
	CH_2Cl_2	501	74%	11.9	1.108	5×10^{-5}	503	84%	13.7	1.165
	Toluene	505	87%	12.6	1.172	1×10^{-5}	502	89%	13.4	1.153
	Hexane	496	80%	12.8	1.06	1×10^{-6}	502	89%	13.3	1.189
2a	CH_3CN	548	79%	27.4	1.073	1×10^{-3}	558	78%	39.1	1.113
	THF	550	88%	25.0	1.100	1×10^{-4}	552	79%	26.1	1.070
	CH_2Cl_2	552	79%	24.0	1.111	5×10^{-5}	550	80%	25.4	1.017
	Toluene	552	83%	23.1	1.189	1×10^{-5}	550	86%	24.8	1.097
	Hexane	550	78%	20.2	1.124	1×10^{-6}	550	92%	24.8	1.065
2b	CH_3CN	484	72%	12.2	1.102	1×10^{-3}	507	57%	21.3	1.149
	THF	486	68%	11.1	1.120	1×10^{-4}	490	59%	12.2	1.064
	CH_2Cl_2	488	66%	10.0	1.056	5×10^{-5}	488	61%	11.7	1.079
	Toluene	489	78%	10.5	1.066	1×10^{-5}	486	66%	11.2	1.114
	Hexane	488	67%	11.3	1.112	1×10^{-6}	485	85%	11.1	1.057
3a	CH_3CN	653	4%	6.6	1.169	1×10^{-3}	627	24%	23.3	1.159
	THF	628	28%	20.8	1.036	1×10^{-4}	627	25%	20.6	1.032
	CH_2Cl_2	623	28%	20.5	1.074	5×10^{-5}	624	26%	20.7	1.026
	Toluene	600	58%	31.0	1.074	1×10^{-5}	628	26%	20.8	1.168
	Hexane	584	61%	34.8	1.040	1×10^{-6}	627	27%	20.9	1.039
3b	CH_3CN	583	48%	8.6	1.044	1×10^{-3}	557	42%	7.5	1.137
	THF	554	63%	6.9	1.028	1×10^{-4}	557	55%	7.0	1.038
	CH_2Cl_2	557	42%	6.8	1.069	5×10^{-5}	557	57%	7.0	1.107
	Toluene	537	45%	5.2	1.074	1×10^{-5}	556	63%	7.0	0.966
	Hexane	517	30%	4.4	1.075	1×10^{-6}	557	64%	7.0	1.040
4a	CH_3CN	528	57%	16.8	1.104	1×10^{-3}	538	53%	18.1	1.039
	THF	527	61%	15.8	1.181	1×10^{-4}	529	58%	16.4	1.077
	CH_2Cl_2	531	57%	14.8	1.153	5×10^{-5}	528	60%	15.9	1.113
	Toluene	529	65%	15.3	1.175	1×10^{-5}	527	60%	15.8	1.112

	Hexane	525	59%	16.0	1.172	1×10^{-6}	527	62%	15.7	1.162
4b	CH_3CN	510	76%	11.1	1.038	1×10^{-3}	522	71%	15.9	1.189
	THF	507	81%	10.3	1.187	1×10^{-4}	510	77%	10.9	1.010
	CH_2Cl_2	511	79%	9.9	1.034	5×10^{-5}	508	79%	10.5	1.146
	Toluene	509	81%	9.4	1.003	1×10^{-5}	507	81%	10.2	1.064
	Hexane	503	81%	10.1	1.015	1×10^{-6}	506	82%	10.2	1.151
5a	CH_3CN	558	77%	23.9	1.061	1×10^{-3}	567	72%	34.1	1.145
	THF	559	82%	21.9	1.147	1×10^{-4}	561	75%	22.7	1.094
	CH_2Cl_2	560	77%	21.4	1.192	5×10^{-5}	559	77%	22.2	1.165
	Toluene	562	79%	20.3	1.161	1×10^{-5}	559	82%	21.9	1.147
	Hexane	560	74%	22.6	1.127	1×10^{-6}	559	83%	21.9	1.146
5b	CH_3CN	486	46%	6.3	1.021	1×10^{-3}	503	37%	8.8	1.116
	THF	487	49%	6.0	1.076	1×10^{-4}	490	43%	6.2	1.038
	CH_2Cl_2	488	44%	5.5	1.003	5×10^{-5}	488	46%	6.1	1.024
	Toluene	490	49%	5.5	1.001	1×10^{-5}	487	49%	6.0	1.076
	Hexane	488	48%	6.0	1.046	1×10^{-6}	487	54%	6.0	1.106

[a] 10^{-5} M in different solution at 298 K. [b] The solution QY was determined in different solution using an integration sphere under N_2.

[c] at different concentratiosn in THF at 298 K.

Fluorescence Spectra of **1a/1b-5a/5b** at 77 K and 298 K

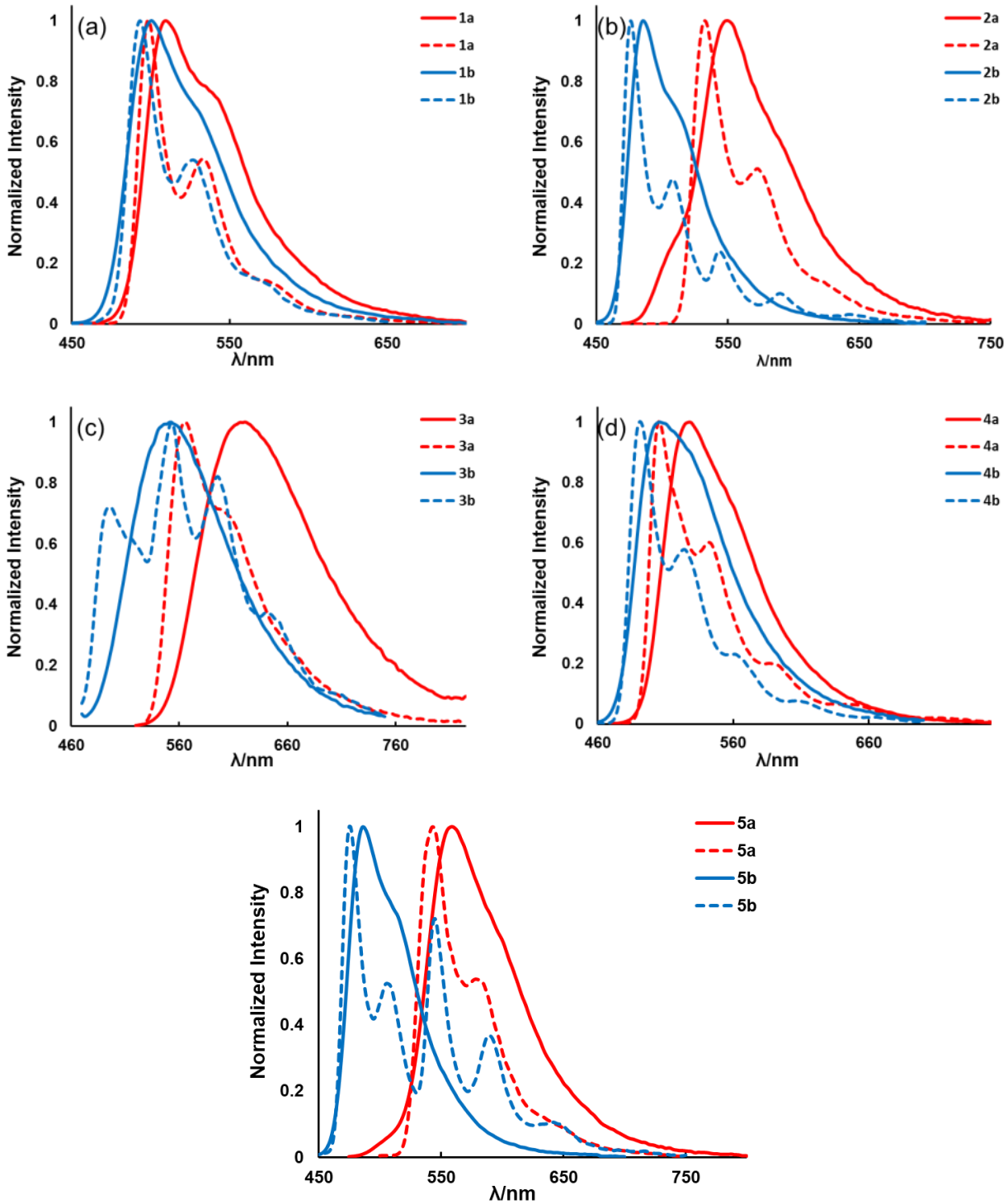


Figure S9: Fluorescence Spectra of Compounds **1a/1b-5a/5b** at 298 K (solid line) and 77 K (dotted lines) in 2-Me-THF (c= 1×10^{-5} mol/L).

Table S3: Fluorescence Data of **1a/1b-5a/5b** at 77 K and 298 K.

	T	λ_{em} (nm)[a]	Φ[b]	$\tau_{av.}$ (ns)	χ^2		T	λ_{em} (nm)[a]	Φ[b]	$\tau_{av.}$ (ns)	χ^2
1a	298 K	509	92%	9.9	1.021	**4a**	298 K	528	60%	16.0	1.165
	77 K	498	100%	7.7	1.170		77 K	505	97%	13.1	1.055
1b	298 K	500	84%	13.6	1.041	**4b**	298 K	506	79%	10.4	1.075
	77 K	493	100%	11.8	1.077		77 K	491	100%	7.9	1.189
2a	298 K	550	82%	25.5	1.000	**5a**	298 K	559	77%	20.4	1.085
	77 K	533	100%	20.2	1.036		77 K	540	100%	17.7	1.106
2b	298 K	485	62%	11.5	1.056	**5b**	298 K	486	52%	5.9	1.005
	77 K	476	100%	8.8	1.171		77 K	475	100%	4.6	1.011
3a	298 K	621	32%	24.7	1.151	**3b**	298 K	552	48%	6.7	1.093
	77 K	566	97%	28.5	0.967		77 K	494	81%	3.3	1.185

[a]10^{-5} M in 2-Me-THF at 298 K/77 K. [b] The solution QY was determined in 2-Me-THF solution using an integration sphere.

Thermochromic Phenomena of **2a/2b, 3a/3b, 5a/5b**

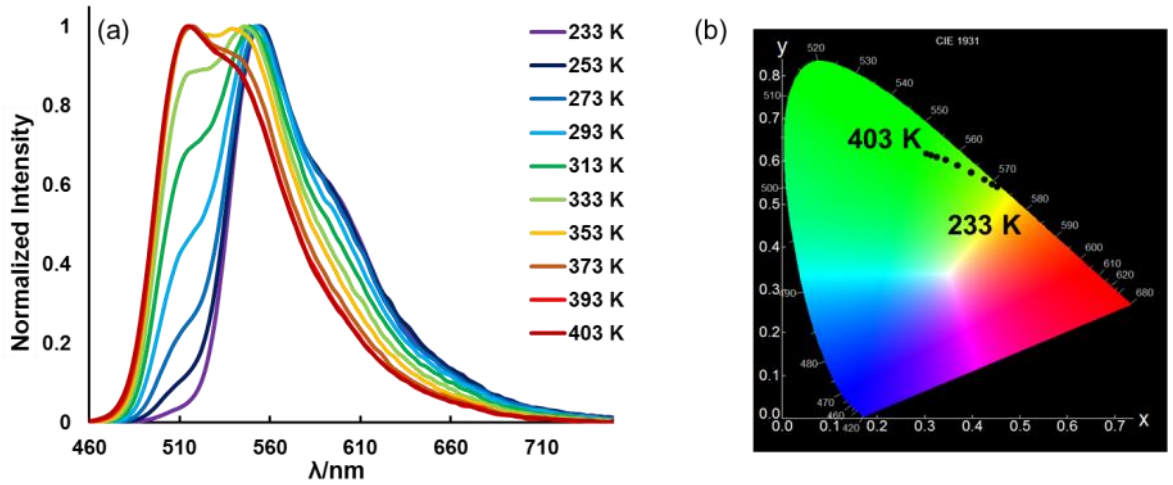


Figure S10: (a) Normalized emission spectra of **2a** recorded between 233 K and 403 K (c = 1×10^{-5} M, in Mesitylene, λ_{ex} = 322 nm, under N_2). (b) CIE coordinates (CIE 1931).

Table S4: The temperature-dependent photoluminescence and lifetime data of **2a** in mesitylene (under N_2, λ_{ex} = 322 nm).

T	λ_{Em1}(nm)	τ_a(ns)	χ^2	λ_{Em2}(nm)	τ_b(ns)	χ^2
233 K	553	22.10	1.015			
253 K	553	20.99	1.030			
273 K	553	19.46	1.022			
293 K	552	17.31	1.013			
313 K	548	15.14	1.084	512	13.17	1.115
333 K	546	13.09	1.122	517	11.90	1.151
353 K	542	11.66	1.116	517	10.95	1.116
373 K	542	10.89	1.111	517	10.29	1.118
393 K	542	10.62	1.165	517	10.04	1.163
403 K				517	10.41	1.207

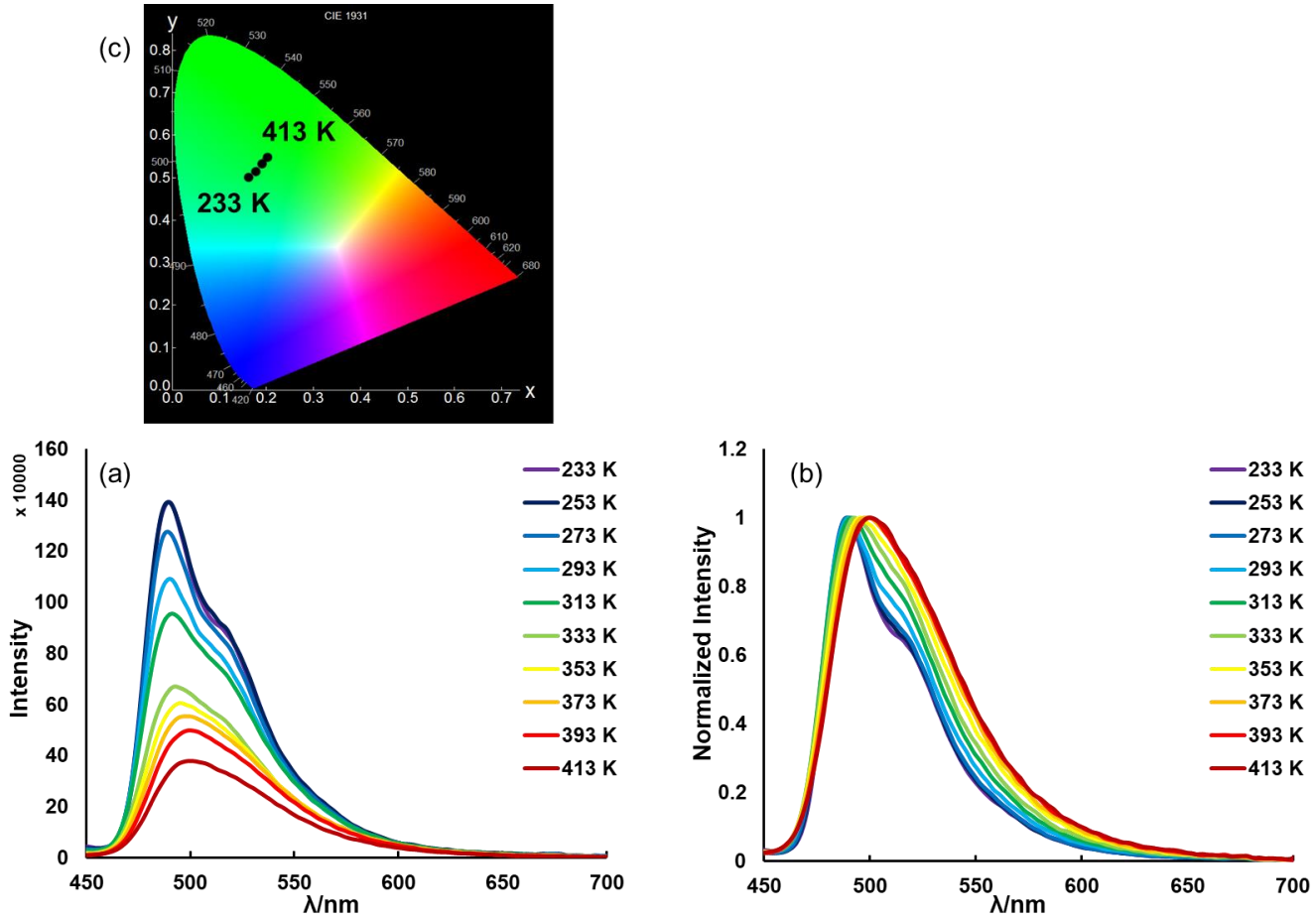


Figure S11: (a) CIE coordinates (CIE 1931) of **2b**. (b) Emission spectra, and (c) Normalized emission spectra of **2b** recorded between 233 K and 413 K (c = 1×10^{-5} M, in mesitylene, λ_{ex} = 320 nm, under N_2)

Table S5: The temperature-dependent photoluminescence and lifetime data of **2b** in mesitylene (under N_2, λ_{ex} = 320 nm).

T	λ_{Em1}(nm)	τ_a(ns)	χ^2
233 K	489	10.1	1.044
253 K	489	10.1	1.022
273 K	489	10.2	1.025
293 K	490	10.3	1.035
313 K	491	10.7	1.036
333 K	493	11.2	1.128
353 K	495	12.5	1.101
373 K	498	13.2	1.180
393 K	500	14.7	1.172
413 K	500	15.3	1.096

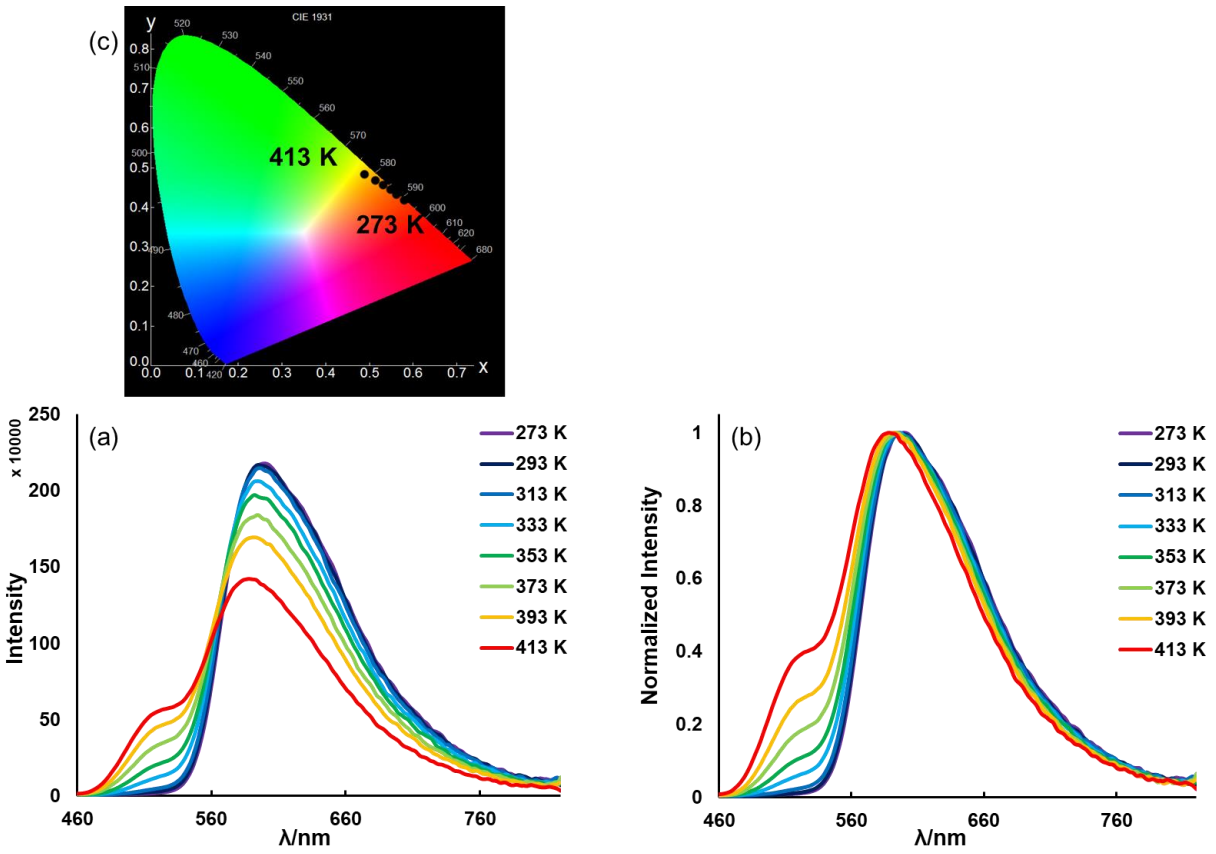


Figure S12: (a) CIE coordinates (CIE 1931) of **3a**. (b) Emission spectra, and (c) Normalized emission spectra of **3a** recorded between 273 K and 413 K (c = 1×10^{-5} M, in mesitylene, λ_{ex} = 370 nm, under N_2)

Table S6: The temperature-dependent photoluminescence and lifetime data of **2b** in mesitylene (under N_2, λ_{ex} = 370 nm).

T	λ_{Em1}(nm)	τ_a(ns)	χ^2
273 K	600	31.2	1.027
293 K	596	31.2	1.148
313 K	596	31.2	1.081
333 K	594	30.8	1.030
353 K	594	30.4	1.098
373 K	593	30.0	1.000
393 K	592	29.5	1.061
413 K	588	29.1	1.048

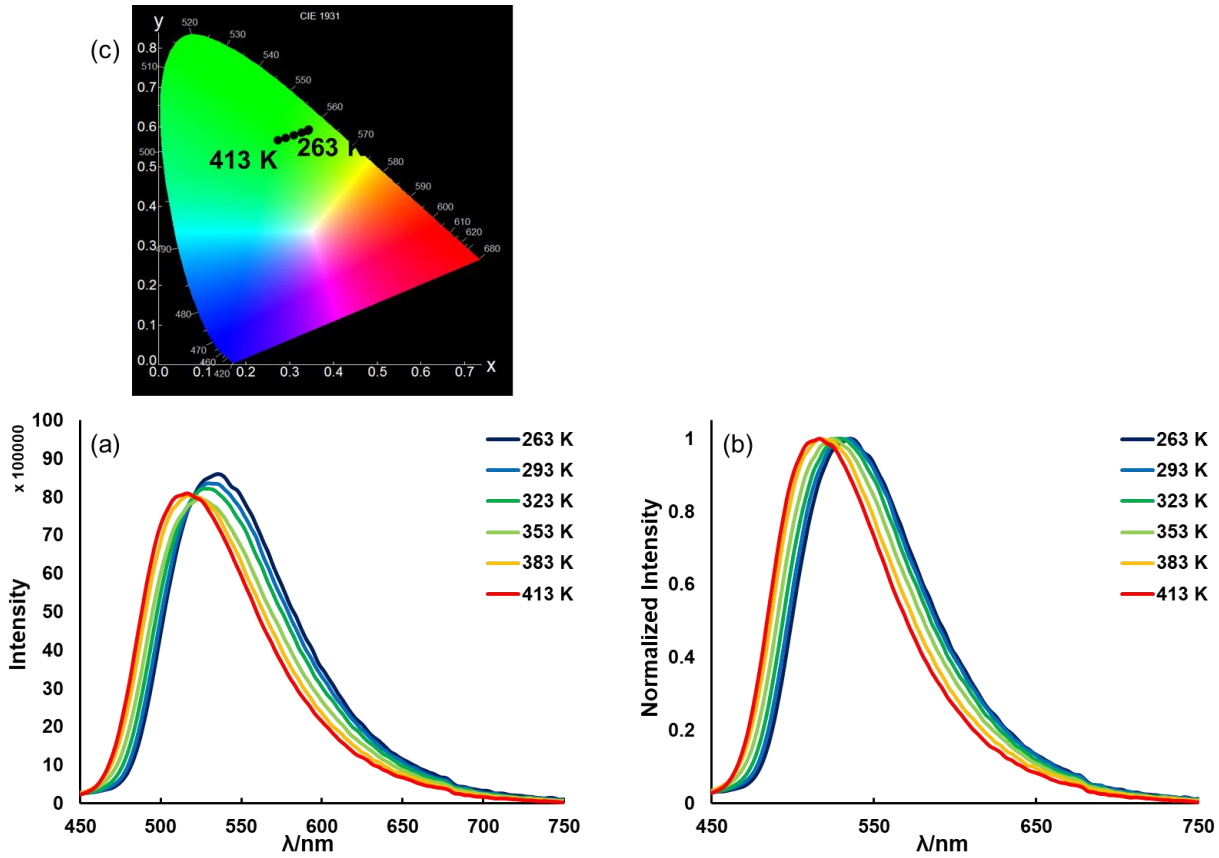


Figure S13: (a) CIE coordinates (CIE 1931) of **3b**. (b) Emission spectra, and (c) Normalized emission spectra of **3a** recorded between 263 K and 413 K (c = 1×10^{-5} M, in mesitylene, λ_{ex} = 360 nm, under N_2)

Table S7: The temperature-dependent photoluminescence and lifetime data of **3b** in mesitylene (under N_2, λ_{ex} = 360 nm).

T	λ_{Em}(nm)	τ_a(ns)	χ^2
263 K	535	5.1	1.127
293 K	529	5.1	1.128
323 K	527	5.0	1.177
353 K	524	5.0	1.182
383 K	517	5.3	1.129
413 K	516	5.6	1.155

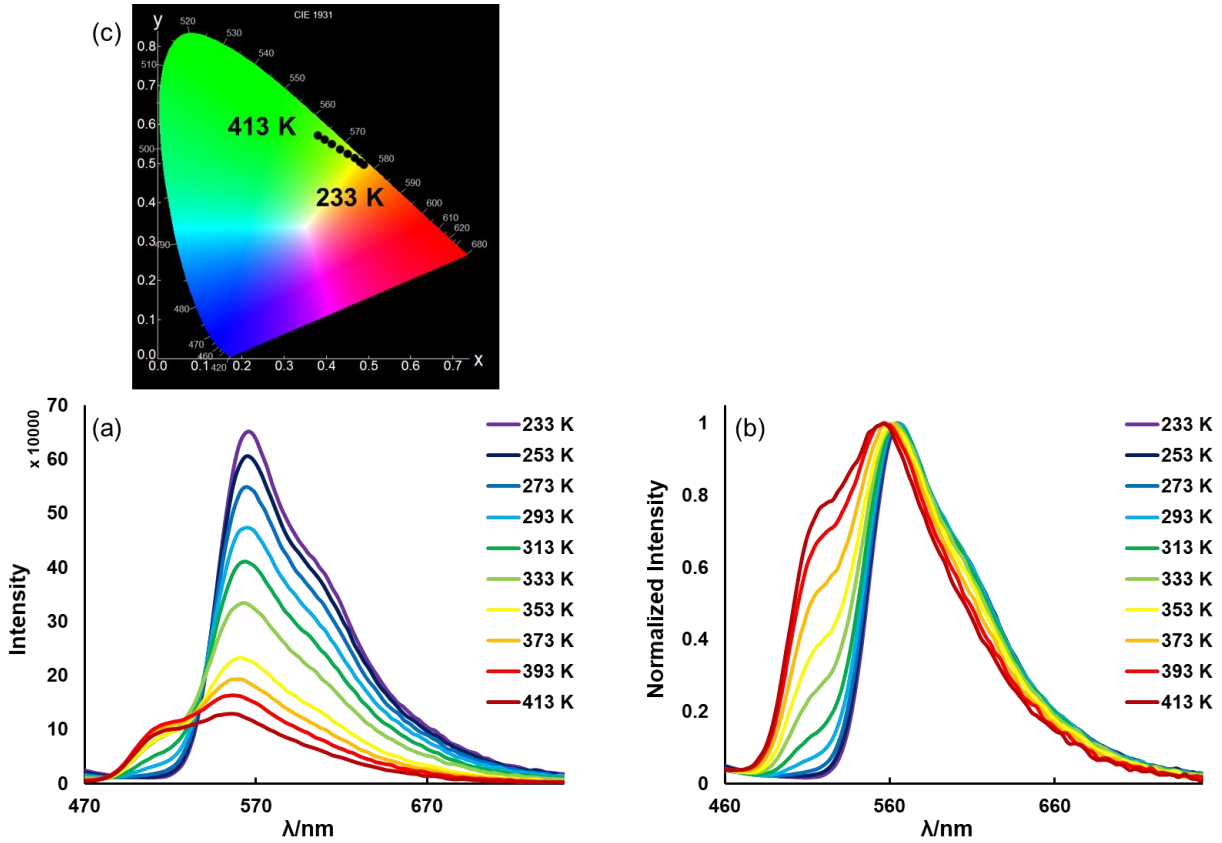


Figure S14: (a) CIE coordinates (CIE 1931) of **5a**. (b) Emission spectra, and (c) Normalized emission spectra of **3a** recorded between 233 K and 413 K (c = 1×10^{-5} M, in mesitylene, λ_{ex} = 320 nm, under N_2)

Table S8: The temperature-dependent luminescence and lifetime data of **5a** in mesitylene (under N_2, λ_{ex} = 320 nm).

T	λ_{Em}(nm)	τ_a(ns)	χ^2
233 K	566	20.8	1.171
253 K	565	20.8	1.104
273 K	565	20.9	1.177
293 K	565	20.9	1.193
313 K	564	20.6	1.091
333 K	563	20.1	1.176
353 K	562	19.3	1.218
373 K	562	17.8	1.199
393 K	556	16.2	1.182
413 K	556	15.7	1.190

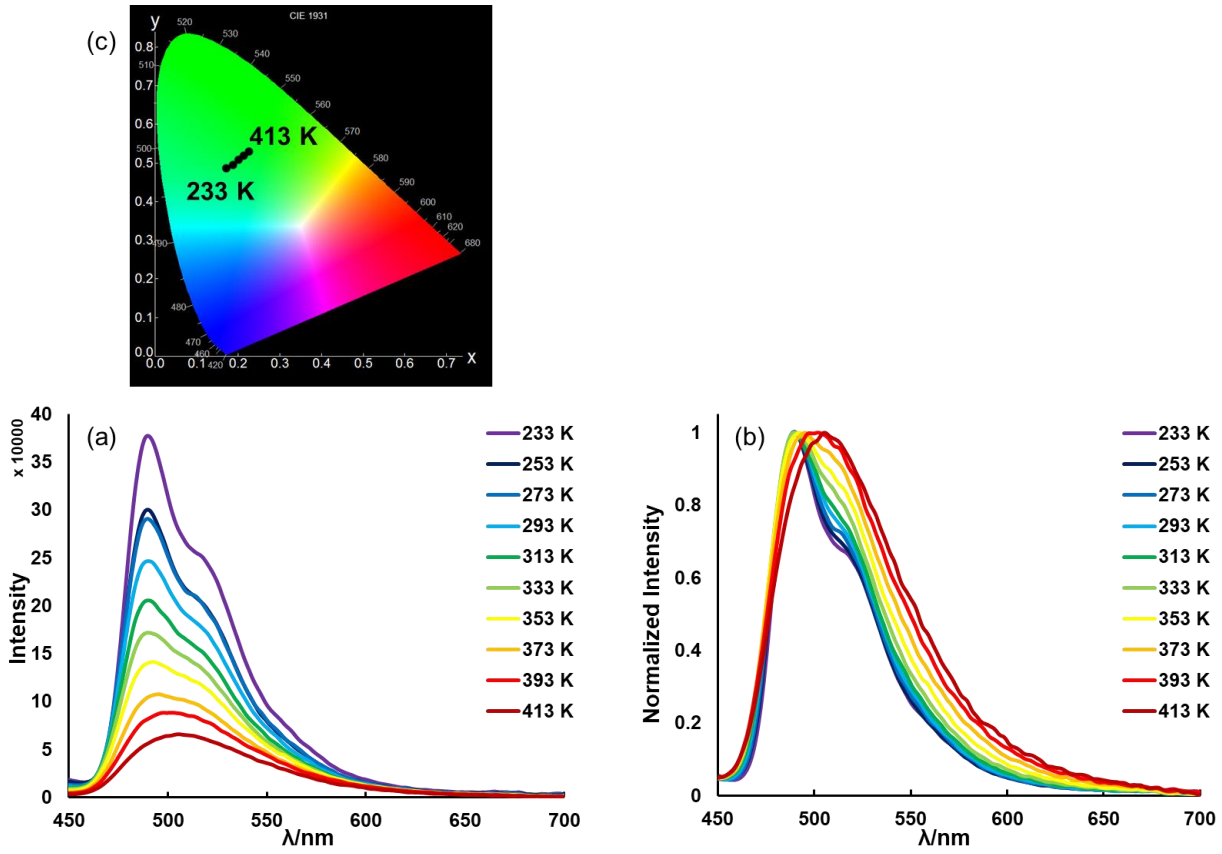


Figure S15: (a) CIE coordinates (CIE 1931) of **5b**. (b) Emission spectra, and (c) Normalized emission spectra of **3a** recorded between 233 K and 413 K (c = 1×10^{-5} M, in mesitylene, λ_{ex} = 320 nm, under N_2)

Table S9: The temperature-dependent photoluminescence and lifetime data of **5b** in mesitylene (under N_2, λ_{ex} = 320 nm).

T	λ_{Em}(nm)	τ_a(ns)	χ^2
233 K	490	5.5	1.114
253 K	490	5.5	1.088
273 K	490	5.5	1.148
293 K	490	5.5	1.149
313 K	490	5.5	1.196
333 K	490	5.7	1.076
353 K	492	5.9	1.142
373 K	495	6.2	1.098
393 K	502	6.3	1.184
413 K	505	6.2	1.207

Fluoride Titration of **1a/1b-5a/5b** in THF solution

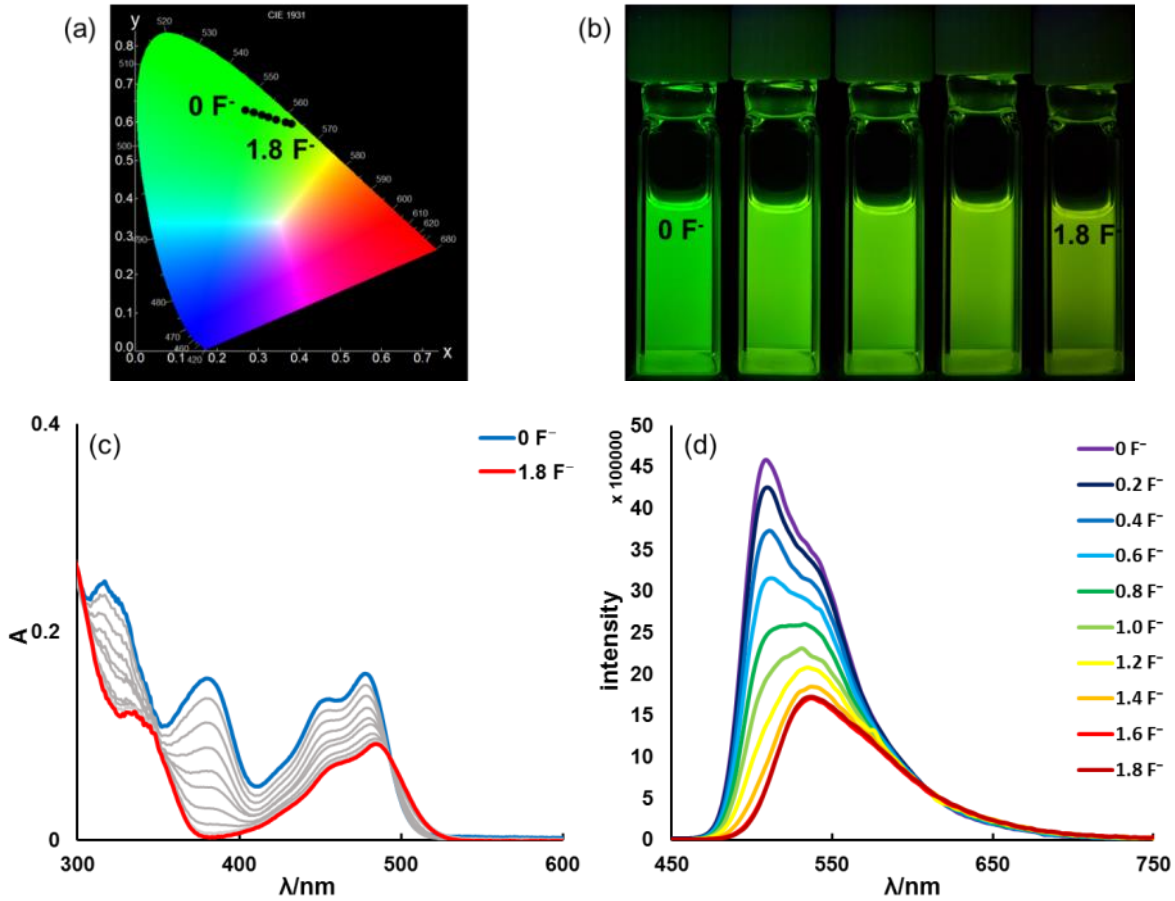


Figure S16. (a): CIE coordinates (CIE 1931). (b): Photographs of the solutions. (c): The UV-Vis titration spectra, (d): Fluorescent titration spectra of **1a** (c = 1×10^{-5} M, λ_{ex} = 320 nm, under air) by TBAF in THF at 298 K.

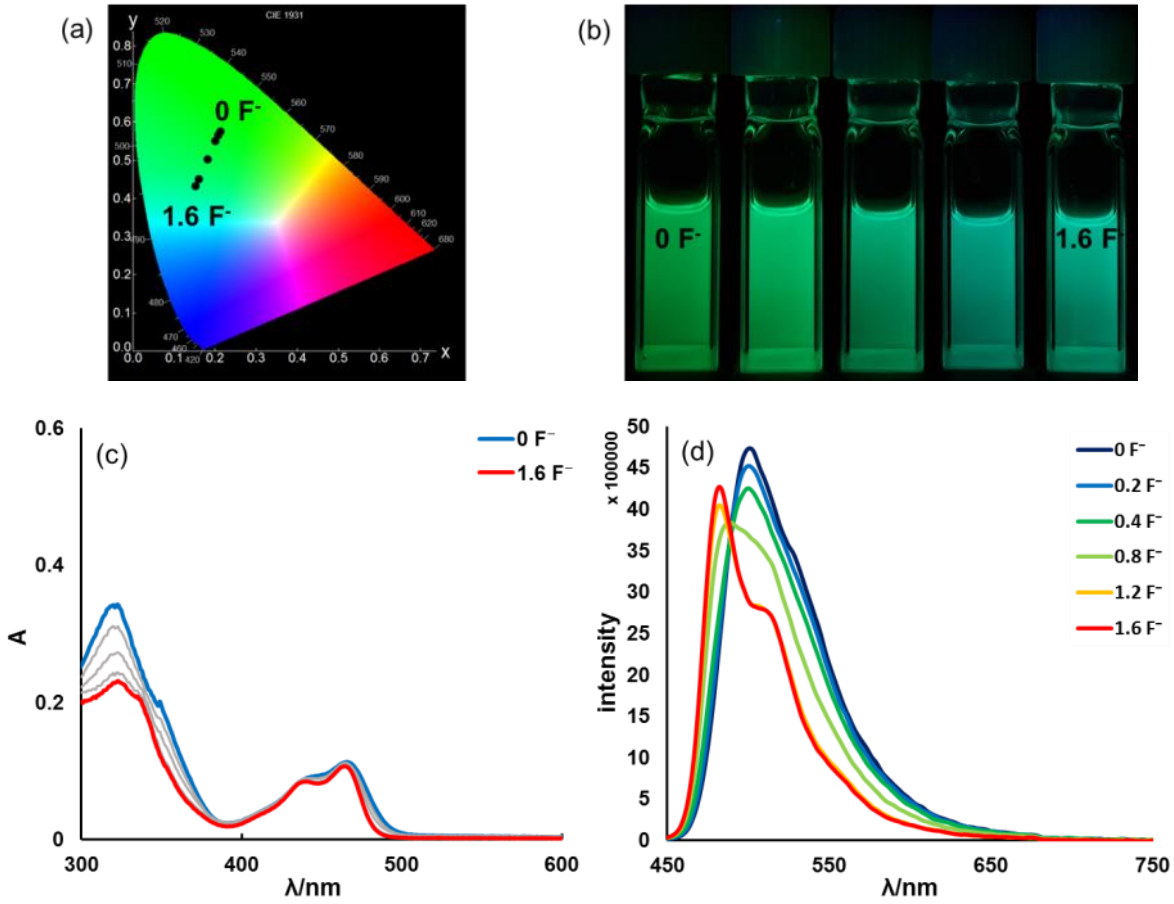


Figure S17: (a): CIE coordinates (CIE 1931). (b): Photographs of the solutions. (c): The UV-Vis titration spectra, and (d): Fluorescent titration of **1b** (c = 1×10^{-5} M, λ_{ex} = 320 nm, under air) by TBAF in THF at 298 K.

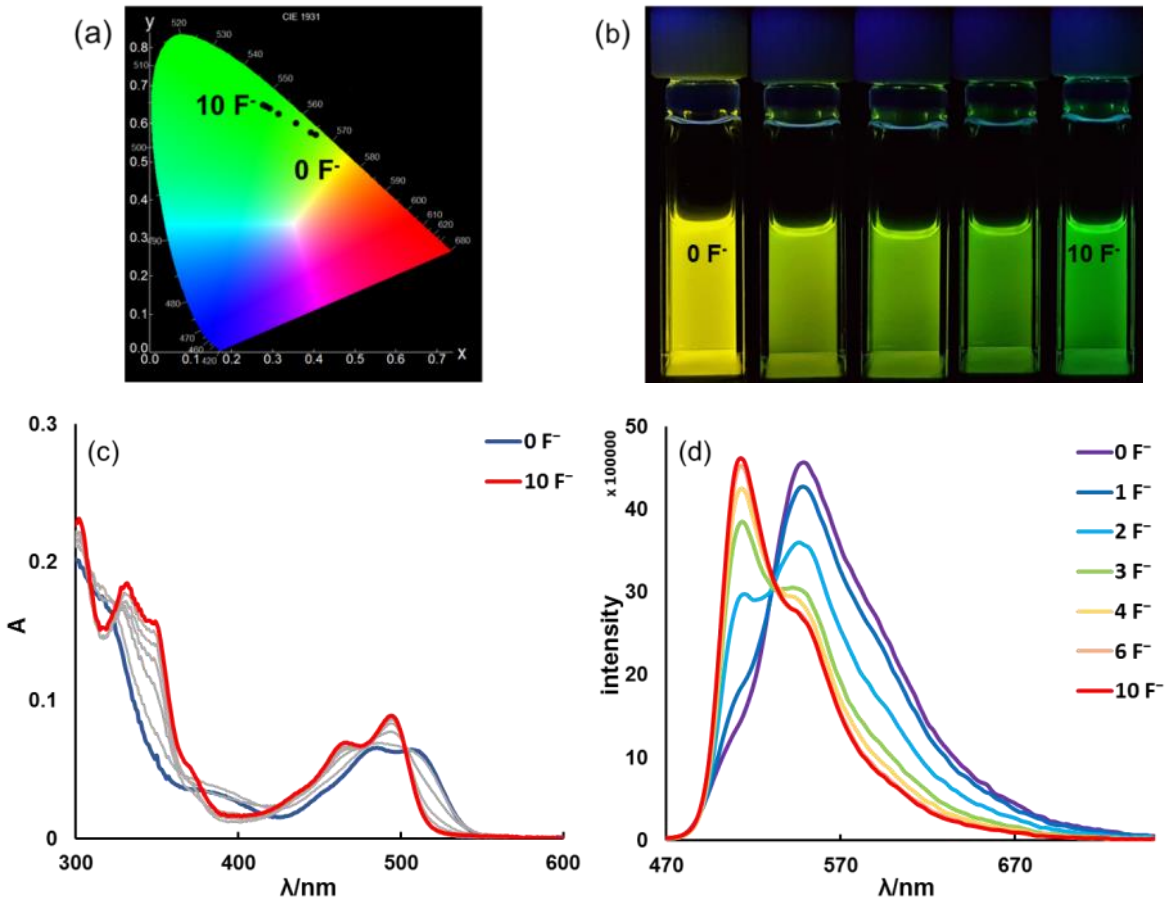


Figure S18. (a): CIE coordinates (CIE 1931). (b): Photographs of the solutions. (c): The UV-Vis titration spectra, and (d): Fluorescent titration spectra of **2a** ($c = 1\times10^{-5}$ M, $\lambda_{ex} = 320$ nm, under air) by TBAF in THF at 298 K.

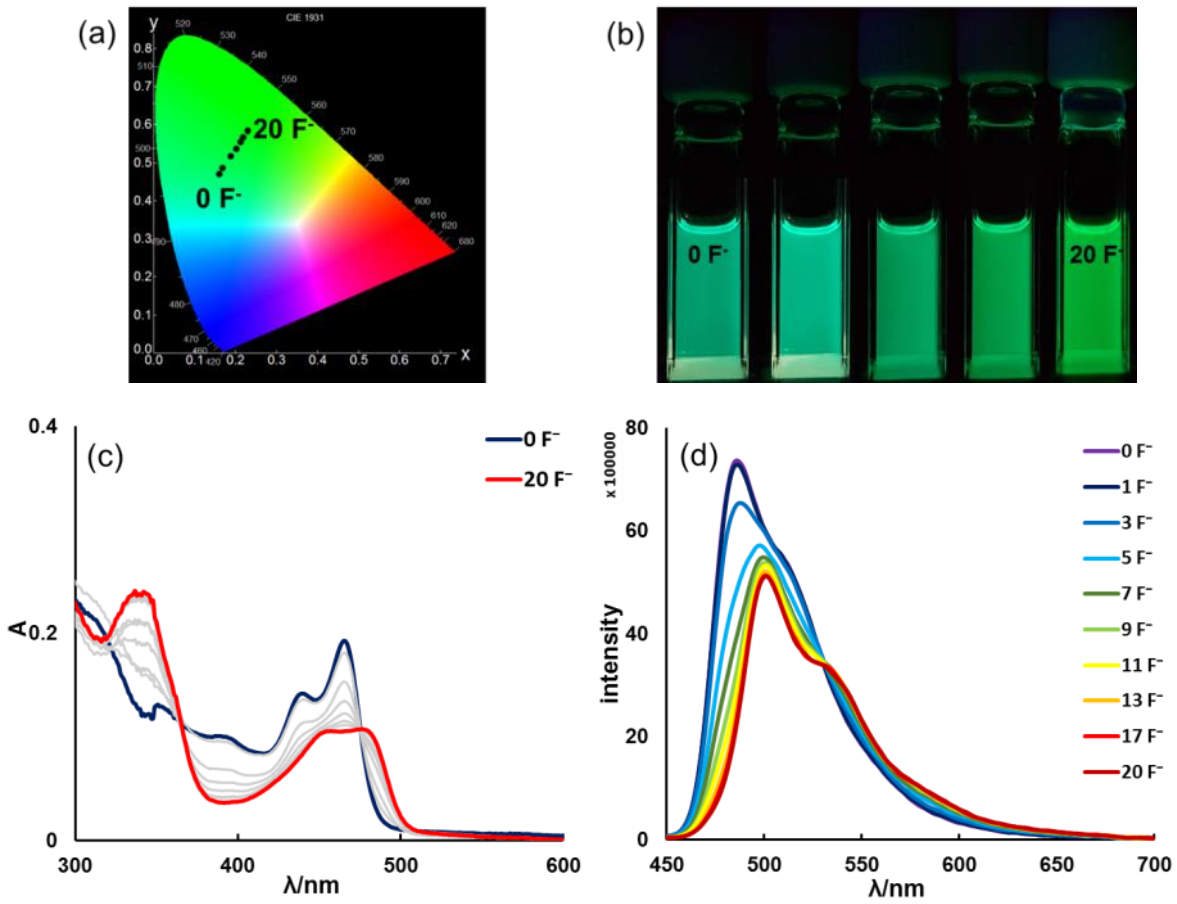


Figure S19. (a): CIE coordinates (CIE 1931). (b): Photographs of the solutions. (c): The UV-Vis titration spectra, and (d): Fluorescent titration spectra of **2b** (c = 1×10^{-5} M, λ_{ex} = 320 nm, under air) by TBAF in THF at 298 K.

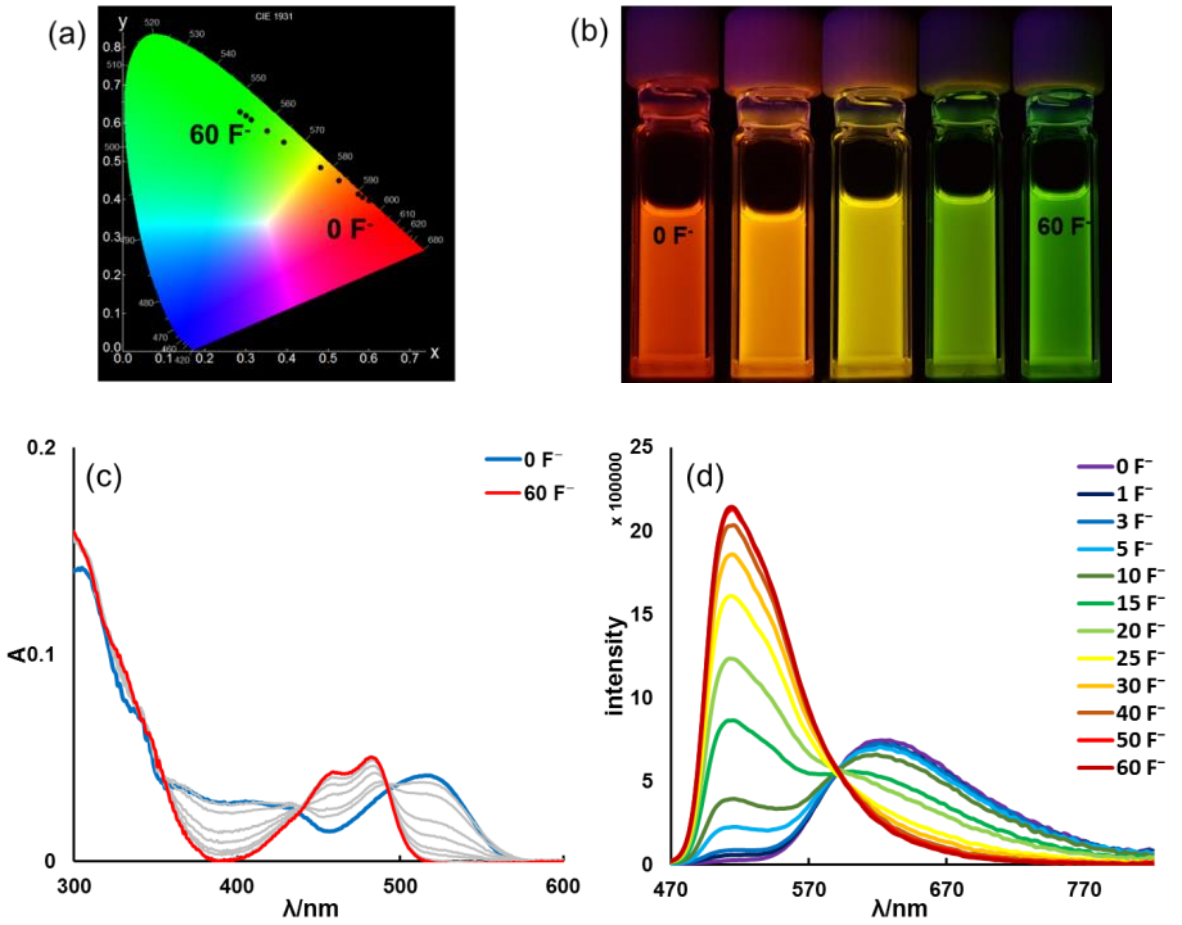


Figure S20. (a): CIE coordinates (CIE 1931). (b): Photographs of the solutions. (c): The UV-Vis titration spectra, and (d): Fluorescent titration spectra of **3a** ($c = 1\times10^{-5}$ M, $\lambda_{ex} = 313$ nm, under air) by TBAF in THF at 298 K.

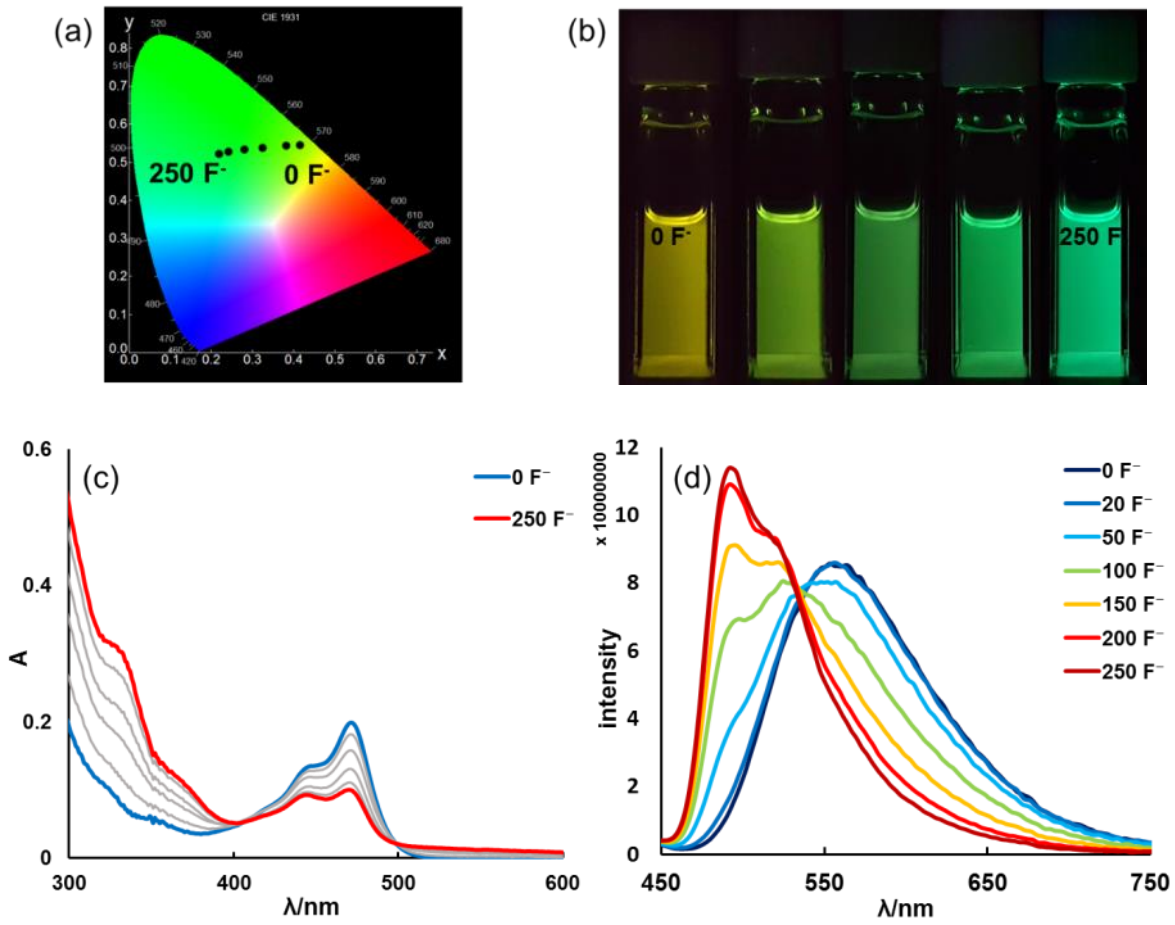


Figure S21. (a): CIE coordinates (CIE 1931). (b): Photographs of the solutions. (c): The UV-Vis titration spectra, and (d): Fluorescent titration spectra of **3b** (c = 1×10^{-5} M, λ_{ex} = 313 nm, under air) by TBAF in THF at 298 K.

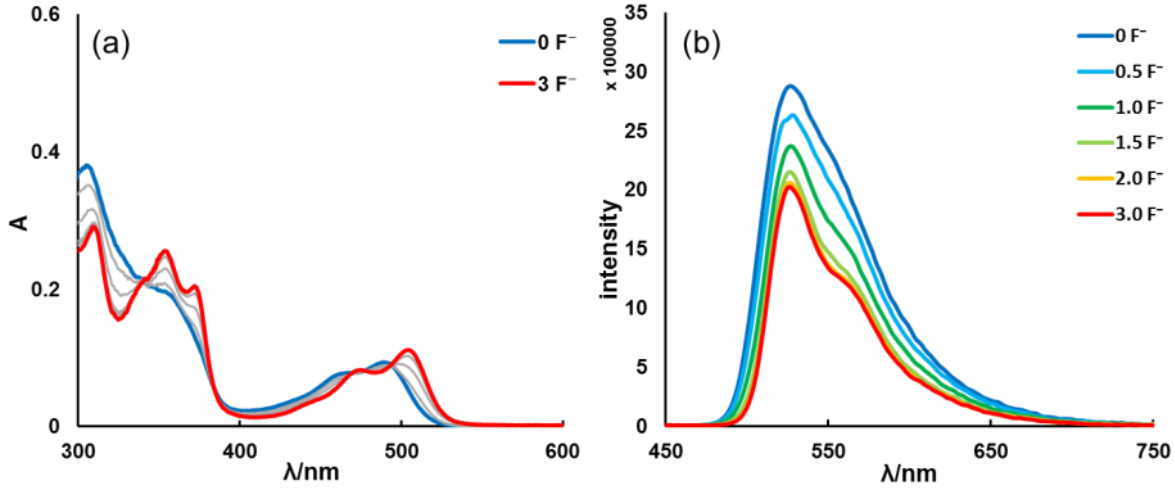


Figure S22. (a): The UV-Vis titration spectra, and (b): Fluorescent titration spectra of **4a** (c = 1×10^{-5} M, λ_{ex} = 320 nm, under air) by TBAF in THF at 298 K.

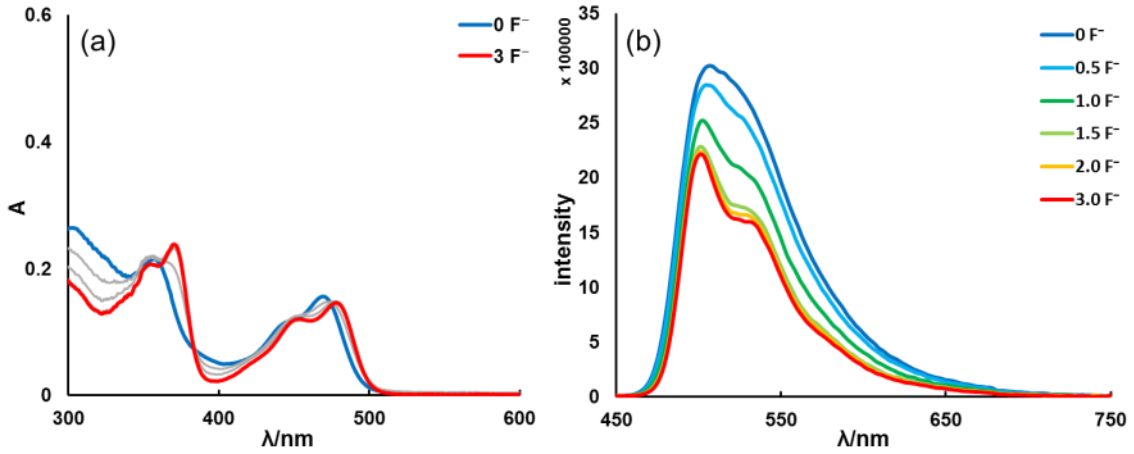


Figure S23: (a): The UV-Vis titration spectra, and (b): Fluorescent titration spectra of **4b** (c = 1×10^{-5} M, λ_{ex} = 320 nm, under air) by TBAF in THF at 298 K.

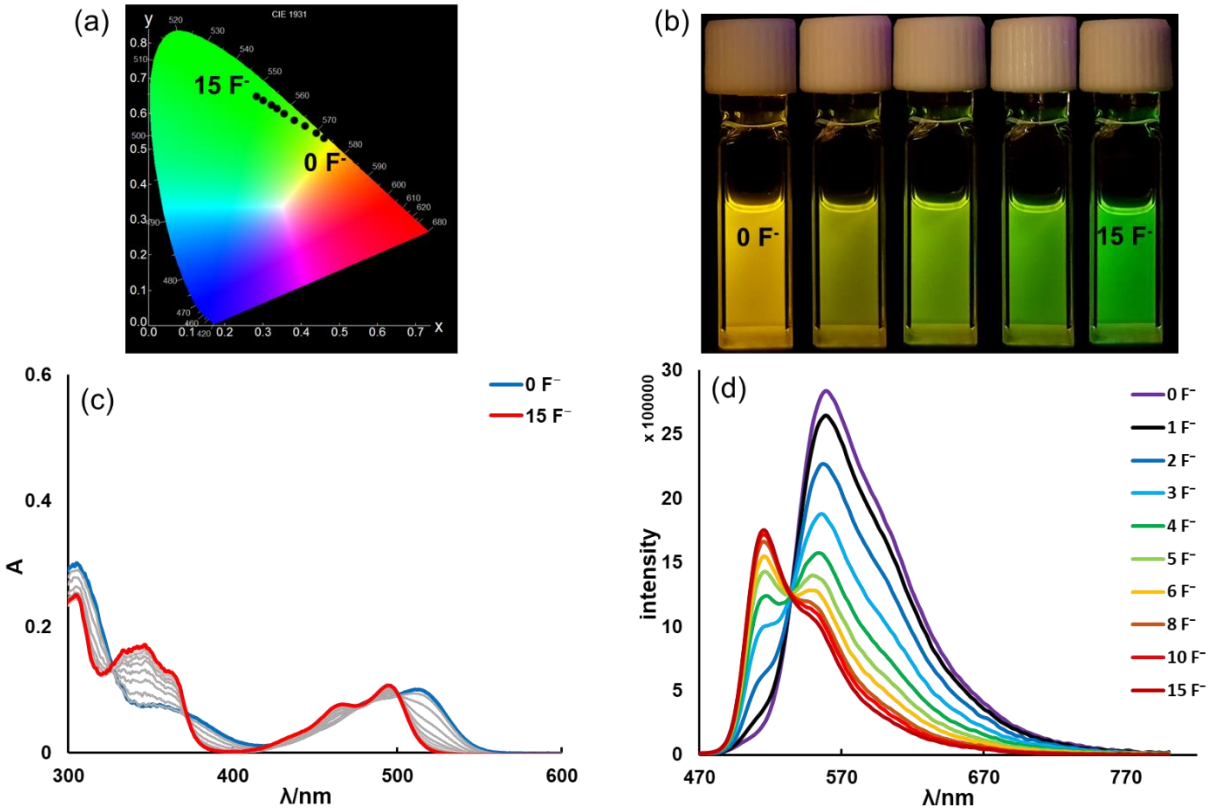


Figure S24. (a): CIE coordinates (CIE 1931). (b): Photographs of the solutions. (c): The UV-Vis titration spectra, and (d): Fluorescent titration spectra of **5a** (c = 1×10^{-5} M, λ_{ex} = 320 nm, under air) by TBAF in THF at 298 K.

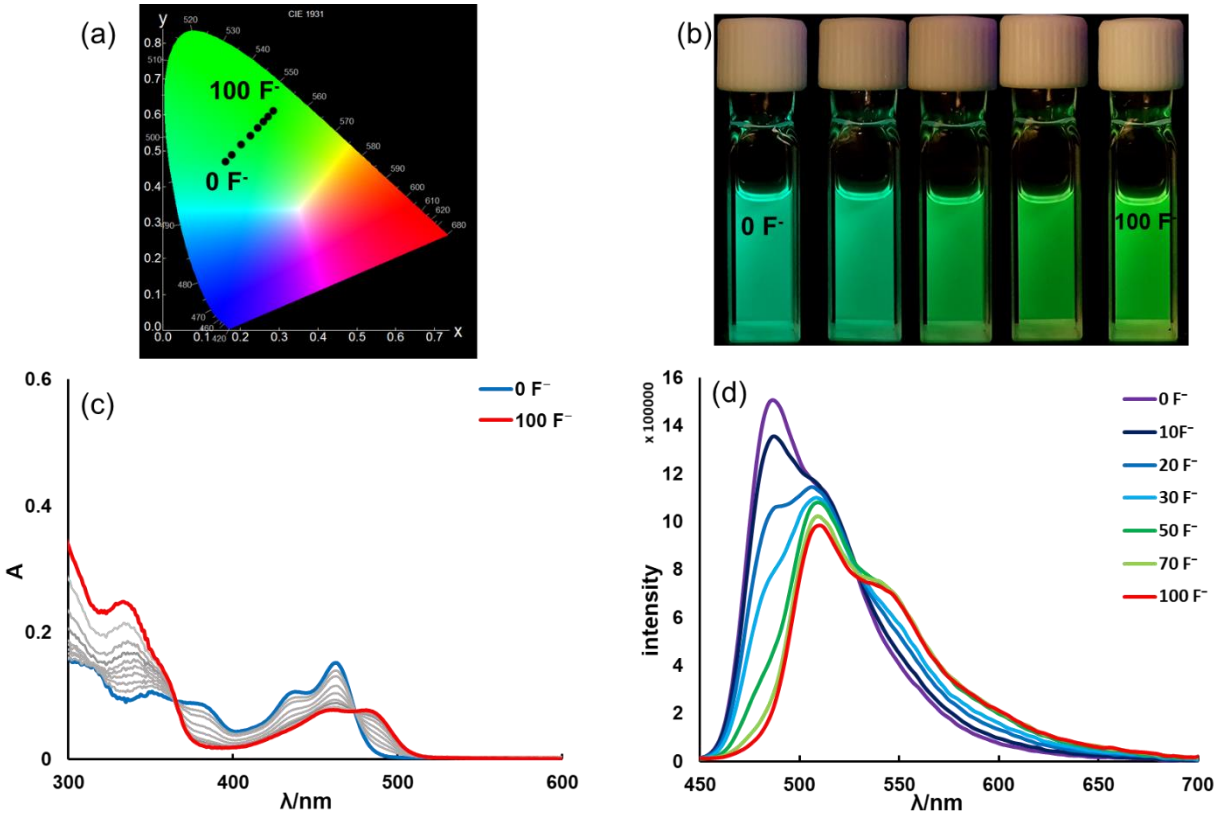


Figure S25. (a): CIE coordinates (CIE 1931). (b): Photographs of the solutions. (c): The UV-Vis titration spectra, and (d): Fluorescent titration spectra of **5b** (c = 1×10^{-5} M, λ_{ex} = 320 nm, under air) by TBAF in THF at 298 K.

Electrochemical Properties of **1a-5b**

Table S10: Electrochemical data of **1a-5b**

	E_{red} (eV)[a]	E_{ox} (eV)[b]	E_{LUMO} (eV)[c]	E_{HOMO} (eV)[c]	E_g^{exp} (eV)[c]	λ_{abs}(nm)[d]	E_g^{opt} (eV)[e]
1a	-2.73	0.22	-2.07	-5.02	2.95	478/505	2.46
1b	-2.60	0.23	-2.20	-5.03	2.83	467/493	2.52
2a	-2.68	0.02	-2.12	-4.82	2.70	507/539	2.30
2b	-2.92	0.15	-1.88	-4.95	3.07	466/484	2.56
3a	-2.42	0.04	-2.38	-4.84	2.46	516/565	2.19
3b	-2.56	0.23	-2.24	-5.03	2.79	471/495	2.51
4a	-2.73	0.16	-2.07	-4.96	2.89	489/517	2.40
4b	-2.84	0.19	-1.96	-4.99	3.03	470/494	2.51
5a	-2.60	0.11	-2.20	-4.91	2.71	511/546	2.27
5b	-2.85	0.20	-1.95	-5.00	3.05	462/484	2.56

[a] Determined from the first reduction peak positions in DPV diagrams, recorded in THF. [b] Determined from the first oxidation peak positions in DPV diagrams, recorded in CH_2Cl_2, [c] $E_{LUMO}/E_{HOMO} = -(4.8 + E_{red}/E_{ox})$, $E_g^{exp} = E_{LUMO}-E_{HOMO}$, [d] Absorption maximum/absorption edge, [e] E_g^{opt} = 1240/absorption edge.

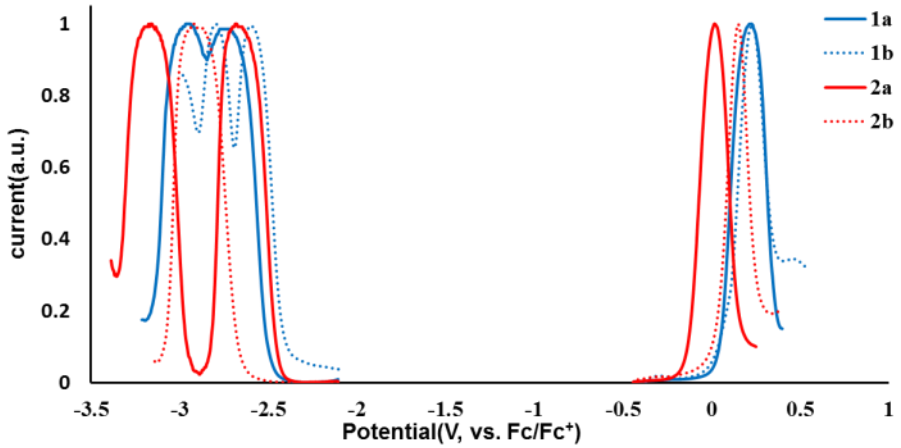


Figure S26: DPV diagrams of **1a/1b-2a/2b** showing the oxidation/ reduction waves (scan rate = 100 mV/s, using 0.1 M of $[NBu_4]PF_6$ as the electrolyte, recorded in CH_2Cl_2 (oxidation), and THF (reduction)).

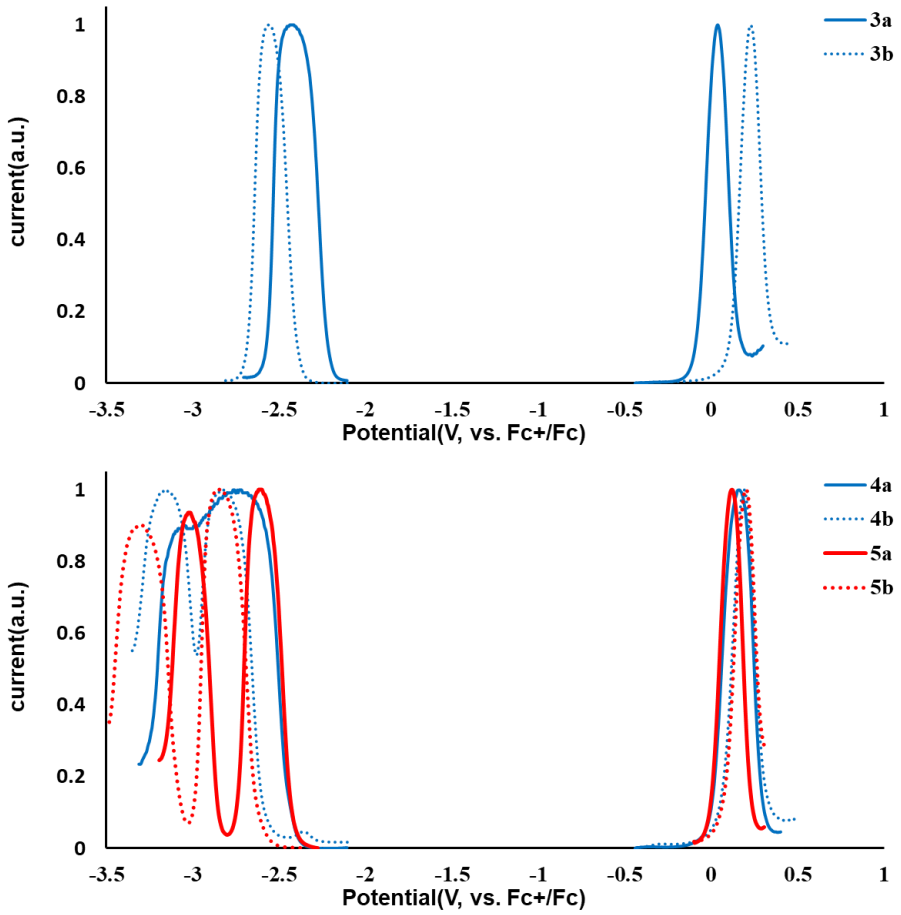


Figure S27: DPV diagrams of **3a/3b-5a/5b** showing the oxidation/ reduction waves (scan rate = 100 mV/s, using 0.1 M of $[NBu_4]PF_6$ as the electrolyte, recorded in CH_2Cl_2 (oxidation), and THF (reduction)).

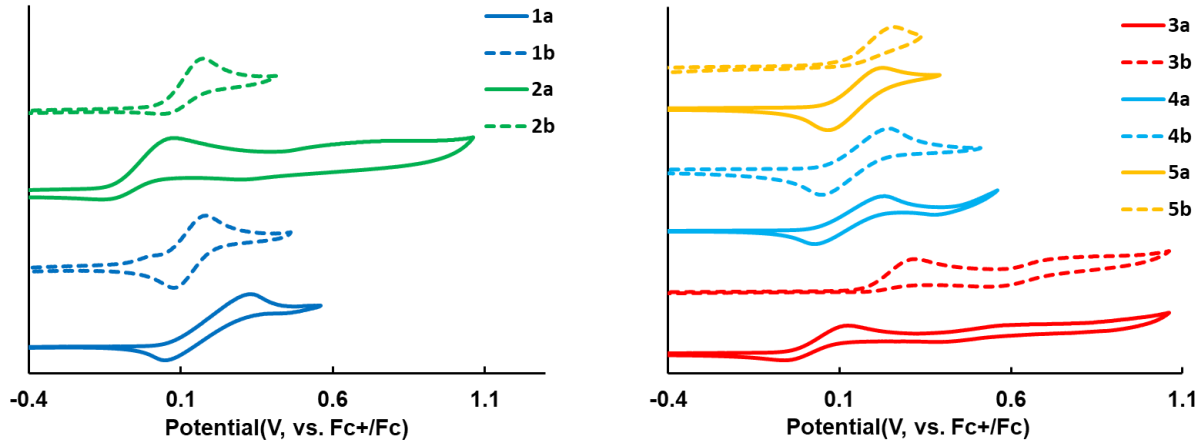


Figure S28: CV diagrams of **1a/1b-5a/5b** showing the oxidation waves at 50 mV/s with 0.1 M of $[NBu_4]PF_6$ as the electrolyte in CH_2Cl_2.

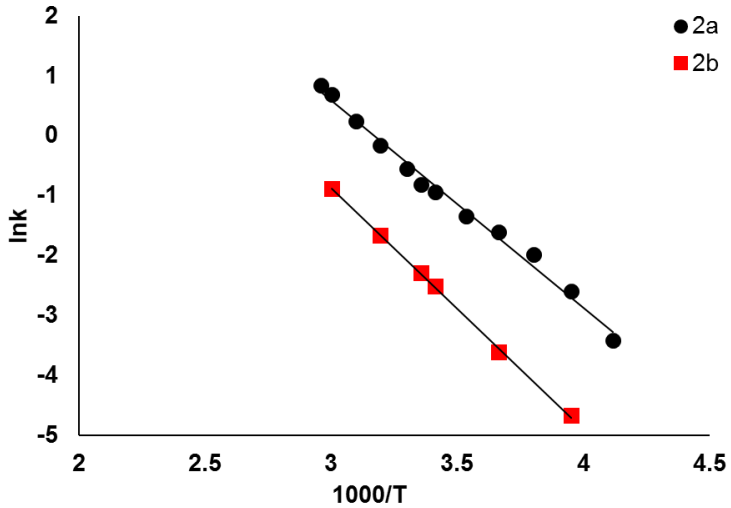


Figure S29: The Ln *K* vs. T^{-1} (kelvin) plots and fittings for **2a** and **2b**, using variable temperature ^{11}B NMR data for the determination of ΔH and ΔS (ΔH = 28.77 kJ/mol for **2a**; 33.5 kJ/mol for **2b**, ΔS = 91 J/mol/K for **2a**; 93 J/mol/K for **2b**).

III. DFT/TD-DFT Computational Data

DFT/TD-DFT calculations and geometry optimizations of all compounds were obtained at the M06-2X[7]/6-31g(d)[8] level of theory in CH_2Cl_2 using PCMs.

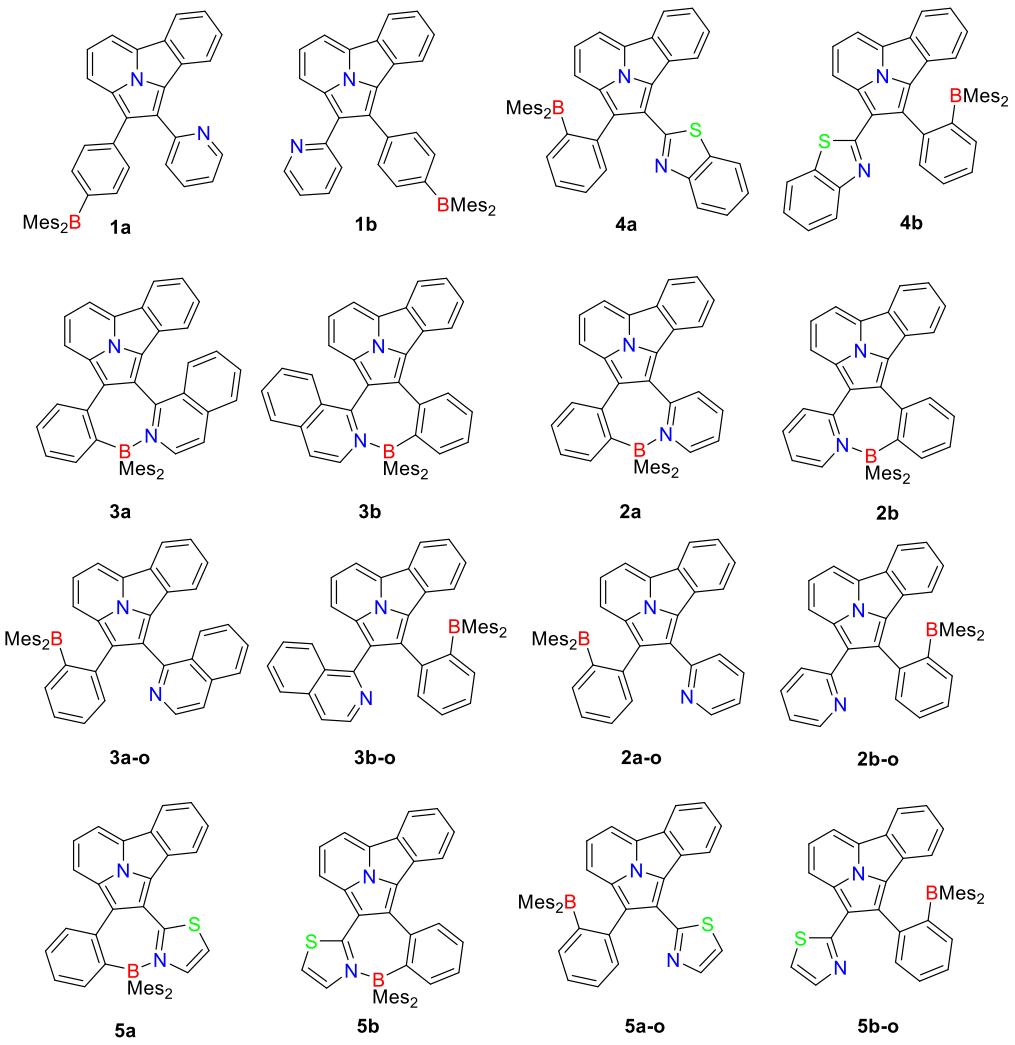


Figure S30: Structures studied by TD-DFT computation.

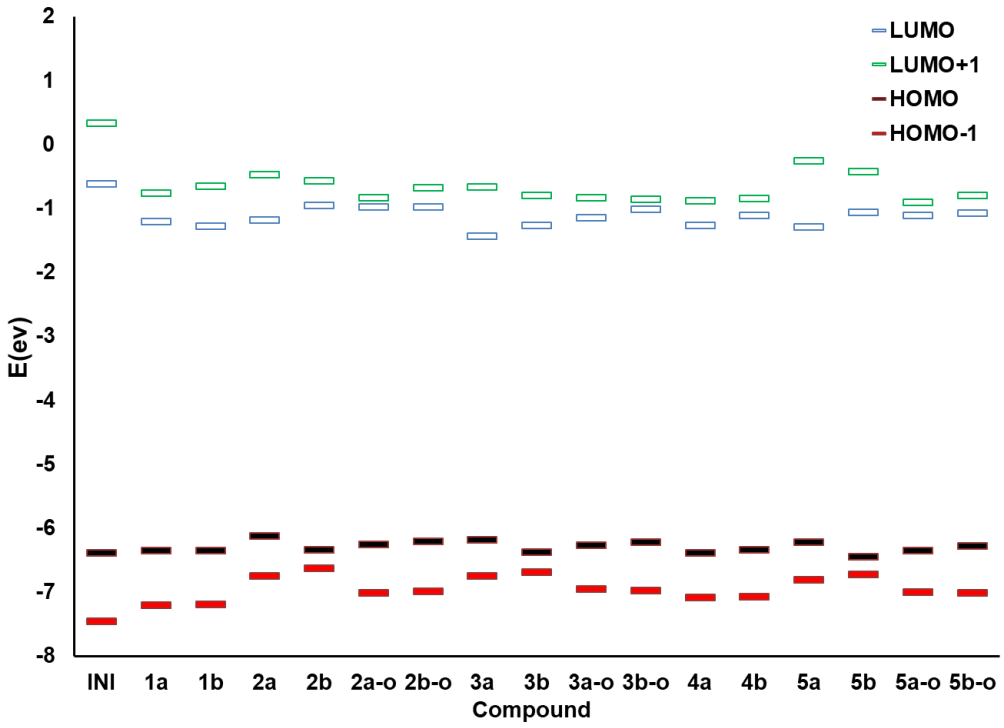


Figure S31: LUMO+1, LUMO, HOMO, and HOMO-1 energy levels from DFT data.

Table S11. TD-DFT calculated electronic transition configurations for **1a** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (77%)	397.33 (3.12)	0.4946
	HOMO → LUMO+1 (17%)		
S_2	HOMO → LUMO+1 (54%)	329.72(3.76)	0.4145
	HOMO → LUMO (14%)		
	HOMO-1 → LUMO (17%)		
S_3	HOMO-2 → LUMO (50%)	300.53 (4.13)	0.1048
	HOMO-2→ LUMO+1 (39%)		
S_4	HOMO-1 → LUMO (43%)	296.75 (4.18)	0.2614
	HOMO-1 → LUMO+1 (14%)		
	HOMO → LUMO+2 (19%)		
S_5	HOMO-3 → LUMO (42%)	284.79 (4.35)	0.0077
	HOMO-3 → LUMO+1 (29%)		
S_6	HOMO-6→LUMO (17%)	273.93(4.53)	0.2830
	HOMO-1→ LUMO (14%)		
	HOMO → LUMO+2 (49%)		
S_7	HOMO-4 →LUMO (50%)	269.03 (4.61)	0.0104
	HOMO-4 → LUMO +1 (36%)		
S_8	HOMO-5→ LUMO (43%)	262.93 (4.73)	0.0164
	HOMO-5→ LUMO+1 (31%)		
S_9	HOMO-7 → LUMO (29%)	261.38 (4.74)	0.0227
	HOMO-7 → LUMO+1 (10%)		
	HOMO → LUMO+3 (11%)		
S_{10}	HOMO-6 → LUMO (14%)	258.35 (4.80)	0.0040
	HOMO-1 → LUMO+1 (17%)		
	HOMO → LUMO+2 (14%)		
	HOMO → LUMO+4 (14%)		

Table S12. Primary orbitals which contribute to the calculated transitions of **1a** (iso = 0.03).

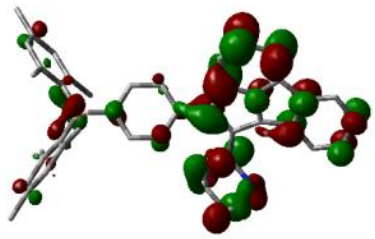
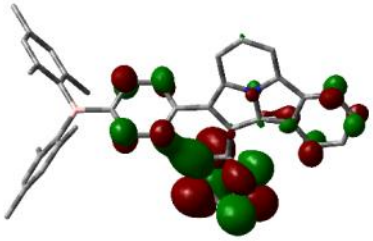
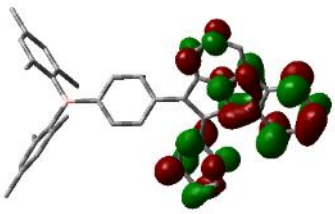
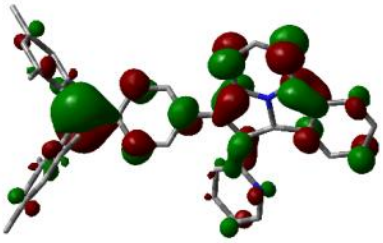
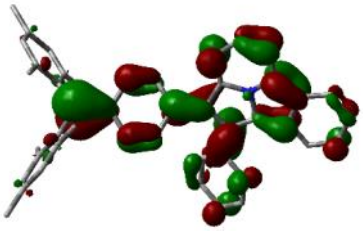
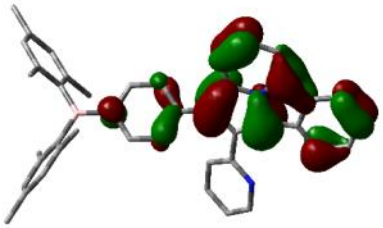
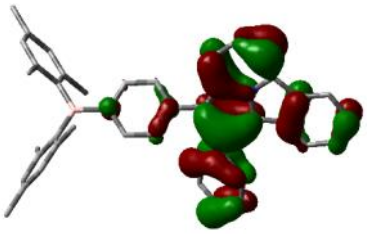
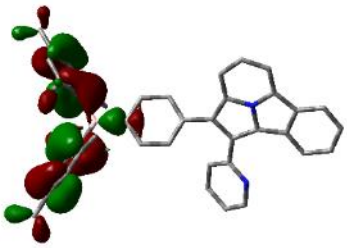
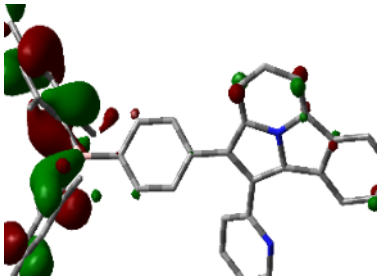
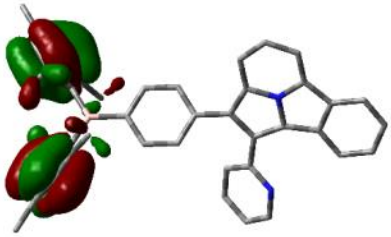
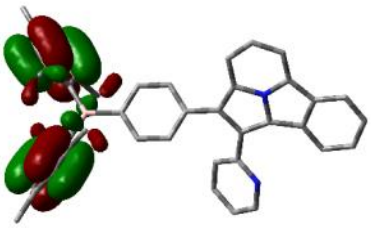
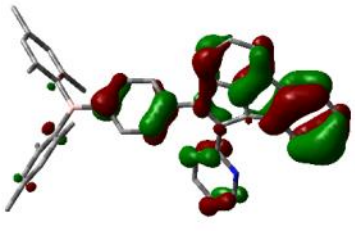
					
LUMO+4	0.53 eV	LUMO+3	0.33 eV	LUMO+2	0.12 eV
					
LUMO+1	-0.76 eV	LUMO	-1.20 eV	HOMO	-6.35 eV
					
HOMO-1	-7.20 eV	HOMO-2	-7.54 eV	HOMO-3	-7.57 eV
					
HOMO-4	-7.64 eV	HOMO-5	-7.76 eV	HOMO-6	-7.91 eV

Table S13. TD-DFT calculated electronic transition configurations for **1b** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (65%)	390.06 (3.18)	0.2915
	HOMO → LUMO+1 (31%)		
S_2	HOMO-1 → LUMO (69%)	316.36 (3.92)	0.5614
S_3	HOMO-2 → LUMO (68%)	308.95 (4.01)	0.1345
	HOMO-2 → LUMO+1 (22%)		
S_4	HOMO → LUMO (27%)	302.53 (4.10)	0.0470
	HOMO → LUMO+1 (50%)		
S_5	HOMO-3 → LUMO (40%)	291.77 (4.25)	0.0947
	HOMO-1 → LUMO+1 (14%)		
	HOMO → LUMO+3 (16%)		
S_6	HOMO-5 → LUMO (15%)	275.74 (4.50)	0.4394
	HOMO-3 → LUMO (13%)		
	HOMO → LUMO+2 (31%)		
S_7	HOMO-4 → LUMO (63%)	274.15 (4.52)	0.0454
	HOMO-4 → LUMO+1 (20%)		
S_8	HOMO-5 → LUMO (14%)	273.79 (4.53)	0.1874
	HOMO → LUMO+2 (33%)		
	HOMO → LUMO+3 (18%)		
S_9	HOMO-6 → LUMO (14%)	270.87 (4.58)	0.0582
	HOMO-5 → LUMO (34%)		
	HOMO-5 → LUMO+1 (13%)		
	HOMO → LUMO+3 (16%)		
S_{10}	HOMO-7 → LUMO (55%),	260.12 (4.77)	0.0356

Table S14. Primary orbitals which contribute to the calculated transitions of **1b** (iso = 0.03).

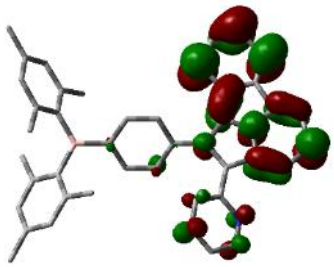
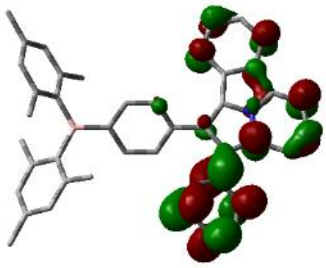
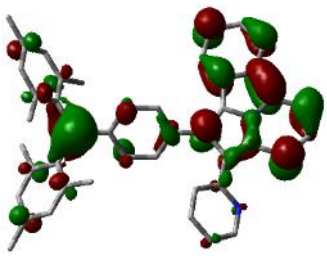
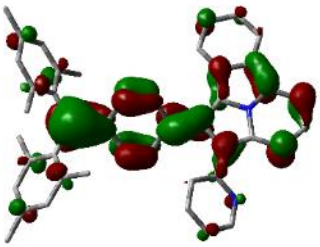
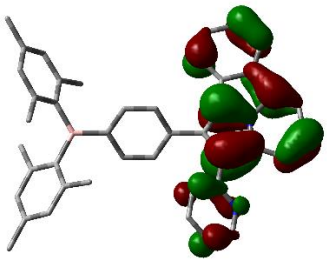
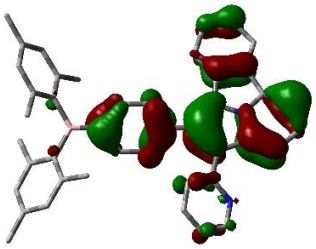
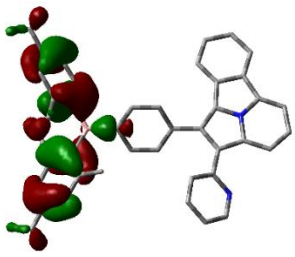
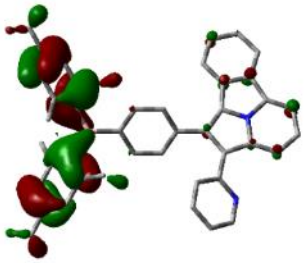
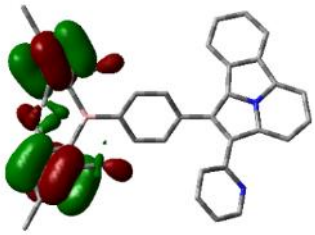
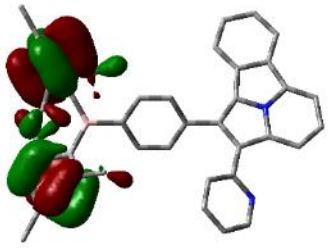
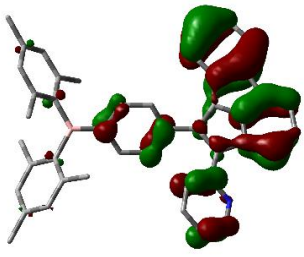
					
LUMO+3	0.21 eV	LUMO+2	0.09 eV	LUMO+1	-0.65 eV
					
LUMO	-1.27 eV	HOMO	-6.35 eV	HOMO-1	-7.19 eV
					
HOMO-2	-7.53 eV	HOMO-3	-7.64 eV	HOMO-4	-7.73 eV
					
HOMO-5	-7.75 eV	HOMO-6	-7.92 eV		

Table S15. TD-DFT calculated electronic transition configurations for **2a** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (89%)	424.31 (2.92)	0.1792
S_2	HOMO-1 → LUMO (81%)	341.29 (3.63)	0.0988
S_3	HOMO-1 → LUMO(10%)	323.26 (3.84)	0.0025
	HOMO → LUMO+1(74%)		
S_4	HOMO-4 → LUMO (25%)	298.87 (4.15)	0.0266
	HOMO-2 → LUMO(31%)		
	HOMO → LUMO+3 (16%)		
S_5	HOMO-4 → LUMO(12%)	292.76 (4.23)	0.0040
	HOMO-3 → LUMO (10%)		
	HOMO-2 → LUMO (56%)		
S_6	HOMO → LUMO+2 (63%)	287.48 (4.31)	0.0610
S_7	HOMO-1 → LUMO+1 (58%)	281.19 (4.41)	0.1519
S_8	HOMO-1 → LUMO+1 (22%)	272.46 (4.55)	0.1247
	HOMO → LUMO+3 (34%)		
S_9	HOMO-4 → LUMO (25%)	264.82(4.68)	0.1407
	HOMO-3 → LUMO (34%)		
S_{10}	HOMO-6 → LUMO (45%),	262.56 (4.72)	0.0559
	HOMO-3 → LUMO (18%)		

Table S16. Primary orbitals which contribute to the calculated transitions of **2a** (iso = 0.03).

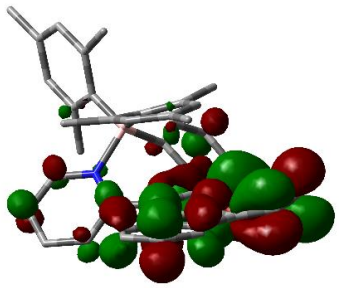
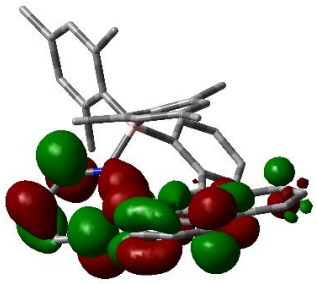
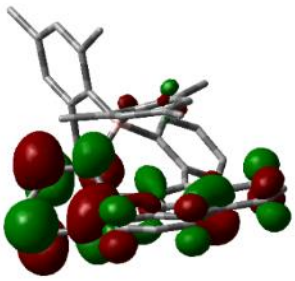
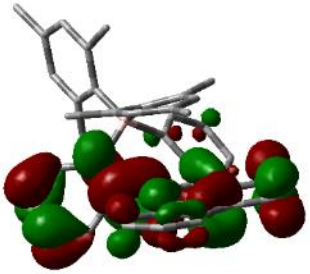
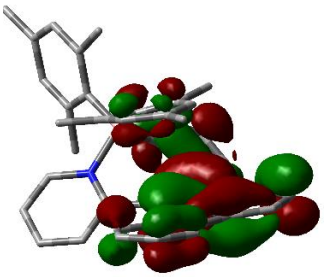
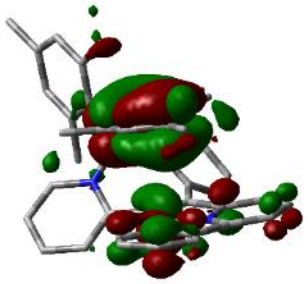
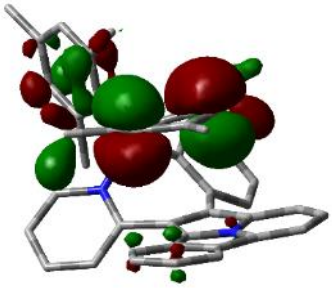
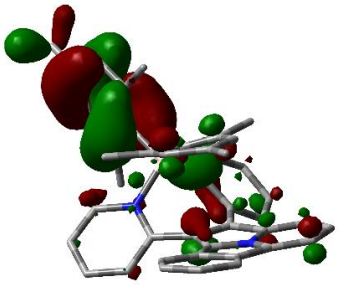
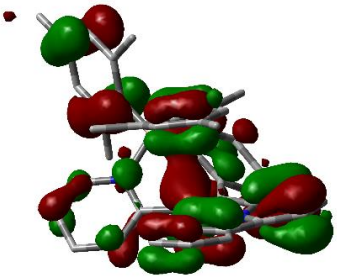
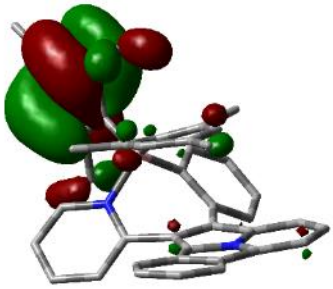
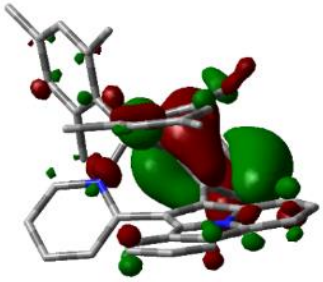
					
LUMO+3	0.34 eV	LUMO+2	0.01 eV	LUMO+1	-0.47 eV
					
LUMO	-1.18 eV	HOMO	-6.12 eV	HOMO-1	-6.74 eV
					
HOMO-2	-7.18 eV	HOMO-3	-7.33 eV	HOMO-4	-7.46 eV
					
HOMO-5	-7.47 eV	HOMO-6	-7.68 eV		

Table S17. TD-DFT calculated electronic transition configurations for **2b** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (86%)	382.39 (3.24)	0.2741
S_2	HOMO-1 → LUMO (41%)	336.94 (3.68)	0.0786
	HOMO → LUMO+1(41%)		
S_3	HOMO-1 → LUMO (51%)	316.11 (3.92)	0.1314
	HOMO → LUMO+1 (36%)		
S_4	HOMO-2 → LUMO (20%)	293.65 (4.22)	0.0144
	HOMO-1 → LUMO+1 (52%)		
	HOMO → LUMO+3 (12%)		
S_5	HOMO-2 → LUMO (38%)	287.89 (4.31)	0.0092
	HOMO-1 → LUMO+1 (31%)		
S_6	HOMO-3 → LUMO (18%)	280.56 (4.42)	0.0490
	HOMO-2 → LUMO (32%)		
	HOMO → LUMO+3 (29%)		
S_7	HOMO-3 → LUMO (13%)	277.32 (4.47)	0.0652
	HOMO → LUMO+2 (61%)		
S_8	HOMO-3 → LUMO (35%)	271.30 (4.57)	0.1318
	HOMO-2 → LUMO+1 (10%)		
	HOMO → LUMO+2 (10%)		
	HOMO → LUMO+3 (21%)		
S_9	HOMO-2 → LUMO+1 (68%)	261.86 (4.73)	0.1385
S_{10}	HOMO-1 → LUMO +2 (44%)	255.63 (4.85)	0.1225
	HOMO-1 → LUMO +3 (15%)		

Table S18. Primary orbitals which contribute to the calculated transitions of **2b** (iso = 0.03).

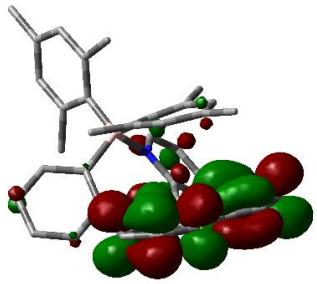
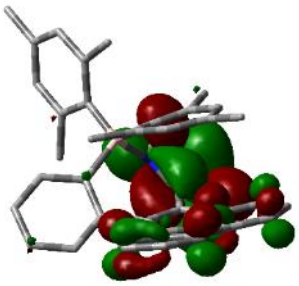
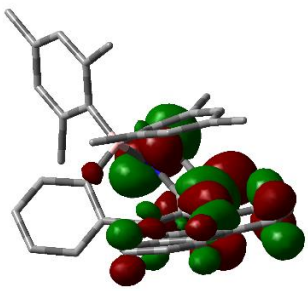
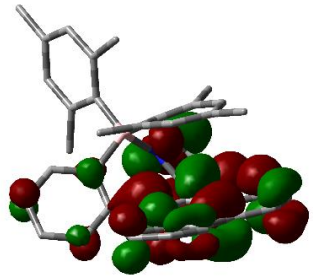
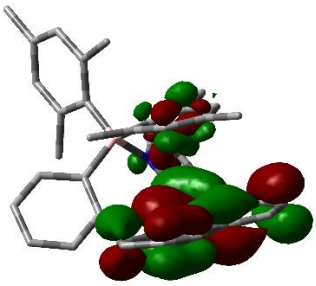
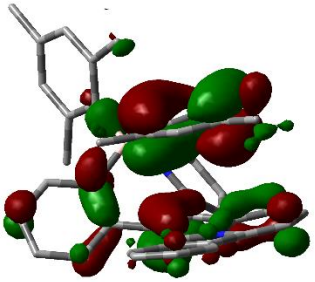
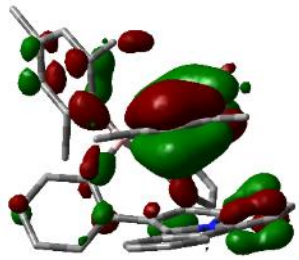
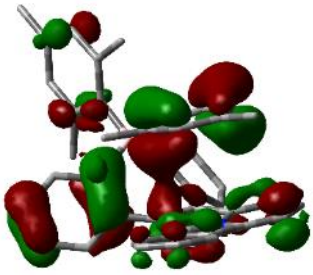
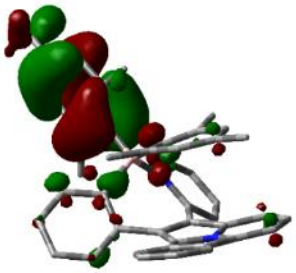
					
LUMO+3	0.20 eV	LUMO+2	0.01 eV	LUMO+1	-0.57 eV
					
LUMO	-0.95 eV	HOMO	-6.34 eV	HOMO-1	-6.63 eV
					
HOMO-2	-7.10 eV	HOMO-3	-7.27 eV	HOMO-4	-7.36 eV

Table S19. TD-DFT calculated electronic transition configurations for **2a-o** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (89%)	397.94 (3.12)	0.1779
S_2	HOMO → LUMO+1 (71%)	348.05 (3.56)	0.0339
S_3	HOMO-2 → LUMO+1 (27%)	312.24 (3.97)	0.0428
	HOMO-1 → LUMO (29%)		
	HOMO-1 → LUMO+1 (22%)		
S_4	HOMO-1 → LUMO (49%),	301.44 (4.11)	0.3129
	HOMO-1 → LUMO+1 (17%)		
S_5	HOMO-4 → LUMO+1 (76%)	290.54 (4.27)	0.1542
S_6	HOMO-2 → LUMO (19%)	284.32 (4.36)	0.0766
	HOMO-1 → LUMO (10%)		
	HOMO → LUMO+2 (51%)		
S_7	HOMO-3 → LUMO+1 (31%)	280.37 (4.42)	0.0364
	HOMO-2 → LUMO+1 (31%)		
	HOMO-1 → LUMO+1 (17%)		
S_8	HOMO-2 → LUMO (61%)	272.08 (4.56)	0.1397
	HOMO → LUMO+2 (24%)		
S_9	HOMO-5 → LUMO+1 (10%)	269.24 (4.61)	0.0513
	HOMO-3 → LUMO (19%)		
	HOMO-3 → LUMO+1 (24%)		
	HOMO-2 → LUMO+1 (11%)		
	HOMO-1 → LUMO+1 (19%)		
S_{10}	HOMO-5 → LUMO+1 (64%)	267.87 (4.63)	0.0250

Table S20. Primary orbitals which contribute to the calculated transitions of **2a-o** (iso = 0.03).

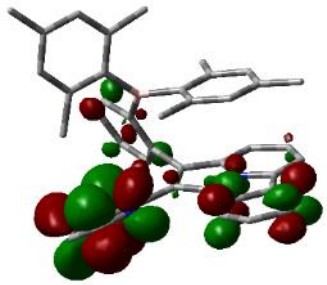
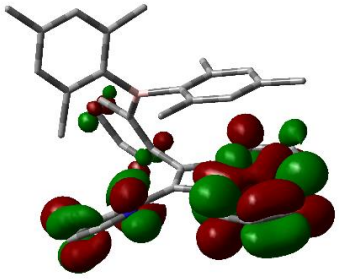
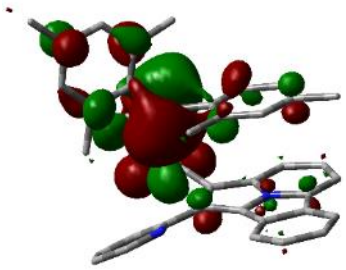
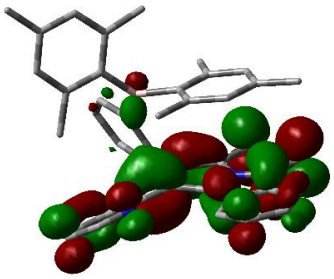
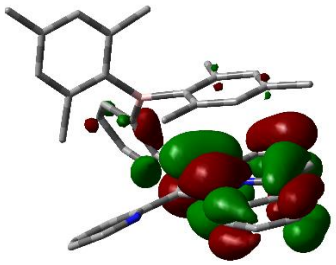
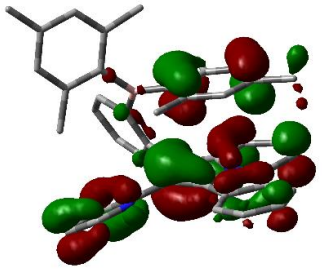
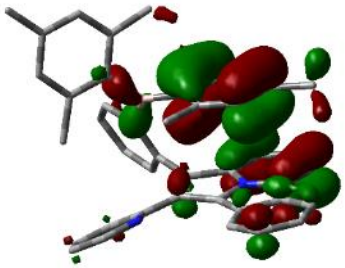
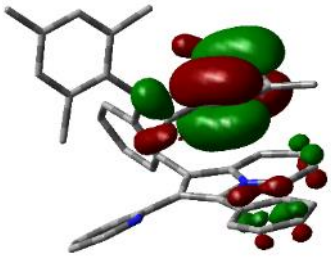
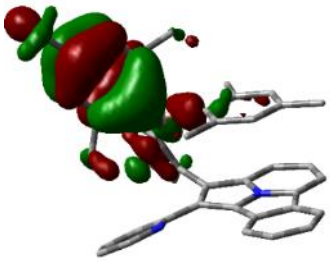
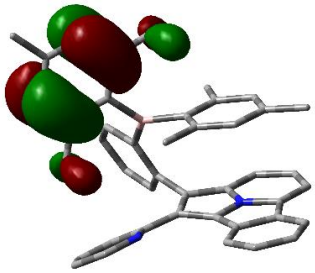
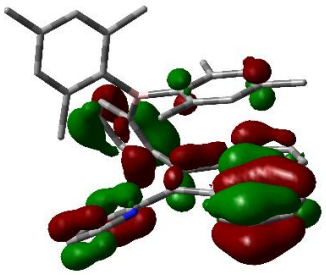
					
LUMO+3	0.38 eV	LUMO+2	0.15 eV	LUMO+1	-0.83 eV
					
LUMO	-0.98 eV	HOMO	-6.25 eV	HOMO-1	-7.01 eV
					
HOMO-2	-7.27 eV	HOMO-3	-7.43 eV	HOMO-4	-7.54 eV
					
HOMO-5	-7.68 eV	HOMO-6	-7.88 eV		

Table S21. TD-DFT calculated electronic transition configurations for **2b-o** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (70%)	394.00 (3.15)	0.2080
	HOMO → LUMO+1 (24%)		
S_2	HOMO-1 → LUMO (18%)	334.91 (3.70)	0.0973
	HOMO → LUMO (16%),		
	HOMO → LUMO+1 (56%)		
S_3	HOMO-1 → LUMO (53%)	321.22 (3.86)	0.0161
	HOMO-1 → LUMO+1 (10%)		
	HOMO → LUMO+1 (16%)		
S_4	HOMO-1 → LUMO+1 (24%)	300.88 (4.12)	0.0837
	HOMO → LUMO+2 (31%)		
S_5	HOMO-3 → LUMO (63%)	292.79 (4.23)	0.2140
	HOMO-1 → LUMO+1 (13%)		
	HOMO → LUMO+2 (10%)		
	HOMO-3 → LUMO+1 (5%)		
	HOMO-2 → LUMO (2%)		
	HOMO-1 → LUMO (2%),		
	HOMO → LUMO+3 (2%)		
S_6	HOMO-2 → LUMO (14%)	286.00 (4.34)	0.2088
	HOMO → LUMO+2 (43%)		
	HOMO → LUMO+3 (27%)		
S_7	HOMO-2 → LUMO (63%)	281.41 (4.41)	0.0161
S_8	HOMO-1 → LUMO (10%)	272.41 (4.55)	0.1295
	HOMO-1 → LUMO+1 (29%)		
	HOMO → LUMO+3 (31%)		
S_9	HOMO-5 → LUMO (23%)	267.14 (4.64)	0.0535
	HOMO-5 → LUMO+1 (14%)		
	HOMO-4 → LUMO (26%)		
S_{10}	HOMO-5 → LUMO (24%)	264.42 (4.69)	0.0788
	HOMO-5 → LUMO+1 (12%)		
	HOMO-4 → LUMO (20%)		

Table S22. Primary orbitals which contribute to the calculated transitions of **2b-o** (iso = 0.03).

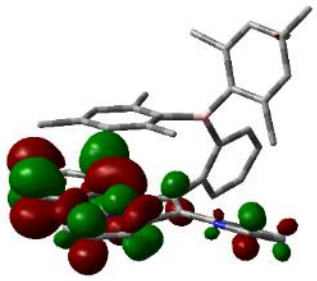
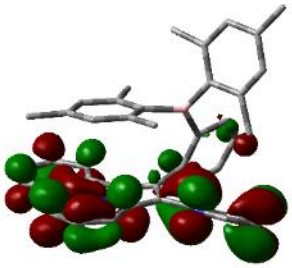
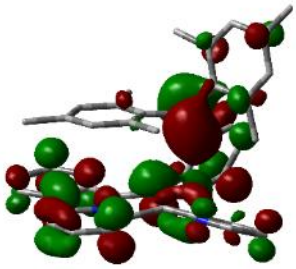
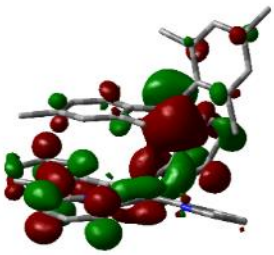
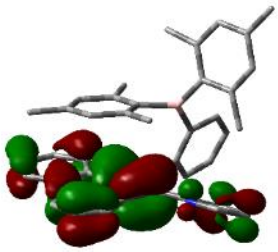
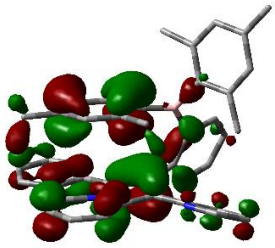
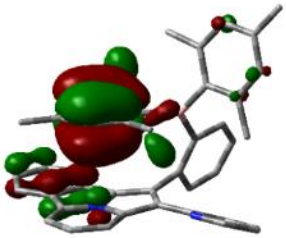
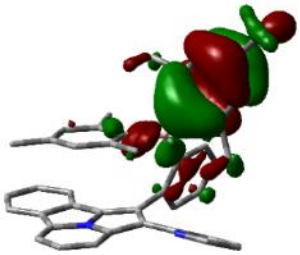
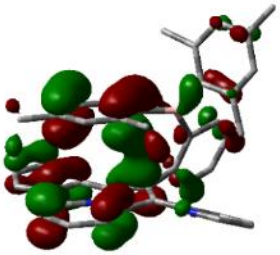
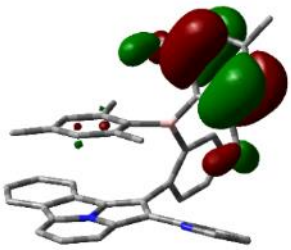
					
LUMO+3	0.28 eV	LUMO+2	0.07 eV	LUMO+1	-0.67 eV
					
LUMO	-0.97 eV	HOMO	-6.20 eV	HOMO-1	-6.98 eV
					
HOMO-2	-7.35 eV	HOMO-3	-7.51 eV	HOMO-4	-7.61 eV
					
HOMO-5	-7.70 eV				

Table S23. TD-DFT calculated electronic transition configurations for **3a** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (87%)	432.55 (2.87)	0.1422
	HOMO → LUMO+1 (10%)		
S_2	HOMO-1 → LUMO (57%)	361.84 (3.43)	0.1045
	HOMO → LUMO+1 (27%)		
S_3	HOMO-1 → LUMO (32%)	353.82 (3.50)	0.0412
	HOMO → LUMO +1 (56%)		
S_4	HOMO-4 → LUMO+1 (14%)	317.34 (3.91)	0.0951
	HOMO-3 → LUMO (10%)		
	HOMO-2 → LUMO (51%)		
S_5	HOMO-5 → LUMO(19%)	304.23 (4.08)	0.0268
	HOMO-4 → LUMO (13%)		
	HOMO-3 → LUMO (16%)		
	HOMO-2 → LUMO (39%)		
S_6	HOMO-1 → LUMO+1 (30%)	294.04 (4.22)	0.0399
	HOMO → LUMO+3 (41%)		
S_7	HOMO-1 → LUMO+1 (55%)	286.40 (4.33)	0.0218
	HOMO → LUMO+3 (20%)		
S_8	HOMO-3 → LUMO (25%)	283.24 (4.38)	0.0016
	HOMO → LUMO+2 (52%)		
S_9	HOMO-4 → LUMO (12%)	281.22 (4.41)	0.0406
	HOMO-3→ LUMO (33%)		
	HOMO → LUMO+2 (34%)		
S_{10}	HOMO-8 → LUMO (13%)	276.10 (4.49)	0.0271
	HOMO-6 → LUMO (64%)		

Table S24. Primary orbitals which contribute to the calculated transitions of **3a** (iso = 0.03).

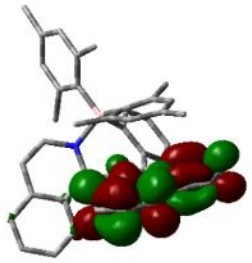
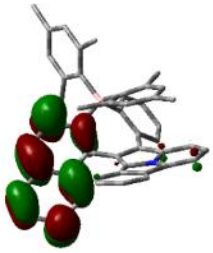
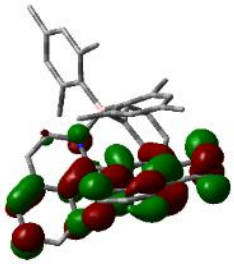
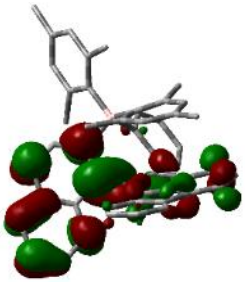
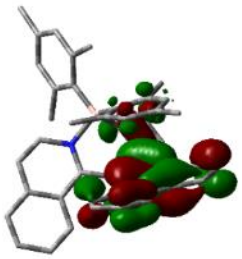
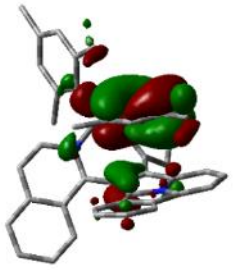
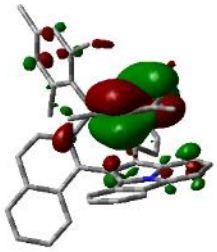
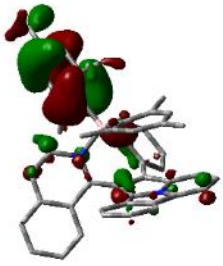
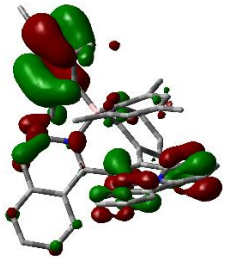
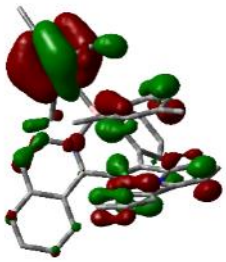
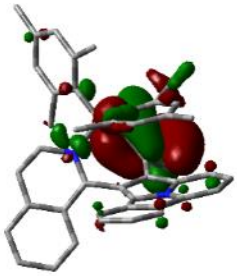
					
LUMO+3	0.18 eV	LUMO+2	-0.28 eV	LUMO+1	-0.66 eV
					
LUMO	-1.43 eV	HOMO	-6.18 eV	HOMO-1	-6.74 eV
					
HOMO-2	-7.09 eV	HOMO-3	-7.30 eV	HOMO-4	-7.42 eV
					
HOMO-5	-7.48 eV	HOMO-6	-7.66 eV		

Table S25. TD-DFT calculated electronic transition configurations for **3b** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (80%) HOMO → LUMO+1 (12%)	395.79 (3.13)	0.4025
S_2	HOMO-1 → LUMO (14%) HOMO → LUMO+1 (70%)	365.75 (3.39)	0.0107
S_3	HOMO-1 → LUMO (77%) HOMO → LUMO+1 (11%)	334.67 (3.70)	0.0287
S_4	HOMO-1 → LUMO+1 (87%)	308.01 (4.03)	0.0209
S_5	HOMO-3 → LUMO (50%) HOMO-2 → LUMO (31%)	304.44 (4.07)	0.0433
S_6	HOMO-3 → LUMO (24%) HOMO-2 → LUMO (54%)	291.54 (4.25)	0.0182
S_7	HOMO-7 → LUMO (20%) , HOMO → LUMO+2 (32%)	283.89 (4.37)	0.0328
S_8	HOMO → LUMO+2 (30%) HOMO → LUMO+3 (30%)	281.09 (4.41)	0.0381
S_9	HOMO-8 → LUMO (20%) HOMO-7 → LUMO(30%) HOMO → LUMO+2 (14%)	274.81 (4.51)	0.0253
S_{10}	HOMO-4 → LUMO (85%)	272.71 (4.54)	0.0196

Table S26. Primary orbitals which contribute to the calculated transitions of **3b** (iso = 0.03).

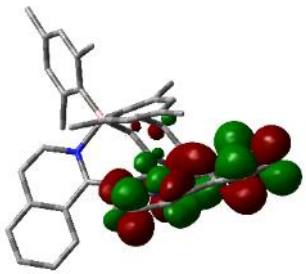
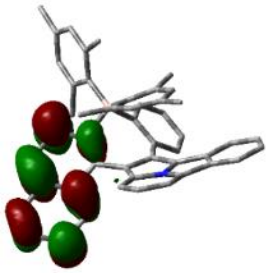
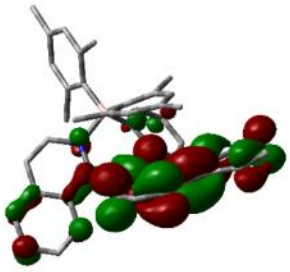
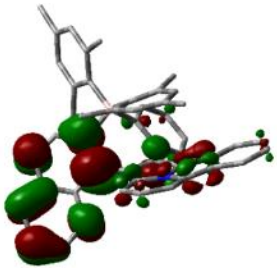
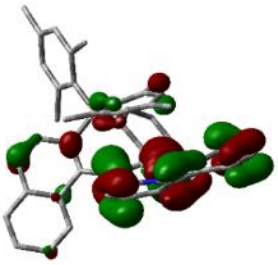
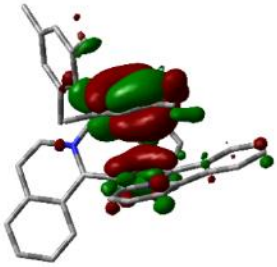
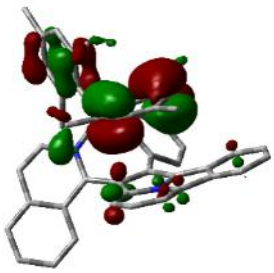
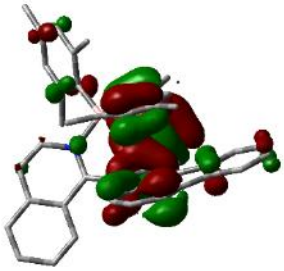
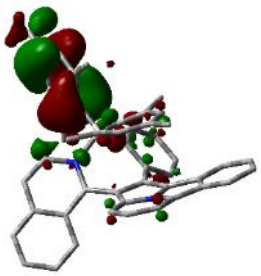
					
LUMO+3	0.21 eV	LUMO+2	-0.23 eV	LUMO+1	-0.80 eV
					
LUMO	-1.26 eV	HOMO	-6.37 eV	HOMO-1	-6.68 eV
					
HOMO-2	-7.14 eV	HOMO-3	-7.20 eV	HOMO-4	-7.34 eV

Table S27. TD-DFT calculated electronic transition configurations for **3a-o** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (84%)	403.91 (3.07)	0.1819
S_2	HOMO → LUMO+1 (76%)	347.16 (3.57)	0.0353
S_3	HOMO-1 → LUMO (81%)	320.53 (3.87)	0.2332
S_4	HOMO-2 → LUMO+1 (33%)	308.56 (4.02)	0.2339
	HOMO-1 → LUMO+1 (28%)		
	HOMO → LUMO+1 (11%)		
S_5	HOMO → LUMO+2 (77%)	300.86 (4.12)	0.0266
S_6	HOMO-4 → LUMO+1 (78%)	289.82 (4.28)	0.1552
S_7	HOMO-5 → LUMO (13%)	284.48 (4.36)	0.0090
	HOMO-2 → LUMO (14%)		
	HOMO → LUMO+4 (29%)		
S_8	HOMO-3 → LUMO+1 (29%)	281.59 (4.40)	0.0316
	HOMO-2 → LUMO (15%)		
	HOMO-2 → LUMO+1 (3%)		
	HOMO-1 → LUMO+1 (25%)		
S_9	HOMO-5 → LUMO (10%)	278.91 (4.45)	0.0410
	HOMO-2 → LUMO (45%)		
	HOMO-1 → LUMO+2 (11%)		
S_{10}	HOMO-12 → LUMO (21%)	277.23 (4.47)	0.0401
	HOMO-11 → LUMO (11%)		
	HOMO-3 →LUMO (13%)		

Table S28. Primary orbitals which contribute to the calculated transitions of **3a-o** (iso = 0.03).

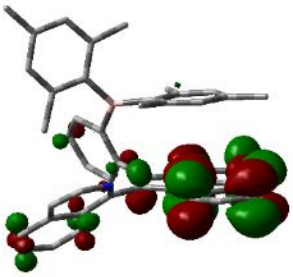
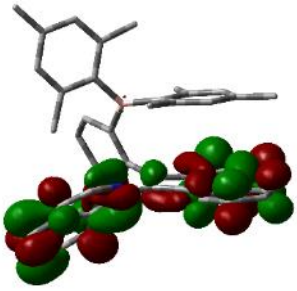
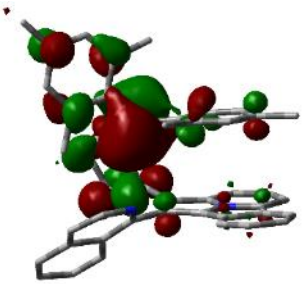
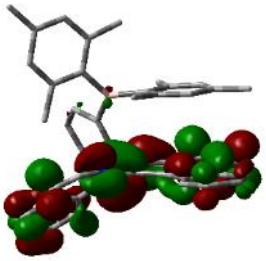
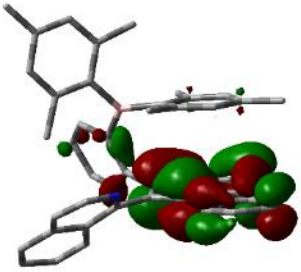
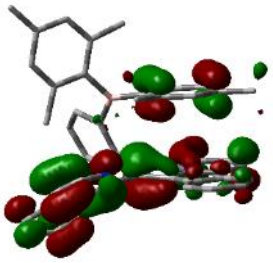
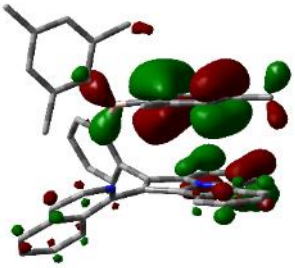
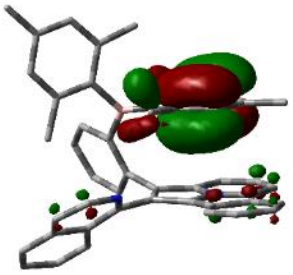
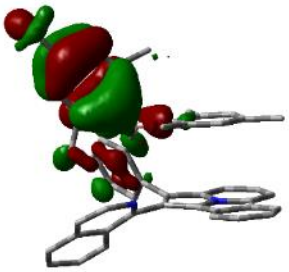
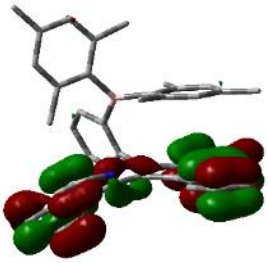
					
LUMO+4	0.32 eV	LUMO+2	-0.25eV	LUMO+1	-0.83 eV
					
LUMO	-1.14 eV	HOMO	-6.26 eV	HOMO-1	-6.95 eV
					
HOMO-2	-7.26 eV	HOMO-3	-7.42eV	HOMO-4	-7.54 eV
					
HOMO-5	-7.67 eV				

Table S29. TD-DFT calculated electronic transition configurations for **3b-o** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (77%)	394.03 (3.15)	0.2857
	HOMO → LUMO+1 (11%)		
S_2	HOMO → LUMO+1 (74%)	344.65 (3.60)	0.1981
	HOMO-1 → LUMO (11%)		
S_3	HOMO-1 → LUMO (43%)	327.87 (3.78)	0.0056
	HOMO-1 → HOMO+1 (26%)		
S_4	HOMO-1 → LUMO (10%)	316.13 (3.92)	0.0631
	HOMO → LUMO (12%),		
	HOMO → LUMO +2 (64%)		
S_5	HOMO-3 → LUMO (23%)	295.32 (4.20)	0.2567
S_6	HOMO-5 → LUMO (12%)	291.64 (4.25)	0.0439
	HOMO-1→ LUMO+1 (17%)		
	HOMO→ LUMO+4 (19%)		
S_7	HOMO-2 → LUMO (62%)	283.13 (4.38)	0.0397
S_8	HOMO-3 → LUMO (11%)	278.48 (4.45)	0.0157
	HOMO-1 → LUMO+1 (24%)		
	HOMO → LUMO+4(19%)		
S_9	HOMO → LUMO+3 (32%)	273.41 (4.53)	0.0270
S_{10}	HOMO-11 → LUMO+1(16%)	272.22 (4.55)	0.0044

Table S30. Primary orbitals which contribute to the calculated transitions of **3b-o** (iso = 0.03).

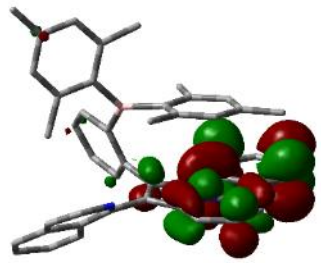
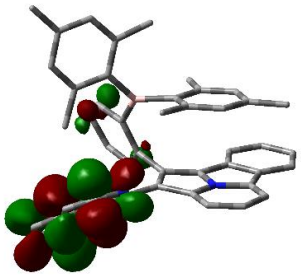
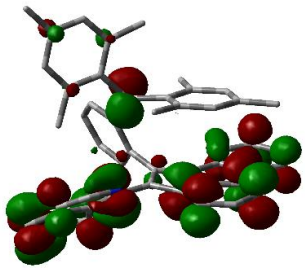
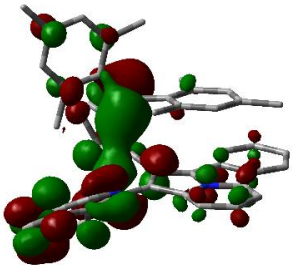
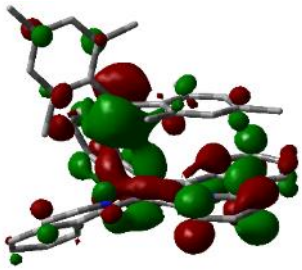
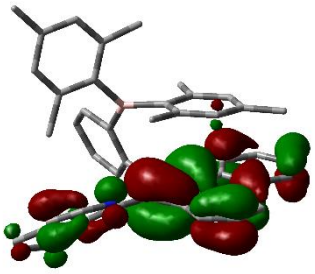
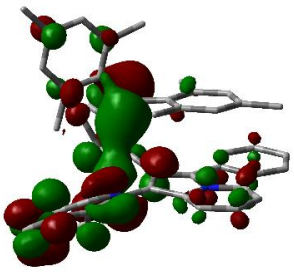
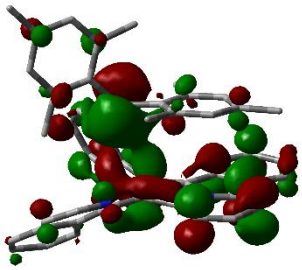
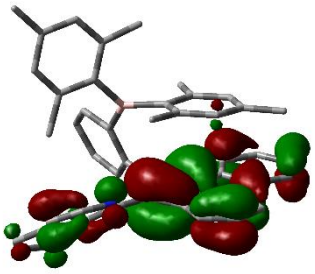
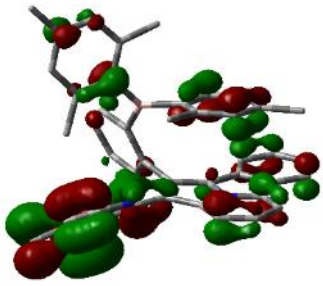
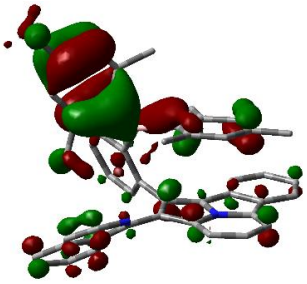
					
LUMO+4	0.29 eV	LUMO+3	0.27 eV	LUMO+2	-0.35 eV
					
LUMO+1	-0.86 eV	LUMO	-1.01 eV	HOMO	-6.22 eV
					
HOMO-1	-6.97 eV	HOMO-2	-7.40 eV	HOMO-3	-7.48 eV
					
HOMO-4	-7.55 eV	HOMO-5	-7.58 eV		

Table S31. TD-DFT calculated electronic transition configurations for **4a** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (93%)	407.08 (3.05)	0.1871
S_2	HOMO → LUMO+1(78%)	342.43 (3.62)	0.0263
S_3	HOMO-1 → LUMO (83%)	319.95 (3.88)	0.3730
S_4	HOMO-4 → LUMO+1 (11%)	304.81 (4.07)	0.2607
	HOMO-2 → LUMO+1 (29%)		
	HOMO-1 → LUMO+1 (21%)		
	HOMO → LUMO+1 (14%)		
S_5	HOMO-4 → LUMO+1 (69%)	295.17 (4.20)	0.0785
S_6	HOMO-2 → LUMO (36%)	290.43 (4.27)	0.0061
	HOMO → LUMO+2 (13%)		
S_7	HOMO-3 → LUMO (49%)	283.33 (4.38)	0.0094
	HOMO-2 → LUMO (15%)		
S_8	HOMO-2 → LUMO (37%)	281.04 (4.41)	0.1044
	HOMO → LUMO+2 (42%)		
S_9	HOMO-3 → LUMO (24%)	278.20 (4.46)	0.0165
	HOMO-3 → LUMO+1 (20%)		
	HOMO-2 → LUMO+1 (20%)		
	HOMO-1 → LUMO+1 (19%)		
S_{10}	HOMO-7 → LUMO (14%)	269.11 (4.61)	0.0863
	HOMO-6 → LUMO (22%)		
	HOMO-5 → LUMO (13%)		
	HOMO → LUMO+3 (17%)		

Table S32. Primary orbitals which contribute to the calculated transitions of **4a** (iso = 0.03).

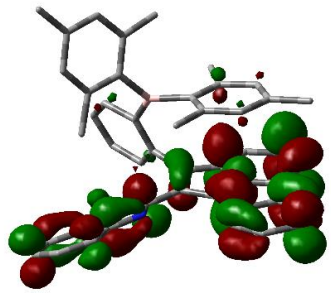
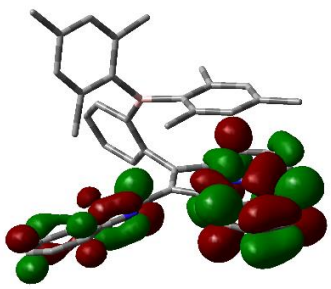
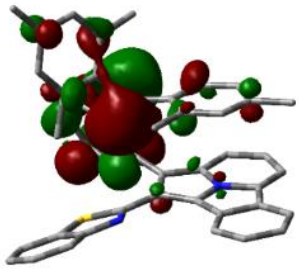
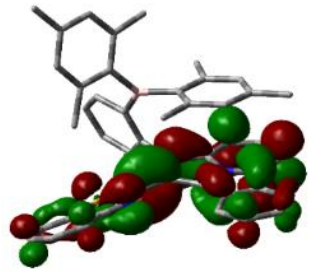
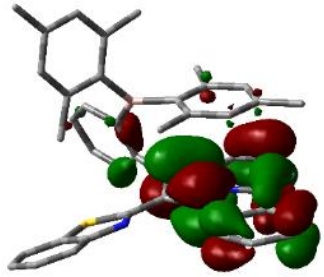
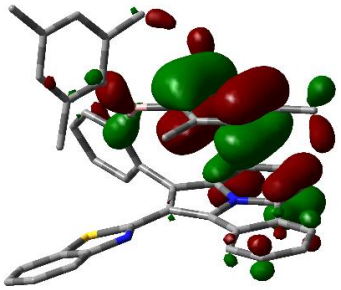
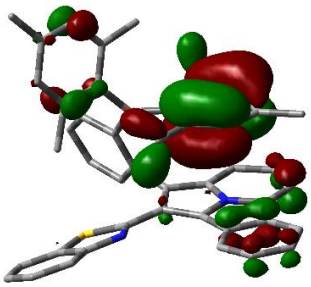
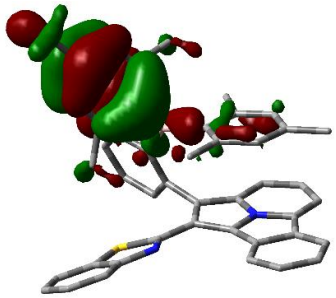
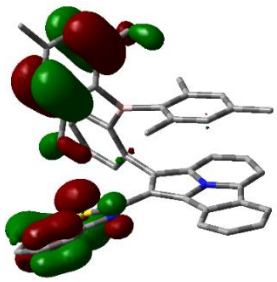
					
LUMO+3	0.38 eV	LUMO+2	-0.02 eV	LUMO+1	-0.88 eV
					
LUMO	-1.26 eV	HOMO	-6.39 eV	HOMO-1	-7.08 eV
					
HOMO-2	-7.34 eV	HOMO-3	-7.44 eV	HOMO-4	-7.50 eV
					
HOMO-5	-7.66 eV				

Table S33. TD-DFT calculated electronic transition configurations for **4b** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (84%)	392.09 (3.16)	0.3653
	HOMO → LUMO+1 (10%)		
S_2	HOMO → LUMO+1 (57%)	334.59 (3.71)	0.1922
	HOMO-1 → LUMO (24%)		
S_3	HOMO-1 → LUMO (33%)	321.92 (3.85)	0.0227
	HOMO-1 → LUMO+1 (24%)		
	HOMO → LUMO+1 (26%)		
S_4	HOMO-1 → LUMO (10%)	309.59 (4.00)	0.1557
	HOMO-1 → LUMO+1 (16%)		
	HOMO → LUMO+2 (49%)		
S_5	HOMO-3 → LUMO(30%)	297.51 (4.17)	0.1829
	HOMO-3 → LUMO+1 (48%)		
S_6	HOMO-1 → LUMO (12%)	288.46 (4.30)	0.1419
	HOMO-1 → LUMO+1 (17%)		
	HOMO → LUMO +2 (31%)		
	HOMO → LUMO+3 (20%)		
S_7	HOMO-2 → LUMO (67%)	283.83 (4.37)	0.0156
S_8	HOMO-5→ LUMO (15%)	276.49 (4.48)	0.0213
	HOMO-1 → LUMO (10%)		
	HOMO-1 → LUMO+1 (18%)		
	HOMO → LUMO+3 (31%)		
S_9	HOMO-6 → LUMO+1 (11%)	269.43 (4.60)	0.0630
	HOMO-4 → LUMO (25%)		
	HOMO-4 → LUMO+1 (19%)		
	HOMO-2 → LUMO+1 (11%)		
S_{10}	HOMO-5 → LUMO (13%)	264.90 (4.68)	0.1505
	HOMO-5 → LUMO+1 (18%)		
	HOMO-2 → LUMO+1 (14%)		
	HOMO → LUMO+3 (11%)		

Table S34. Primary orbitals which contribute to the calculated transitions of **4b** (iso = 0.03).

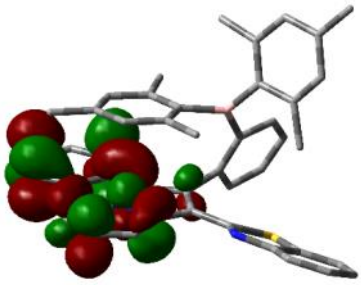
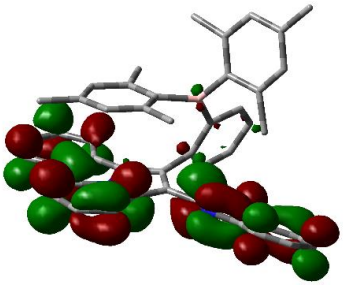
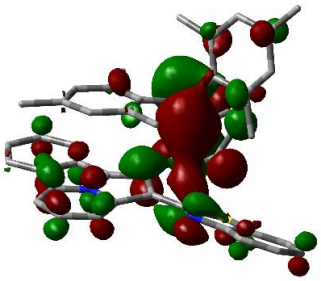
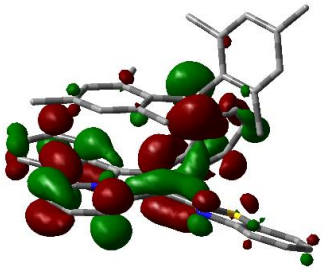
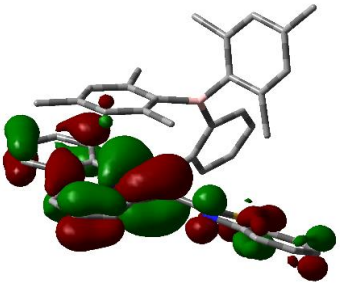
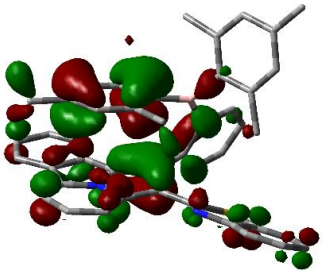
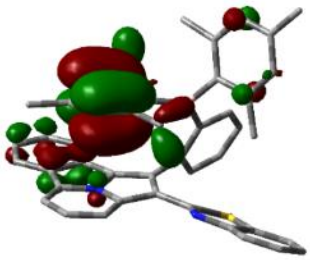
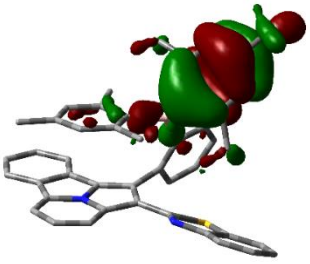
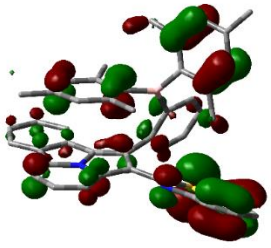
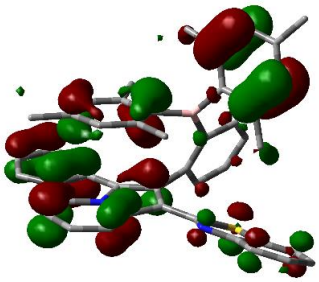
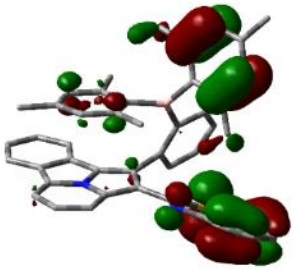
					
LUMO+3	0.20 eV	LUMO+2	-0.20 eV	LUMO+1	-0.84 eV
					
LUMO	-1.11 eV	HOMO	-6.34 eV	HOMO-1	-7.07 eV
					
HOMO-2	-7.41 eV	HOMO-3	-7.51 eV	HOMO-4	-7.59 eV
					
HOMO-5	-7.68 eV	HOMO-6	-7.77 eV		

Table S35. TD-DFT calculated electronic transition configurations for **5a** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (94%)	429.04 (2.89)	0.1907
S_2	HOMO -1 → LUMO (89%)	344.40 (3.60)	0.0658
S_3	HOMO → LUMO+1 (88%)	314.03 (3.95)	0.0094
S_4	HOMO-5 → LUMO (30%)	305.33 (4.06)	0.0650
	HOMO-2 → LUMO (50%)		
S_5	HOMO-5 → LUMO (26%)	299.43 (4.14)	0.0385
	HOMO-3 → LUMO (17%)		
	HOMO-2 → LUMO (41%)		
S_6	HOMO-7 → LUMO (14%)	278.09 (4.46)	0.1333
	HOMO → LUMO+2 (44%)		
S_7	HOMO-6 → LUMO (29%)	269.22 (4.61)	0.1535
	HOMO-1 → LUMO+1 (33%)		
S_8	HOMO-5 → LUMO (13%)	266.39 (4.65)	0.0078
	HOMO-3 → LUMO (60%)		
S_9	HOMO-7 → LUMO (11%)	265.15 (4.68)	0.0952
	HOMO-6 → LUMO (35%)		
	HOMO-1 → LUMO+1 (18%)		
	HOMO → LUMO+3 (14%)		
S_{10}	HOMO-1 → LUMO+1 (22%)	260.60 (4.76)	0.2305
	HOMO → LUMO+3 (64%)		

Table S36. Primary orbitals which contribute to the calculated transitions of **5a** (iso = 0.03).

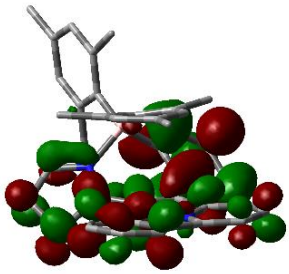
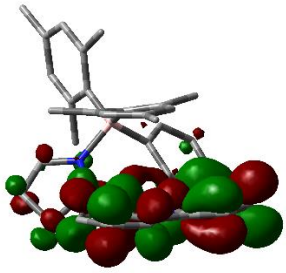
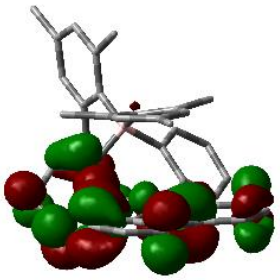
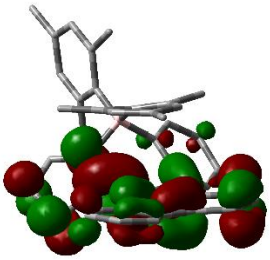
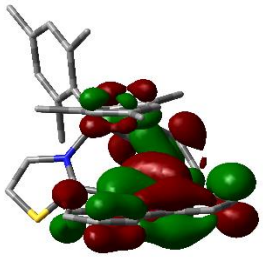
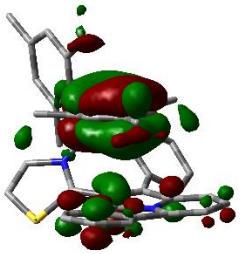
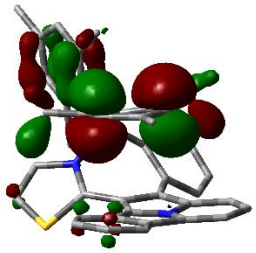
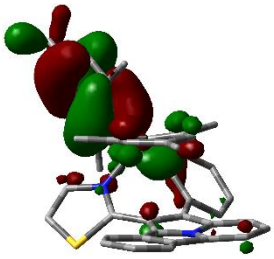
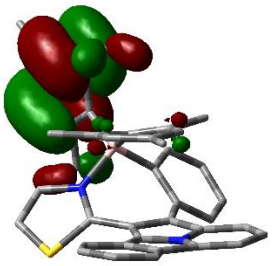
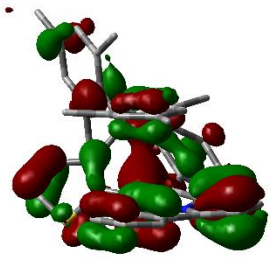
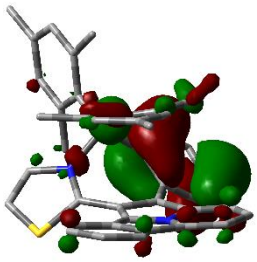
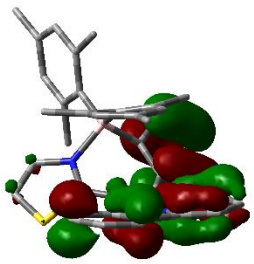
					
LUMO+3	0.53 eV	LUMO+2	0.26 eV	LUMO+1	-0.25 eV
					
LUMO	-1.29 eV	HOMO	-6.22 eV	HOMO-1	-6.81 eV
					
HOMO-2	-7.19 eV	HOMO-3	-7.33 eV	HOMO-4	-7.46 eV
					
HOMO-5	-7.49 eV	HOMO-6	-7.71 eV	HOMO-7	-7.89 eV

Table S37. TD-DFT calculated electronic transition configurations for **5b** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (93%)	382.75 (3.24)	0.3076
S_2	HOMO-1 → LUMO (63%)	337.13 (3.68)	0.0690
	HOMO → LUMO+1 (25%)		
S_3	HOMO-1 → LUMO (33%)	314.06 (3.95)	0.1245
	HOMO → LUMO+1 (54%)		
S_4	HOMO-3 → LUMO (11%)	294.88 (4.20)	0.0659
	HOMO-2 → LUMO (61%)		
	HOMO → LUMO+2 (10%)		
S_5	HOMO-3 → LUMO (41%)	285.52 (4.34)	0.0501
	HOMO-2 → LUMO (28%)		
	HOMO → LUMO+2 (15%)		
S_6	HOMO-3 → LUMO (11%)	282.42 (4.39)	0.0075
	HOMO-1->LUMO+1 (70%)		
S_7	HOMO-7 → LUMO (12%)	273.36 (4.54)	0.1363
	HOMO-3 → LUMO (13%)		
	HOMO-1 → LOMO+1 (14%)		
	HOMO → LOMO+2 (43%)		
S_8	HOMO-6 → LUMO (37%)	257.05 (4.82)	0.1068
	HOMO-4 → LUMO (32%)		
S_9	HOMO-6 → LUMO (19%)	254.88 (4.86)	0.0216
	HOMO-4 → LUMO (39%)		
S_{10}	HOMO-2 → LUMO+1 (65%)	253.92 (4.88)	0.1185

Table S38. Primary orbitals which contribute to the calculated transitions of **5b** (iso = 0.03).

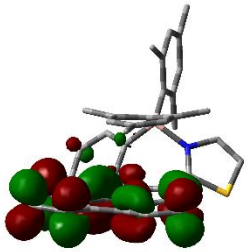
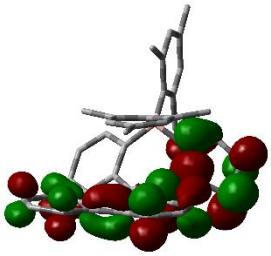
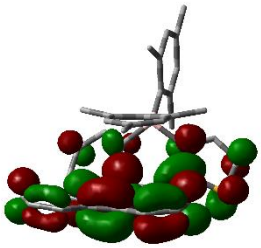
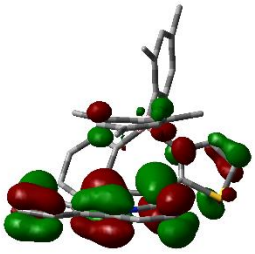
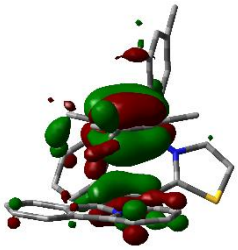
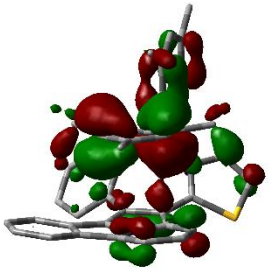
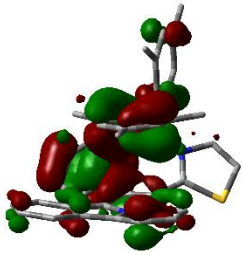
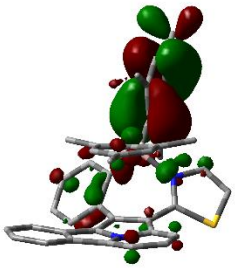
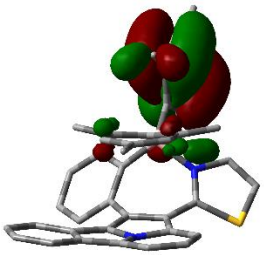
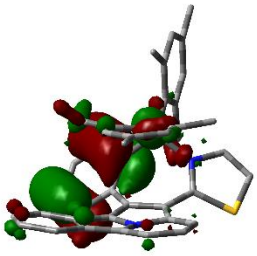
					
LUMO+2	0.12 eV	LUMO+1	-0.42 eV	LUMO	-1.06 eV
					
HOMO	-6.45 eV	HOMO-1	-6.72 eV	HOMO-2	-7.14 eV
					
HOMO-3	-7.29 eV	HOMO-4	-7.36 eV	HOMO-5	-7.46 eV
					
HOMO-6	-7.77 eV				

Table S39 TD-DFT calculated electronic transition configurations for **5a-o** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (92%)	400.35 (3.10)	0.1868
S_2	HOMO-1 → LUMO+1 (12%)	347.07 (3.57)	0.0293
	HOMO → LUMO+1 (75%)		
S_3	HOMO-2 → LUMO+1 (13%)	317.85 (3.90)	0.1096
	HOMO-1 → LUMO (65%)		
S_4	HOMO-2 → LUMO+1 (21%)	307.74 (4.03)	0.3027
	HOMO-1 → LUMO (21%)		
	HOMO-1 → LUMO+1 (28%)		
	HOMO → LUMO+1 (12%)		
S_5	HOMO-4 → LUMO+1 (74%)	293.39 (4.23)	0.1587
S_6	HOMO-2 → LUMO (36%)	286.78 (4.32)	0.0158
	HOMO → LUMO+2 (46%)		
S_7	HOMO-3 → LUMO+1 (21%)	282.59 (4.39)	0.0351
	HOMO-2 → LUMO+1 (37%)		
	HOMO-1 → LUMO+1 (24%)		
S_8	HOMO-2 → LUMO (53%)	277.16 (4.47)	0.1155
	HOMO → LUMO+2 (35%)		
S_9	HOMO-3 → LUMO (58%)	272.93 (4.54)	0.0089
	HOMO-1 → LUMO+1 (12%)		
S_{10}	HOMO-5 → LUMO+1 (43%)	271.12 (4.57)	0.0332
	HOMO-3 → LUMO (18%)		
	HOMO-3 → LUMO+1 (18%)		

Table S40. Primary orbitals which contribute to the calculated transitions of **5a-o** (iso = 0.03).

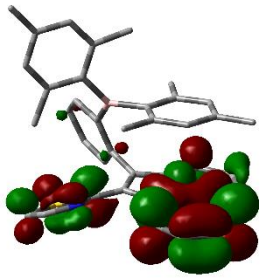
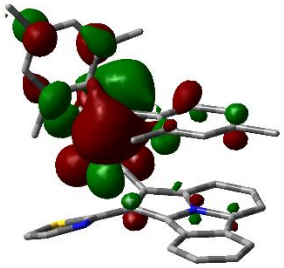
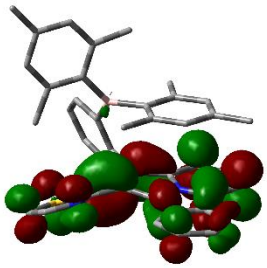
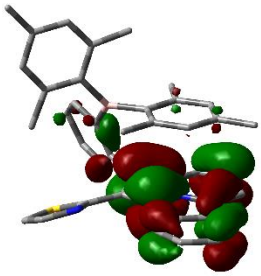
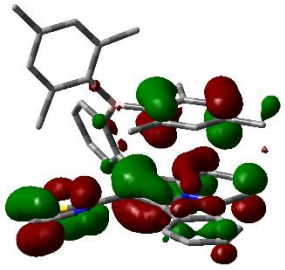
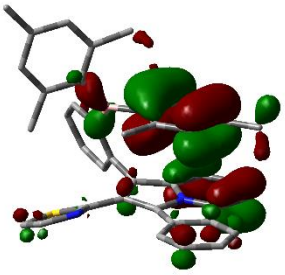
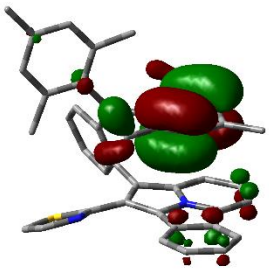
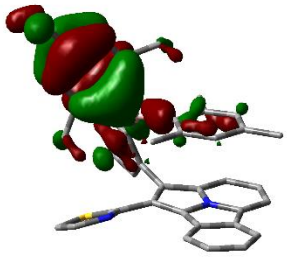
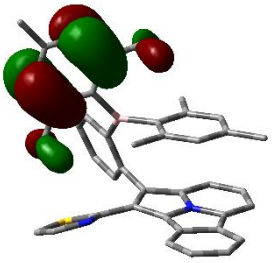
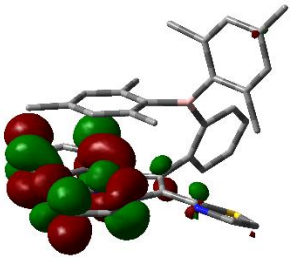
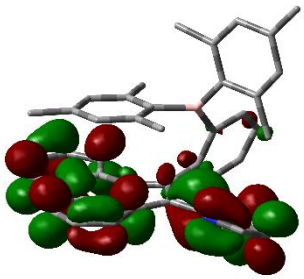
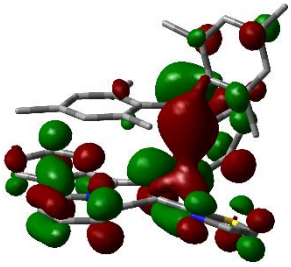
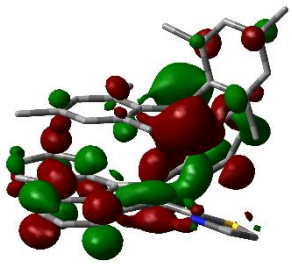
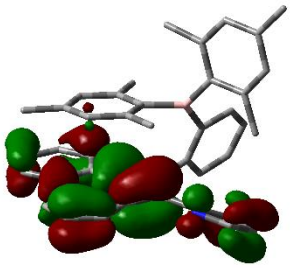
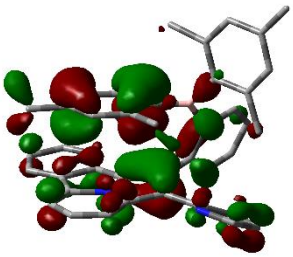
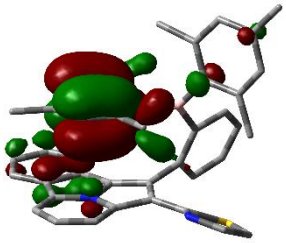
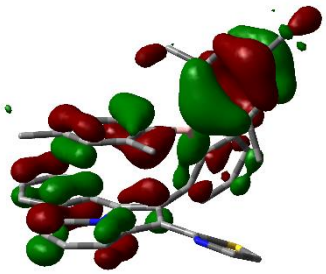
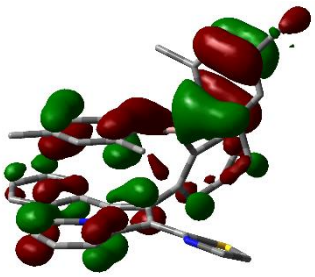
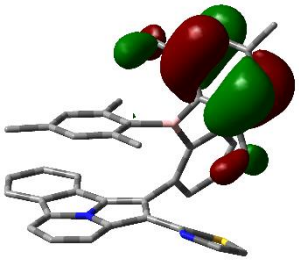
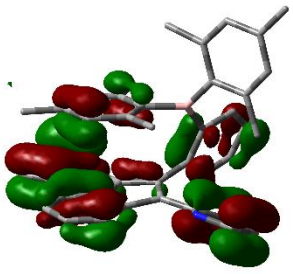
					
LUMO+2	0.10 eV	LUMO+1	-0.90 eV	LUMO	-1.11 eV
					
HOMO	-6.35 eV	HOMO-1	-7.00 eV	HOMO-2	-7.31 eV
					
HOMO-3	-7.47 eV	HOMO-4	-7.56 eV	HOMO-5	-7.69 eV

Table S41. TD-DFT calculated electronic transition configurations for **5b-o** along with their corresponding excitation energies and oscillator strengths

Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
S_1	HOMO → LUMO (70%)	393.29 (3.15)	0.2332
	HOMO → LOMO+1 (25%)		
S_2	HOMO-1 → LUMO (23%)	339.40 (3.65)	0.1137
	HOMO → LUMO (14%)		
	HOMO → LOMO+1 (53%)		
S_3	HOMO-1 → LUMO (50%)	330.38 (3.75)	0.0113
	HOMO-1 → LOMO+1 (12%)		
	HOMO → LUMO (11%)		
	HOMO → LOMO+1 (19%)		
S_4	HOMO-3 → LUMO (12%)	304.85 (4.07)	0.0874
	HOMO-1 → LOMO+1 (28%)		
	HOMO → LOMO+2 (30%)		
	HOMO → LOMO+3 (10%)		
S_5	HOMO-4 → LUMO (14%)	297.42 (4.17)	0.2526
	HOMO-3 → LUMO (21%)		
	HOMO-3 → LOMO+1 (16%)		
	HOMO-2 → LUMO (17%)		
S_6	HOMO → LOMO+2 (50%)	287.07 (4.32)	0.1651
	HOMO → LOMO+3 (19%)		
S_7	HOMO-4 → LUMO (13%)	284.14 (4.36)	0.0291
	HOMO-2 → LUMO (59%)		
S_8	HOMO-4 → LUMO (11%)	276.92 (4.48)	0.0221
	HOMO-1 → LOMO+1 (33%)		
	HOMO → LOMO+3 (25%)		
S_9	HOMO-5 → LUMO (43%)	272.80 (4.54)	0.0378
	HOMO-5 → LUMO+1 (28%)		
S_{10}	HOMO-6 → LUMO (13%)	267.23 (4.64)	0.1888
	HOMO-4 → LUMO (15%)		
	HOMO-3 → LUMO (12%)		

Table S42. Primary orbitals which contribute to the calculated transitions of **5b-o** (iso = 0.03).

					
LUMO+3	0.25 eV	LUMO+2	0.01 eV	LUMO+1	-0.80 eV
					
LUMO	-1.07 eV	HOMO	-6.28 eV	HOMO-1	-7.01 eV
					
HOMO-2	-7.43 eV	HOMO-3	-7.54 eV	HOMO-4	-7.60 eV
					
HOMO-5	-7.70 eV	HOMO-6	-7.87 eV		

The orbital composition analysis of **1a/1b-5a/5b** calculated with Ros-Schuit (C-squared Population Analysis, SCPA) method, based on the results of DFT calculations (M06-2X / 6-31G(d)) in CH_2Cl_2.

Table S43: Orbital composition analysis of **1a/1b-5a/5b**

	Fragment	**HOMO**	**LUMO**		**Fragment**	**HOMO**	**LUMO**
1a	Pyridine	1%	12%	**4a**	Benzothiazole	1%	30%
	$BMes_2$-Ph	13%	42%		$BMes_2$-Ph	11%	11%
1b	Pyridine	13%	5%	**4b**	Benzothiazole	19%	11%
	$BMes_2$-Ph	1%	62%		$BMes_2$-Ph	5%	35%
2a	Pyridine	1%	41%	**2a-o**	Pyridine	1%	21%
	Ph	15%	4%		Ph	7%	5%
	$BMes_2$-Ph	25%	9%		$BMes_2$-Ph	12%	15%
2b	Pyridine	8%	31%	**2b-o**	Pyridine	12%	4%
	Ph	2%	8%		Ph	1%	21%
	$BMes_2$-Ph	10%	12%		$BMes_2$-Ph	5%	55%
3a	Isoquinoline	1%	67%	**3a-o**	Isoquinoline	2%	42%
	Ph	13%	3%		Ph	7%	4%
	$BMes_2$-Ph	20%	8%		$BMes_2$-Ph	12%	10%
3b	Isoquinoline	13%	70%	**3b-o**	Isoquinoline	17%	9%
	Ph	2%	4%		Ph	1%	16%
	$BMes_2$-Ph	10%	9%		$BMes_2$-Ph	5%	46%
5a	Thiazole	1%	39%	**5a-o**	Thiazole	1%	25%
	Ph	15%	4%		Ph	7%	5%
	$BMes_2$-Ph	26%	9%		$BMes_2$-Ph	12%	13%
5b	Thiazole	12%	26%	**5a-o**	Thiazole	18%	5%
	Ph	2%	7%		Ph	1%	19%
	$BMes_2$-Ph	11%	12%		$BMes_2$-Ph	5%	55%

The electrostatic potential surfaces of **1a-5b** based on the results of DFT calculations (M06-2X/6-31G(d)) in CH_2Cl_2, negatively charged regions are shown in red, positively charged regions in blue.

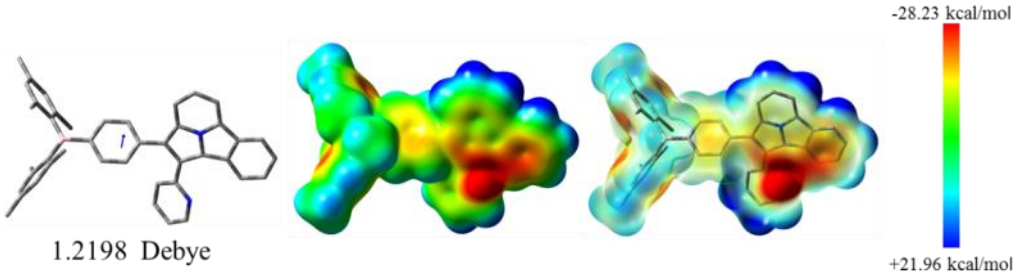


Figure S32: Electrostatic potential surfaces of **1a** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

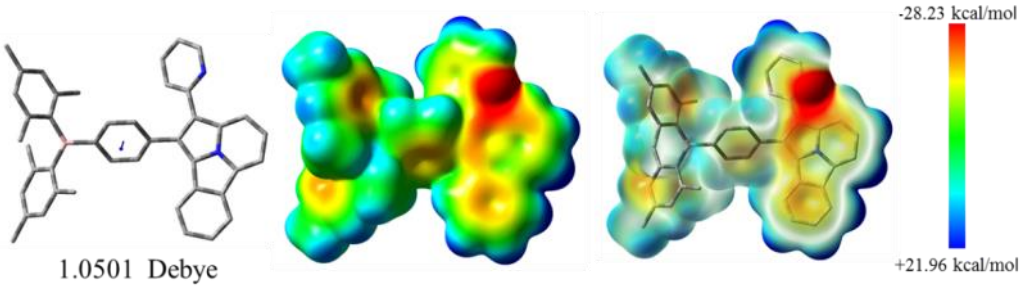


Figure S33: Electrostatic potential surfaces of **1b** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

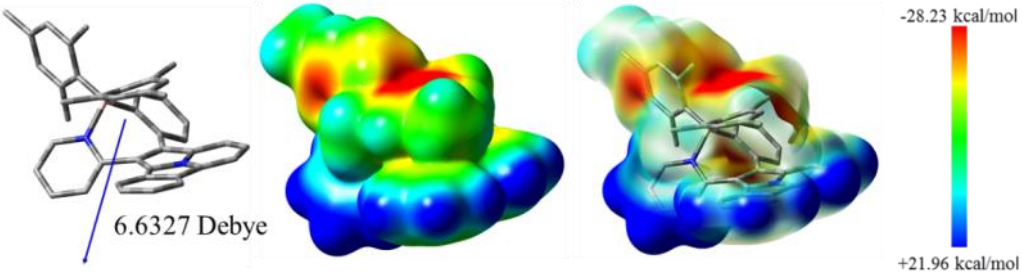


Figure S34: Electrostatic potential surfaces of **2a** calculated at the (M062X/6-31g(d) theory) and visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

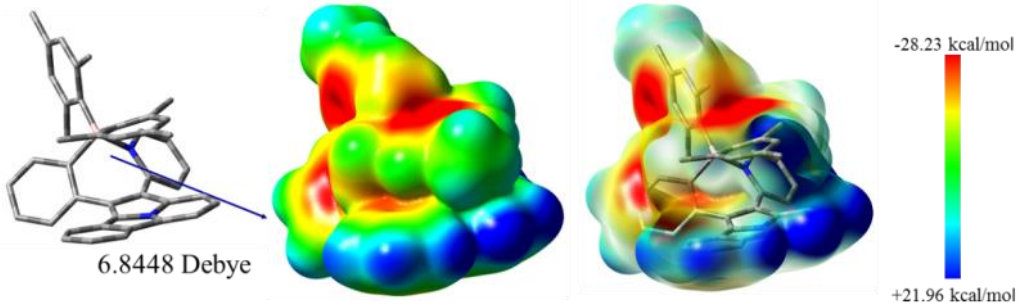


Figure S35: Electrostatic potential surfaces of **2b** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

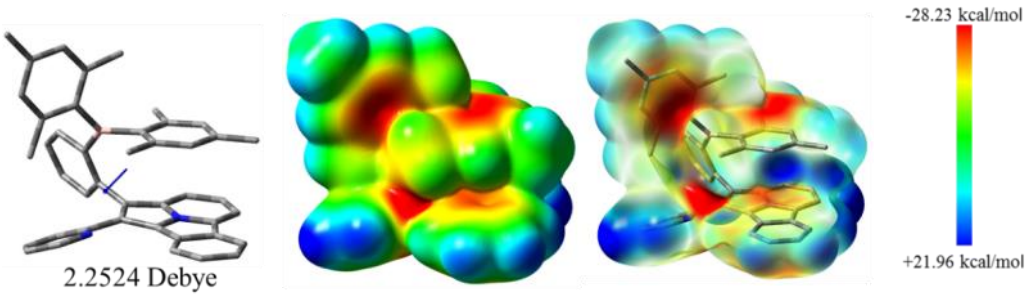


Figure S36: Electrostatic potential surfaces of **2a-o** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

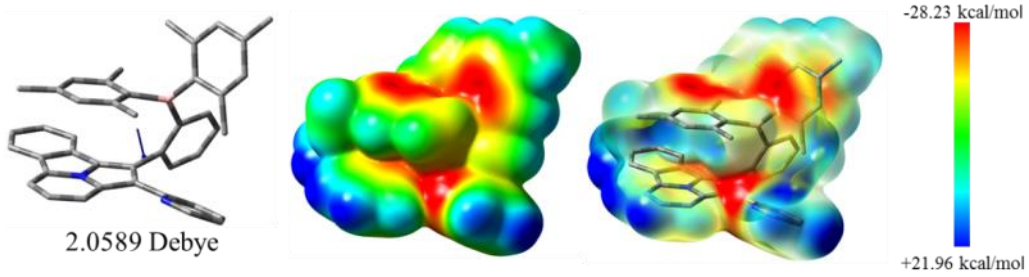


Figure S37: Electrostatic potential surfaces of **2b-o** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

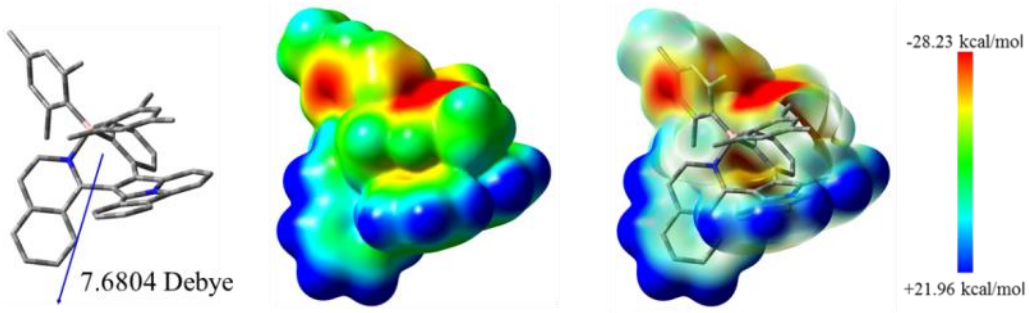


Figure S38: Electrostatic potential surfaces of **3a** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

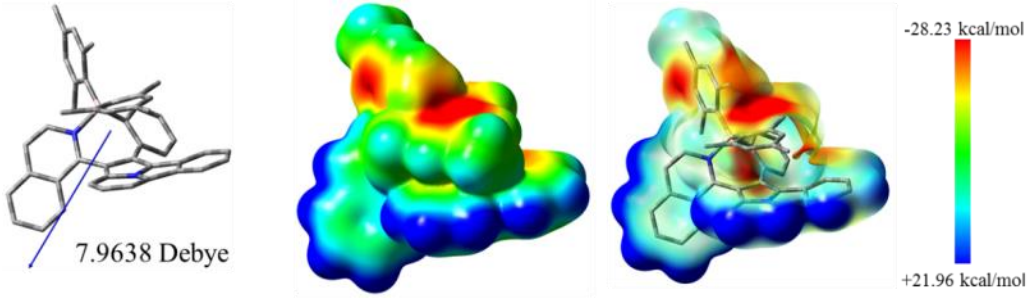


Figure S39: Electrostatic potential surfaces of **3b** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

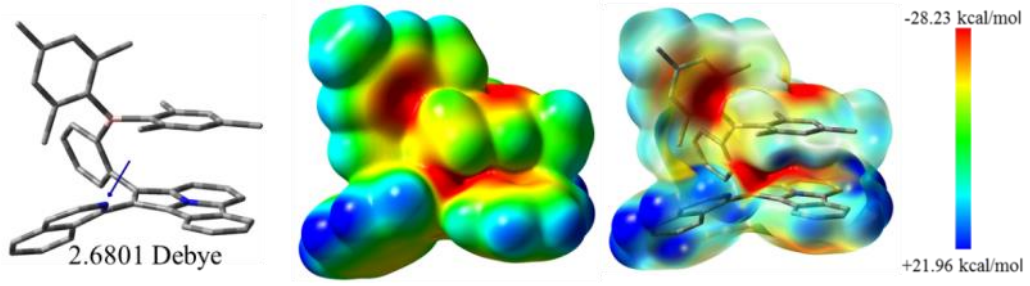


Figure S40: Electrostatic potential surfaces of **3a-o** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

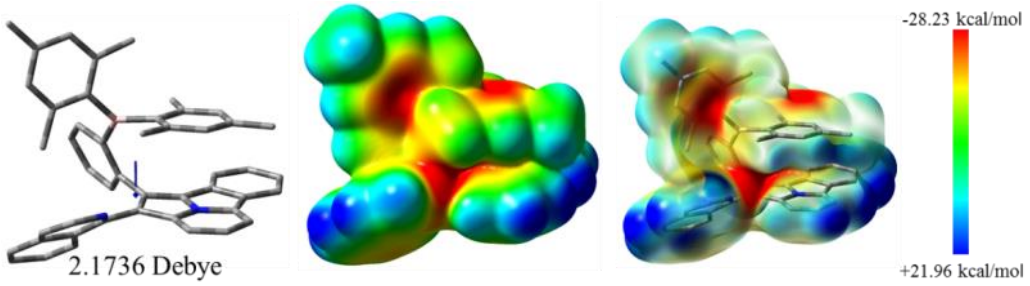


Figure S41: Electrostatic potential surfaces of **3b-o** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

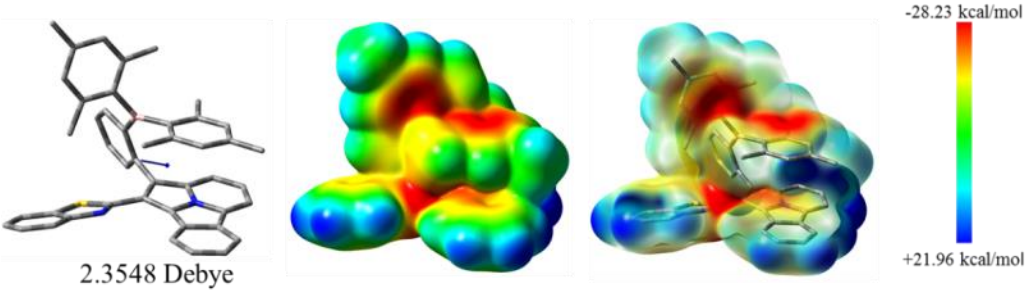


Figure S42: Electrostatic potential surfaces of **4a** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

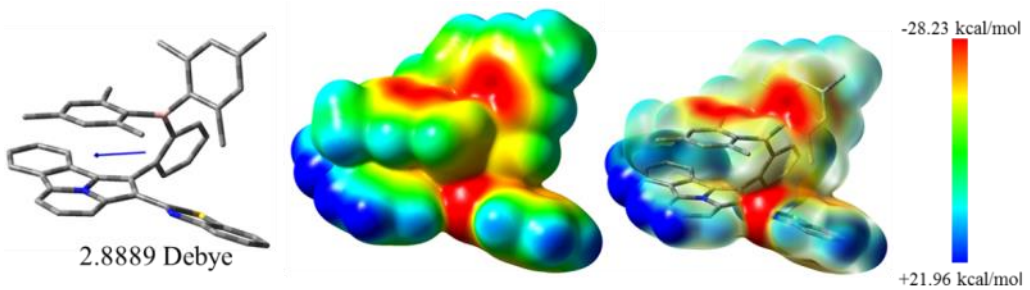


Figure S43: Electrostatic potential surfaces of **4b** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

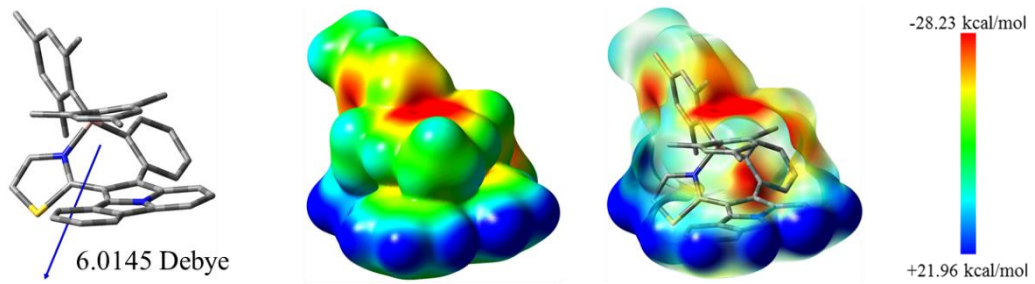


Figure S44: Electrostatic potential surfaces of **5a** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

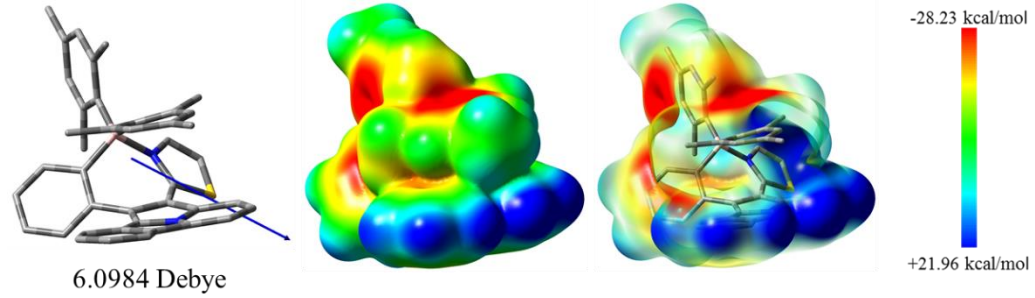


Figure S45: Electrostatic potential surfaces of **5b** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

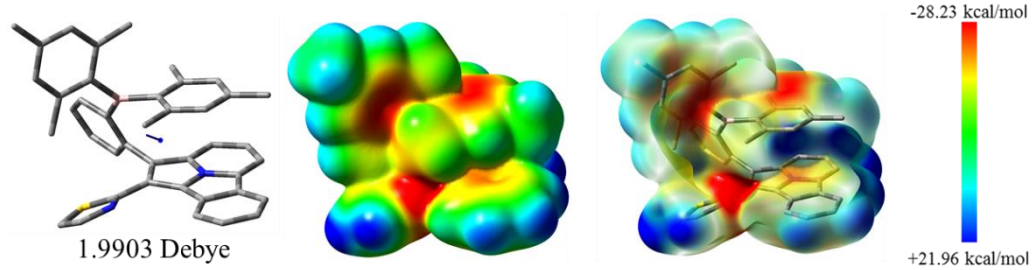


Figure S46: Electrostatic potential surfaces of **5a-o** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

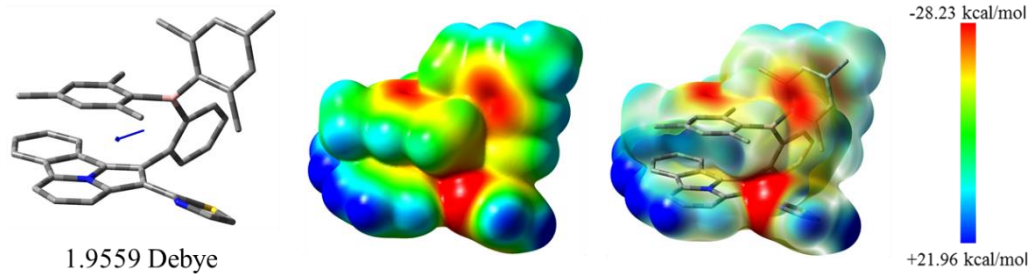


Figure S47: Electrostatic potential surfaces of **5b-o** visualized in GaussView 5.0 (isovalue = 0.002). The arrow indicates the direction of the dipole moment.

The estimated absorption spectra of **1a/1b-5a/5b** formed by TD-DFT calculations (M06-2X/6-31G(d)) in CH_2Cl_2 using PCMs are shown below:

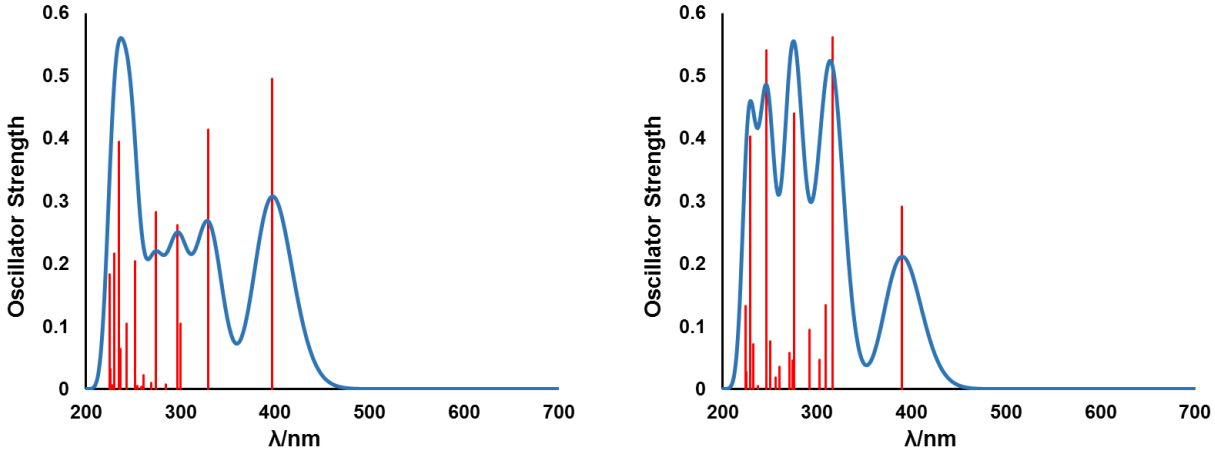


Figure S48. Predicted UV/Vis spectrum of **1a** (left) and **1b** (right).

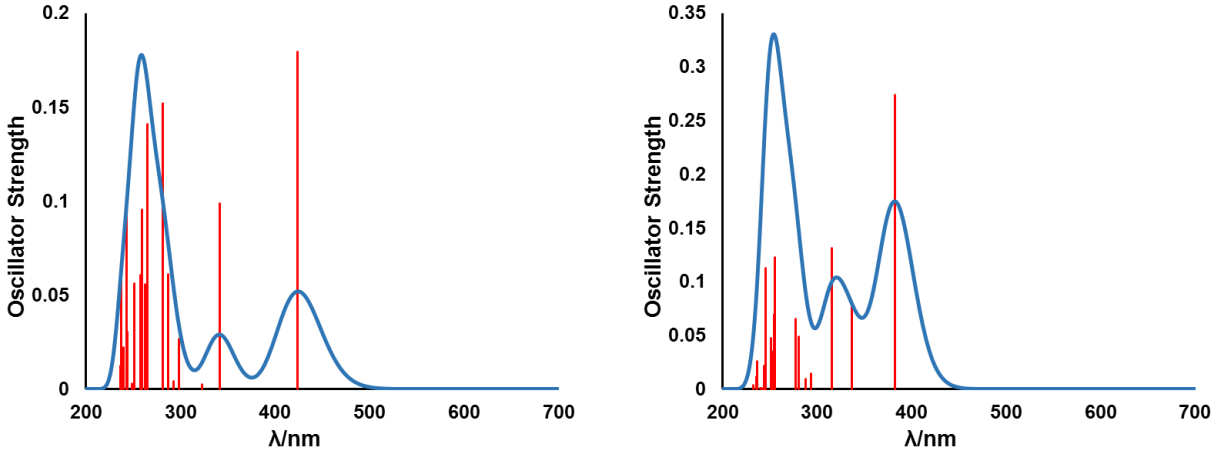


Figure S49. Predicted UV/Vis spectrum of **2a** (left) and **2b** (right).

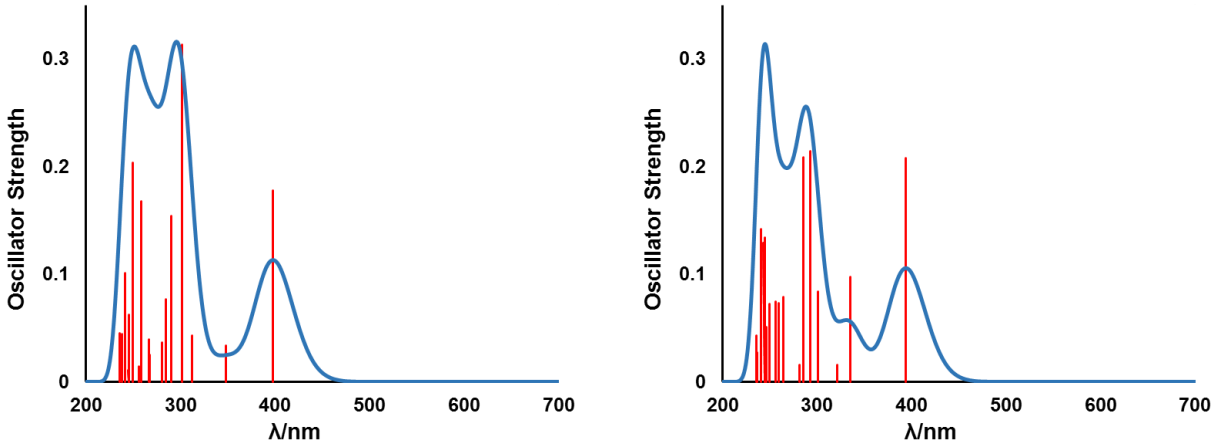


Figure S50. Predicted UV/Vis spectrum of **2a-o** (left) and **2b-o** (right).

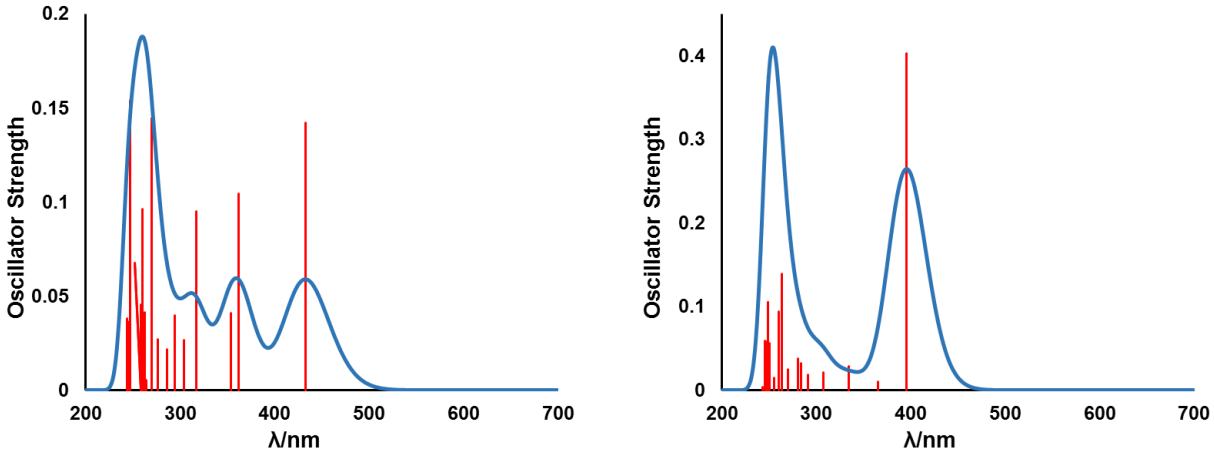


Figure S51. Predicted UV/Vis spectrum of **3a** (left) and **3b** (right).

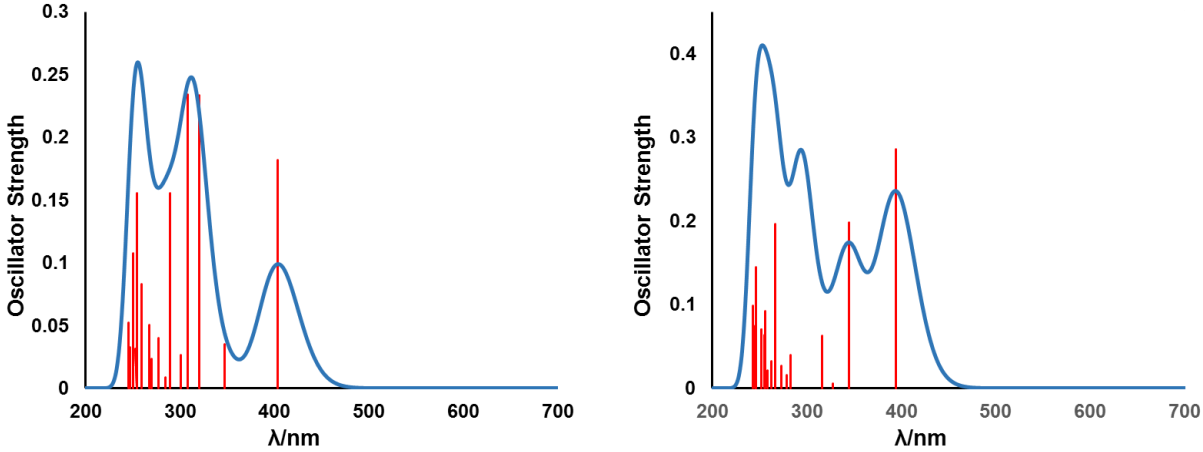


Figure S52. Predicted UV/Vis spectrum of **3a-o** (left) and **3b-o** (right).

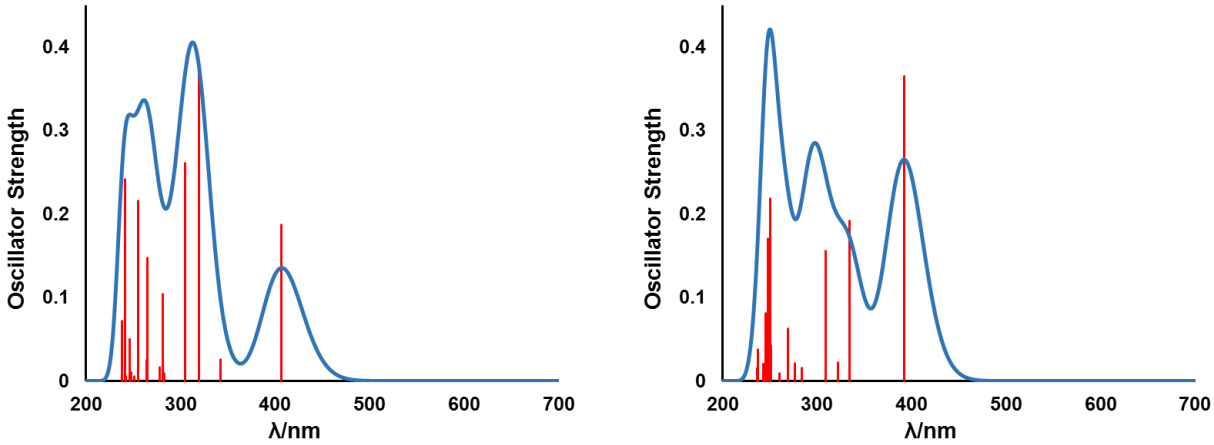


Figure S53. Predicted UV/Vis spectrum of **4a** (left) and **4b** (right).

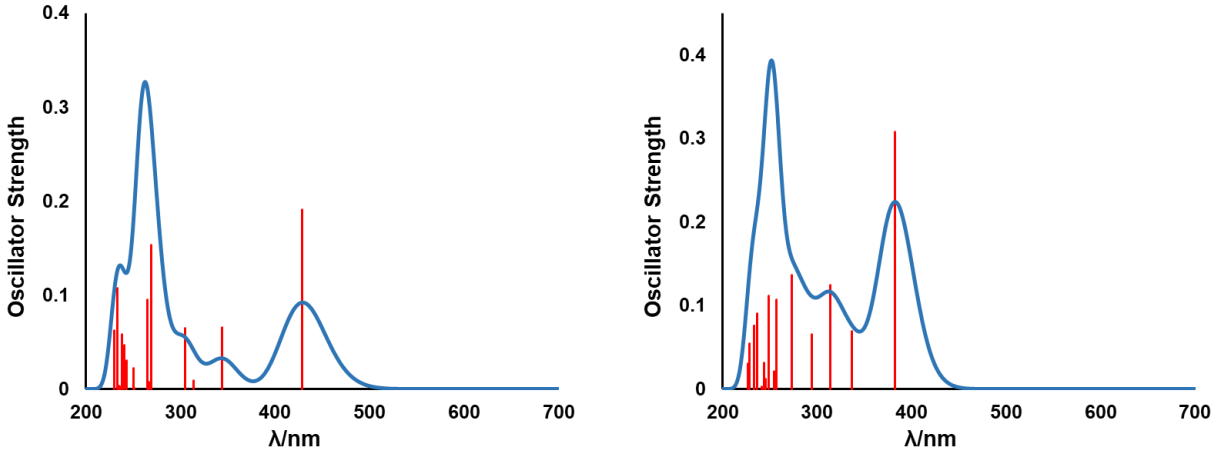


Figure S54. Predicted UV/Vis spectrum of **5a** (left) and **5b** (right).

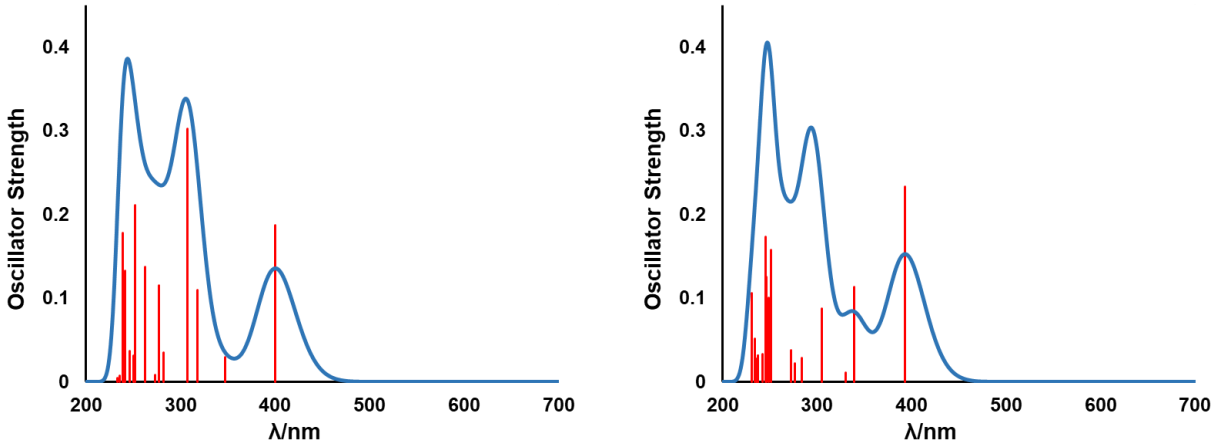


Figure S55. Predicted UV/Vis spectrum of **5a-o** (left) and **5b-o** (right).

The NBO calculations for **2a/2b, 3a/3b, 5a/5b** based on the results of Geometry optimization (M06-2X/6-31G(d)) in CH_2Cl_2 are shown below:

Table S44: NBO calculations for selected compounds/bonds

	B-N Bond Lengths (in Å)	Wiberg Bond Indices	NBO	
			Molecular unit	Occupancy
2a	1.73138	0.5505	LP*(1) B	0.39443
			LP (1) N	1.63427
2b	1.72271	0.5614	LP*(1) B	0.39963
			LP (1) N	1.62960
3a	1.72106	0.5613	LP*(1) B	0.39878
			LP (1) N	1.63104
3b	1.71143	0.5709	LP*(1) B	0.40397
			LP (1) N	1.62555
5a	1.70511	0.5840	LP*(1) B	0.39217
			LP (1) N	1.62984
5b	1.69168	0.5962	LP*(1) B	0.39957
			LP (1) N	1.62360

Table S45: The calculated ^{11}B-NMR of **2a/2a-open**

	Isotropic	**^{11}B-NMR(ppm)**
2a	100.0468	4.5
2a open	36.8130	67.7
$BF_3 \cdot OET_2$	104.5221	0

The differences on solvent effects in the Gibbs free energy (△G) for compounds **2a/2a-open** and **3a/3a-open** were also examined by DFT calculations (M06-2X/6-31G(d) level of theory) using appropriate Polarizable Continuum Models (PCMs).

Table: S46: The Summary of the Solvent Effects on the Gibbs Free Energy of **2a/2a-open**, **2b/2b-open, 3a/3a open**, **3b/3b-open,5a/5a-open** and **5b/5b-open**.

Solvent	**2a**			**3a**		
	$\triangle S_{closed\rightarrow open}$ (cal/mol)	$\triangle H_{closed\rightarrow open}$ (kcal/mol)	$\triangle G_{closed\rightarrow open}$ (kcal/mol)	$\triangle S_{closed\rightarrow open}$ (cal/mol)	$\triangle H_{closed\rightarrow open}$ (kcal/mol)	$\triangle G_{closed\rightarrow open}$ (kcal/mol)
CH_3CN	14.26	3.66	-0.59	16.42	6.17	1.27
THF	13.87	3.45	-0.69	12.15	6.23	2.61
CH_2Cl_2	13.96	3.49	-0.67	12.63	6.24	2.47
Toluene	14.21	2.90	-1.34	14.58	5.93	1.58
Hexane	14.00	2.72	-1.45	13.97	5.80	1.64
	2b			**3b**		
CH_2Cl_2	14.38	5.08	0.80	8.91	6.31	3.65
	5a			**5b**		
CH_2Cl_2	12.97	4.24	0.37	12.18	5.55	1.92

Table S47: Gibbs Free Energies calculated by DFT calculations (M06-2X/6-31G(d) level of theory) in CH_2Cl_2 using PCMs.

	Gibbs Free Energy (kcal/mol)		**Gibbs Free Energy (kcal/mol)**	**$\triangle G_{a-b}$ (kcal/mol)**
1a	-1125702.1706	**1b**	-1125702.7655	-0.5949
2a	-1125700.2636	**2b**	-1125701.8016	-1.5380
2a-o	-1125700.9319	**2b-o**	-1125701.0028	-0.0709
3a	-1222046.8242	**3b**	-1222048.8529	-2.0287
3a-o	-1222044.3500	**3b-o**	-1222045.1984	-0.8484
4a	-1423356.8634	**4b**	-1423358.4246	-1.5612
5a	-1327014.8046	**5b**	-1327017.9491	-3.1445
5a-o	-1327014.4319	**5b-o**	-1327016.0320	-1.6001

The electrostatic potential surfaces of INI based on the results of DFT calculations (M06-2X/6-31G(d)) in CH_2Cl_2 using PCMs, negatively charged regions are shown in red, positively charged regions in blue. Electrostatic potential (ESP) charge calculated according to Merz-Kollman (MK) Methods[14].

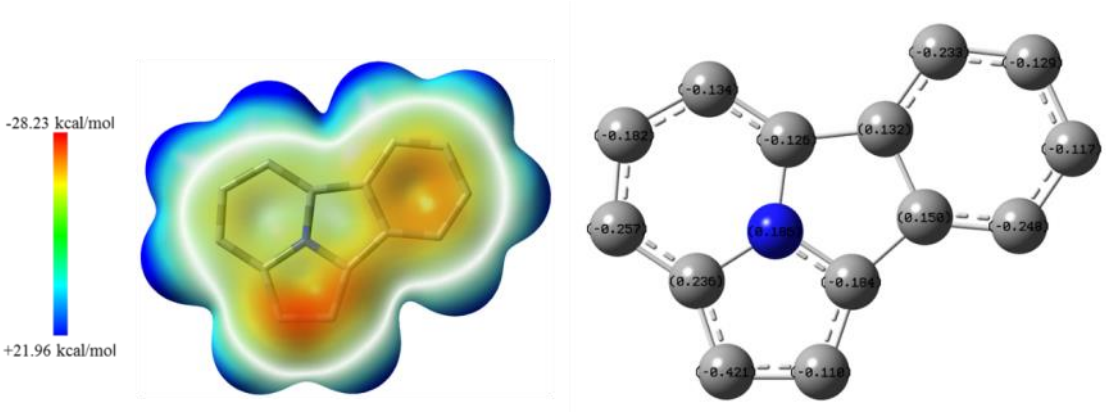


Figure S56: Electrostatic potential surfaces of **INI** visualized in GaussView 5.0 (isovalue = 0.002). the number on the atom are the value of ESP charges.

IV. NMR Spectra

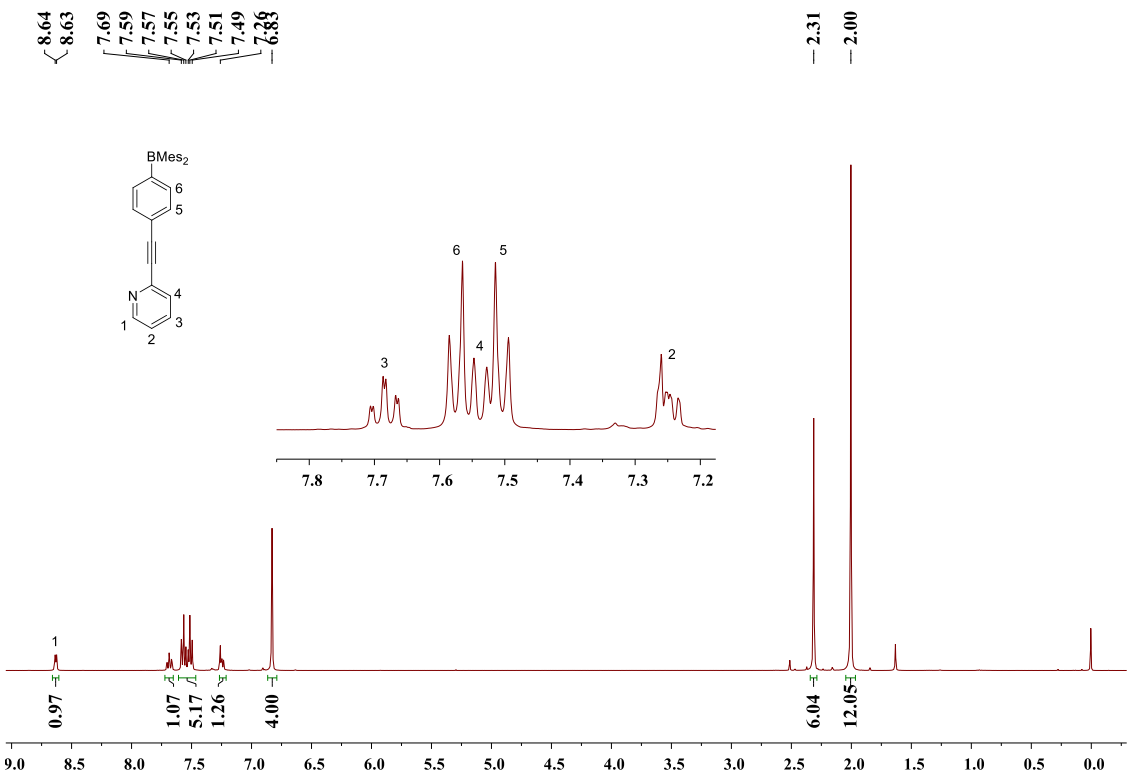


Figure S57: ^{1}H NMR spectrum of compound **1** in $CDCl_3$

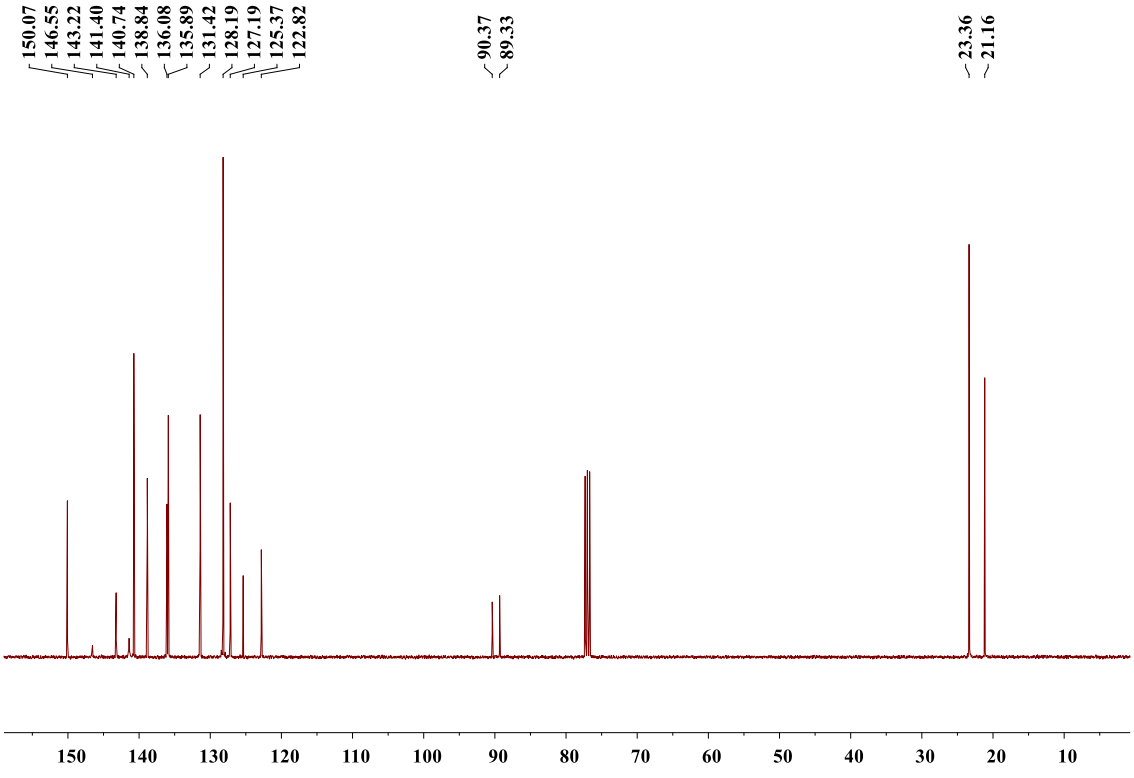


Figure S58: ^{13}C NMR spectrum of compound **1** in $CDCl_3$.

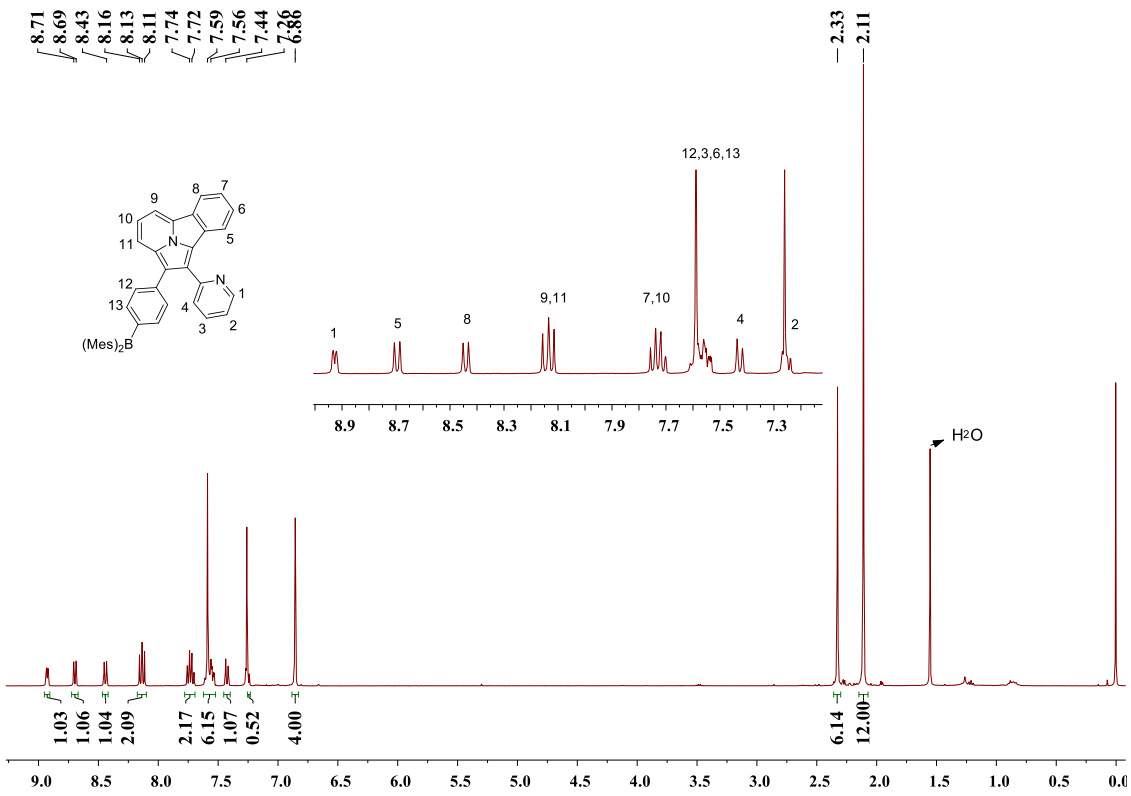


Figure S59: ^{1}H NMR spectrum of compound **1a** in $CDCl_3$

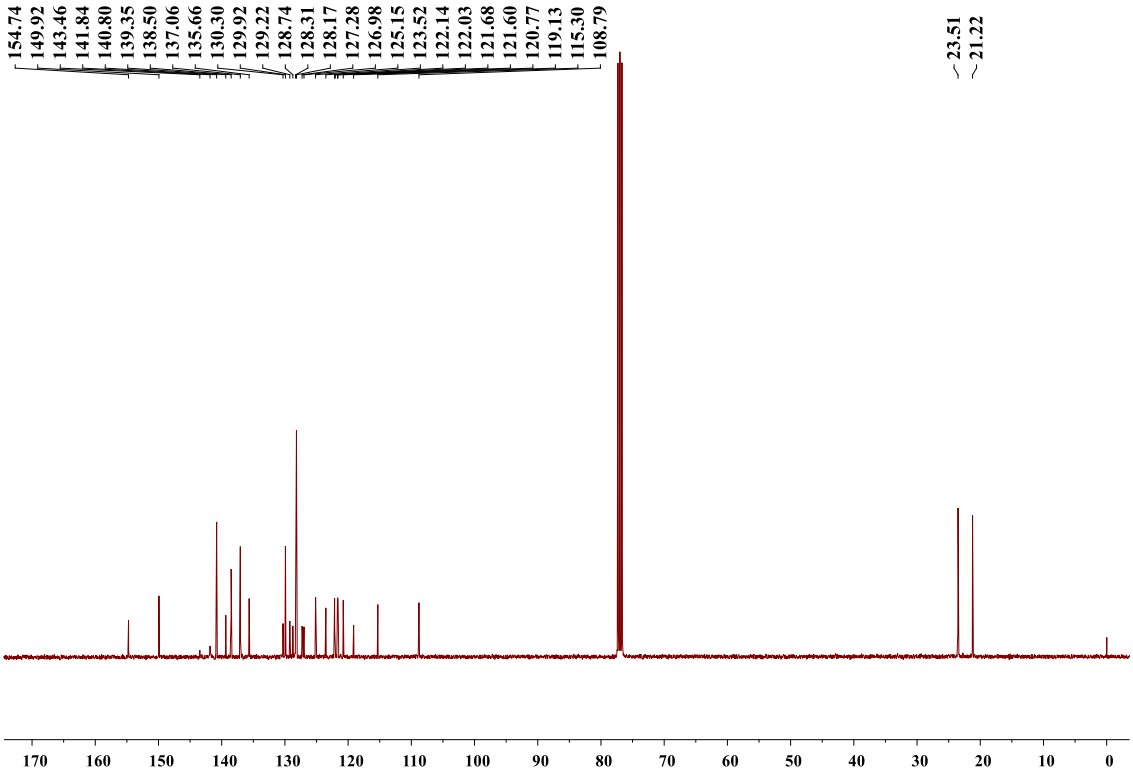


Figure S60: ^{13}C NMR spectrum of compound **1a** in $CDCl_3$

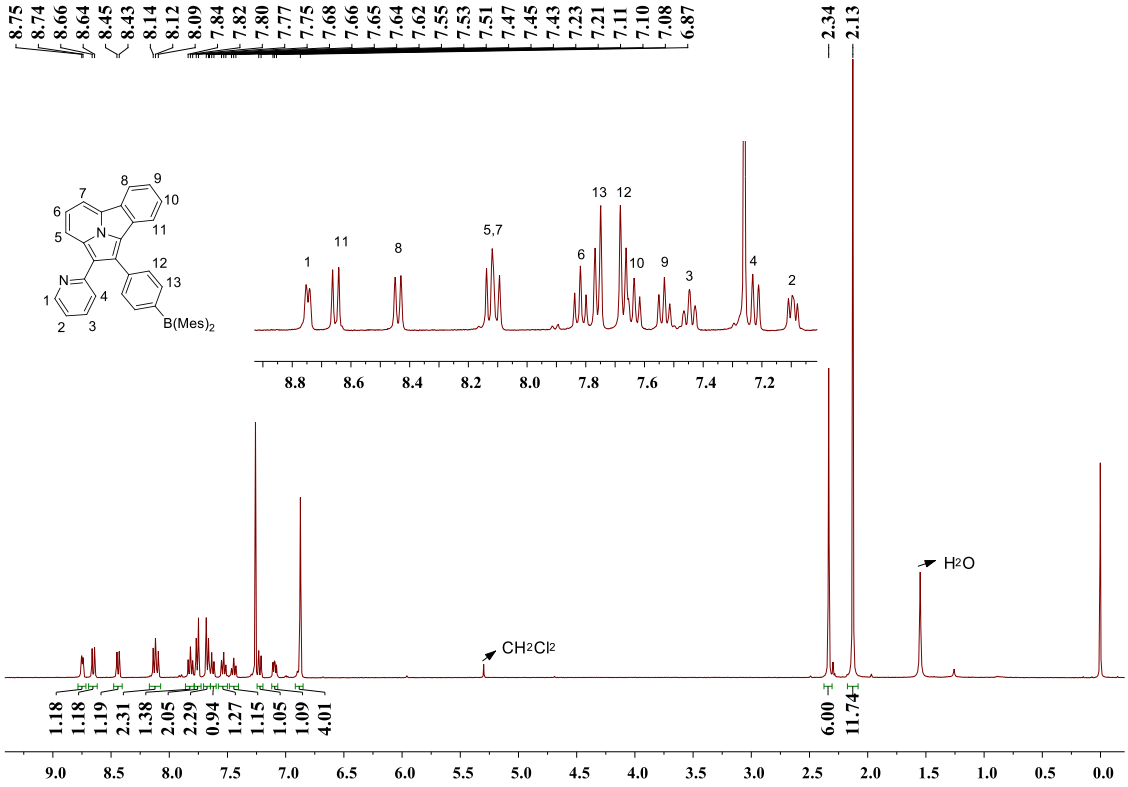


Figure S61: ^{1}H NMR spectrum of compound **1b** in $CDCl_3$

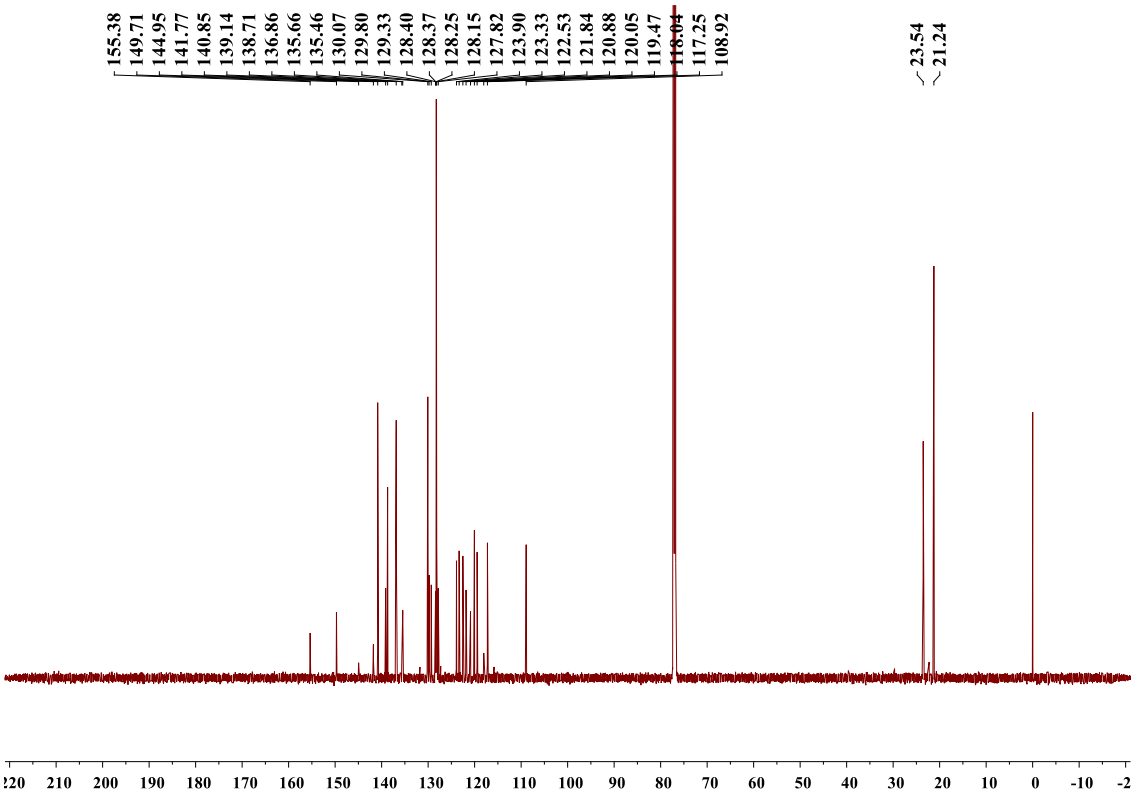


Figure S62: ^{13}C NMR spectrum of compound **1b** in $CDCl_3$

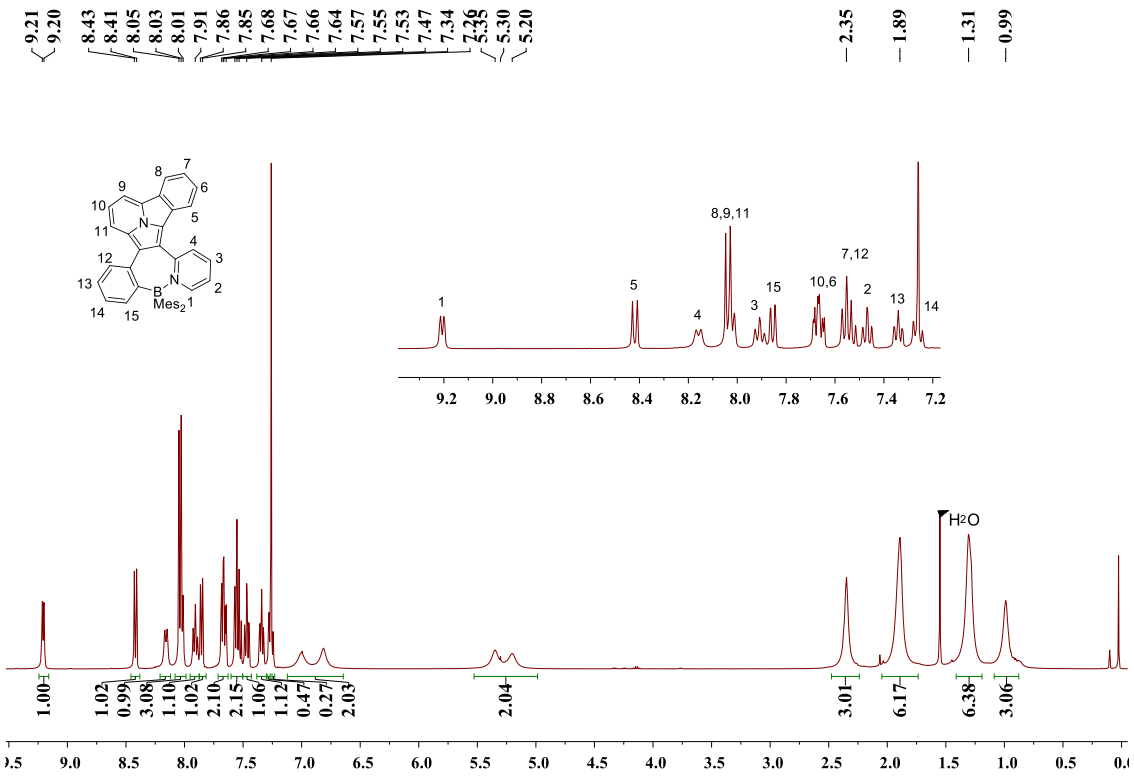


Figure S63: ^{1}H NMR spectrum of compound 2**a** in $CDCl_3$

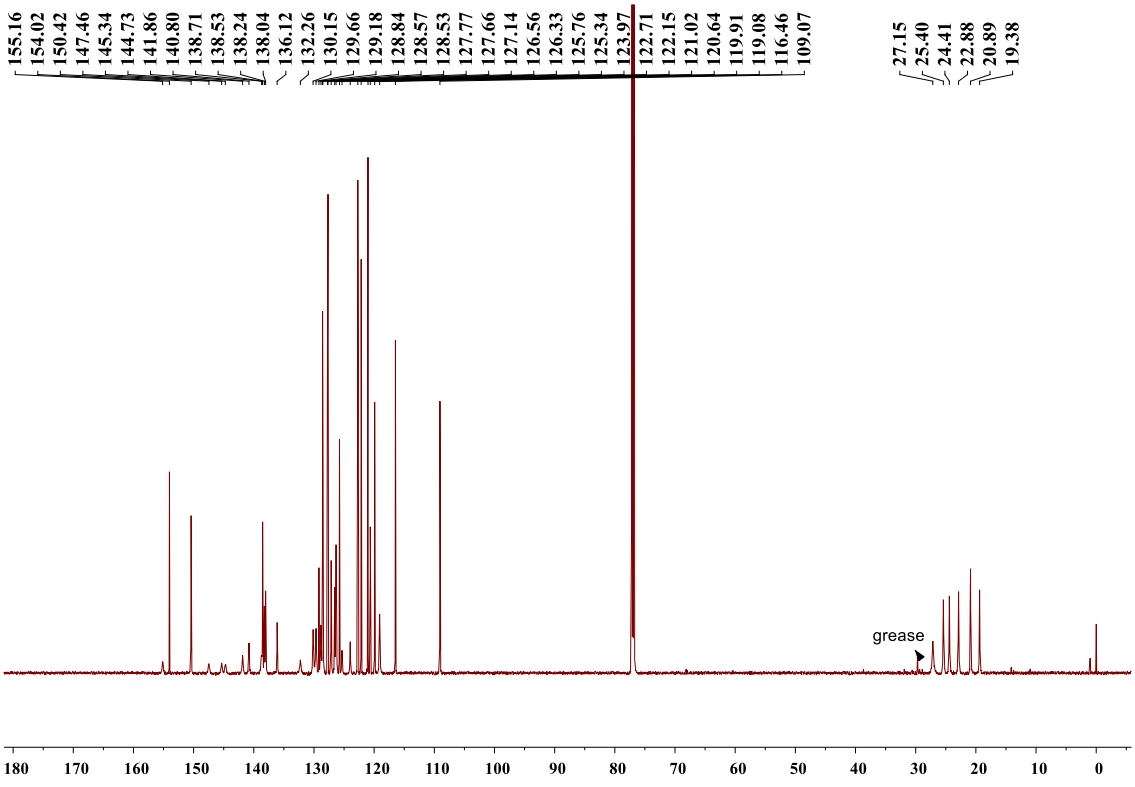


Figure S64: ^{13}C NMR spectrum of compound **2a** in $CDCl_3$

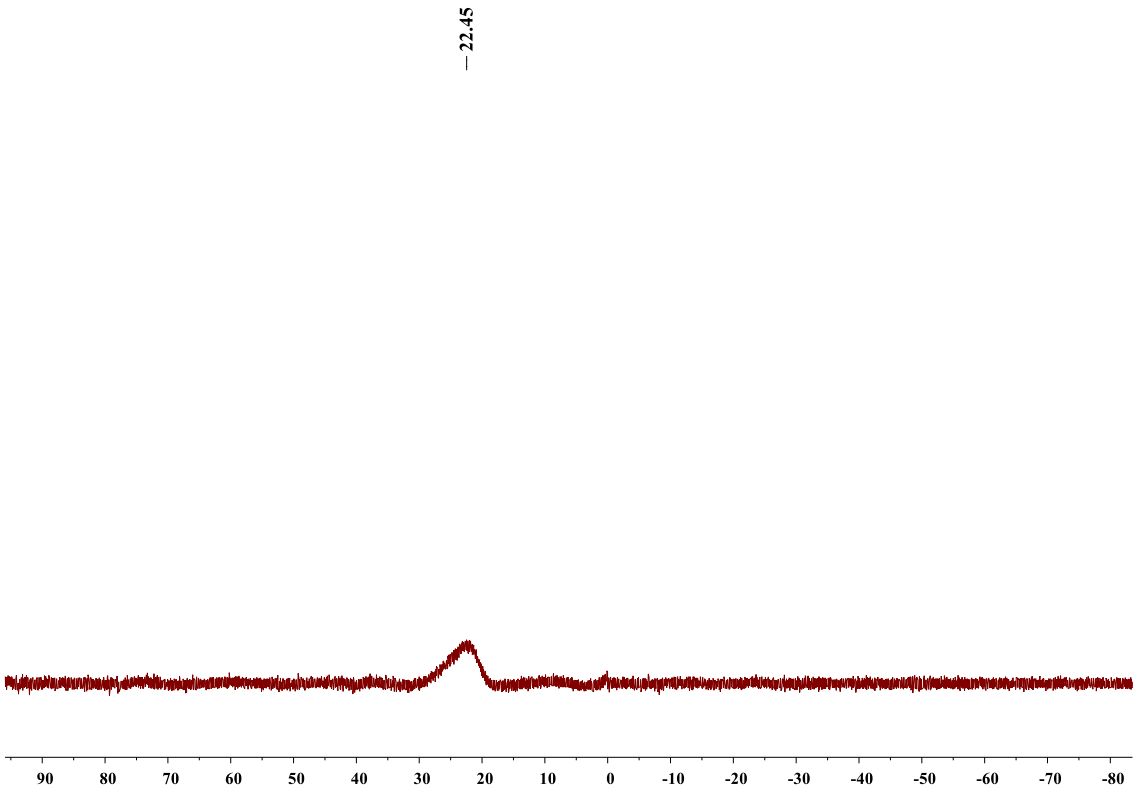


Figure S65: ^{11}B NMR spectrum of compound **2a** in $CDCl_3$

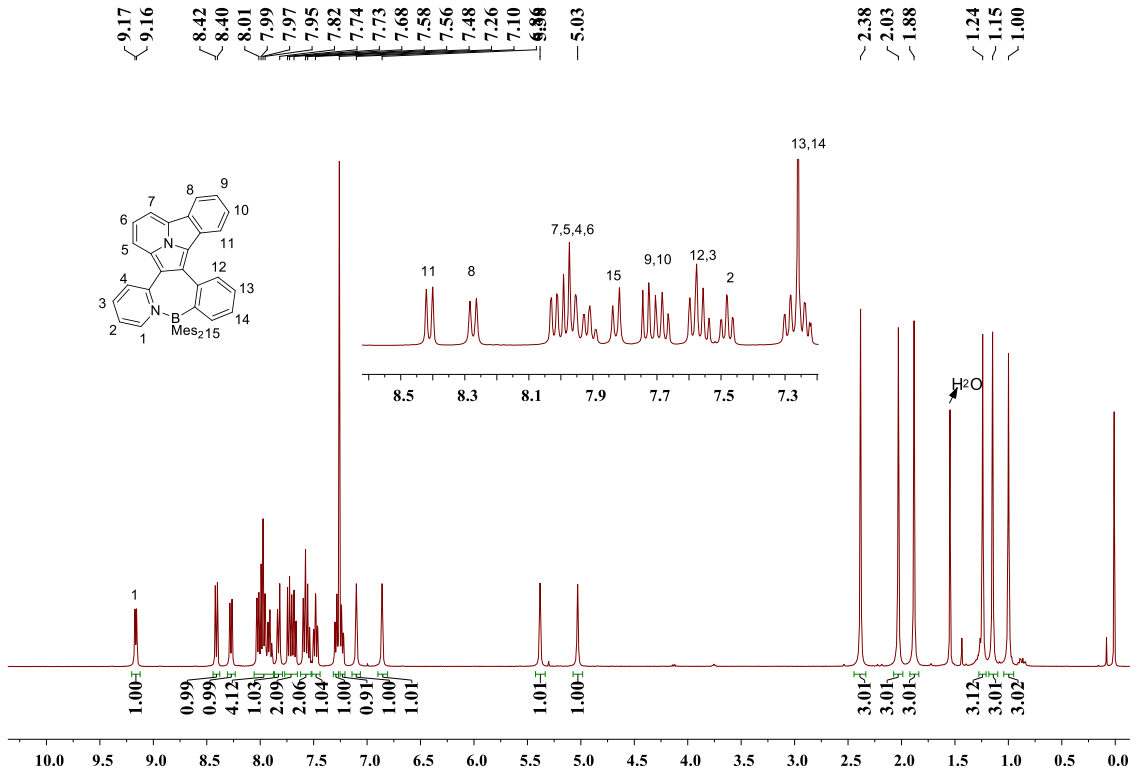


Figure S66: ^{1}H NMR spectrum of compound **2b** in $CDCl_3$

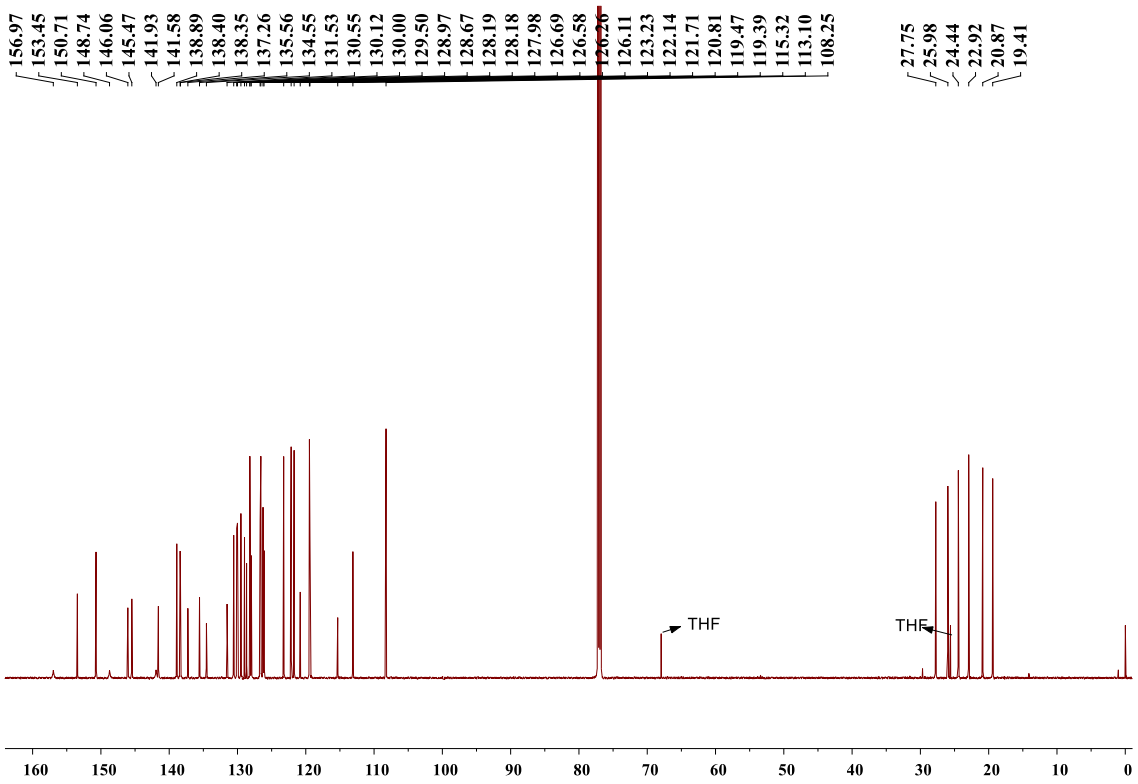


Figure S67: ^{13}C NMR spectrum of compound 2**b** in $CDCl_3$

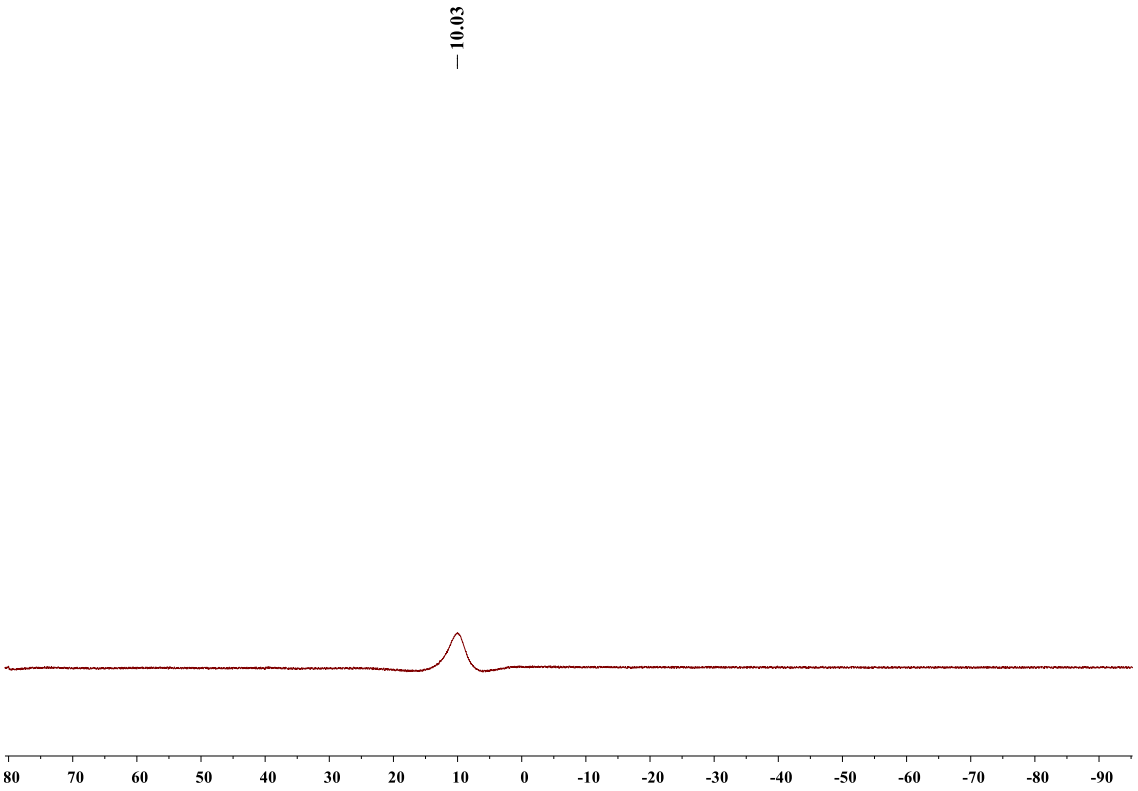


Figure S68: ^{11}B NMR spectrum of compound **2b** in $CDCl_3$

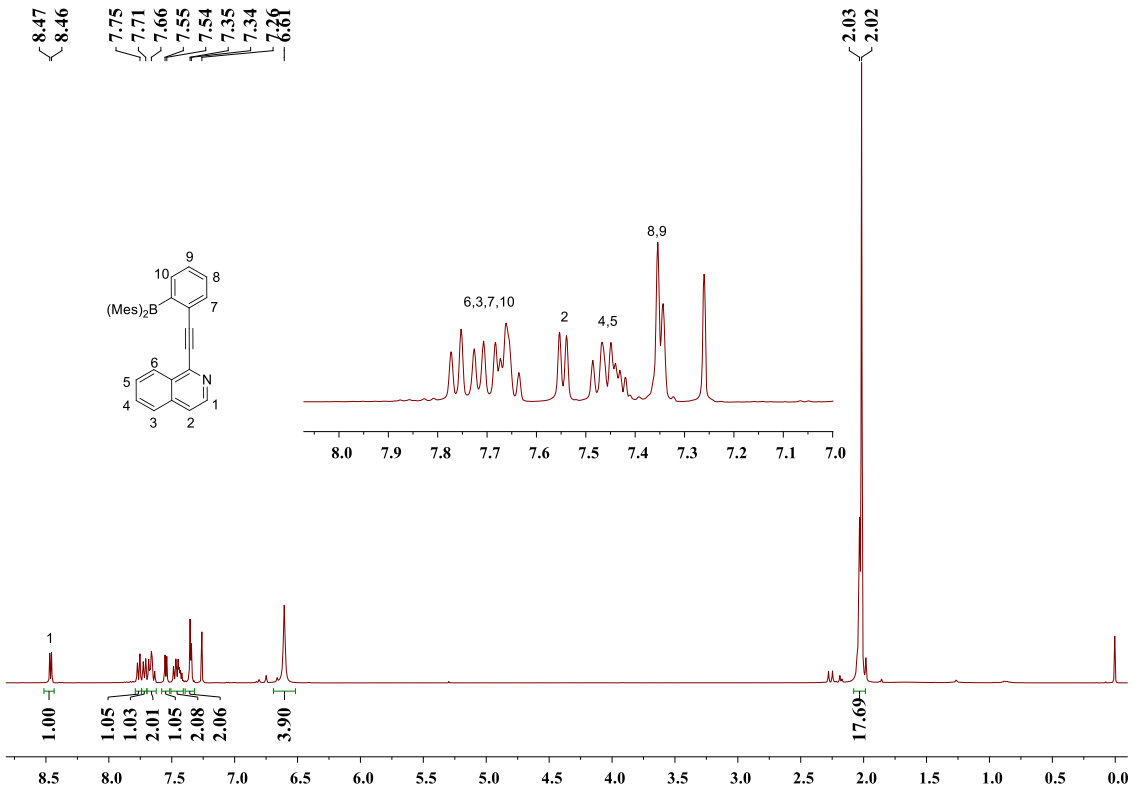


Figure S69: ^{1}H NMR spectrum of compound **3** in $CDCl_3$

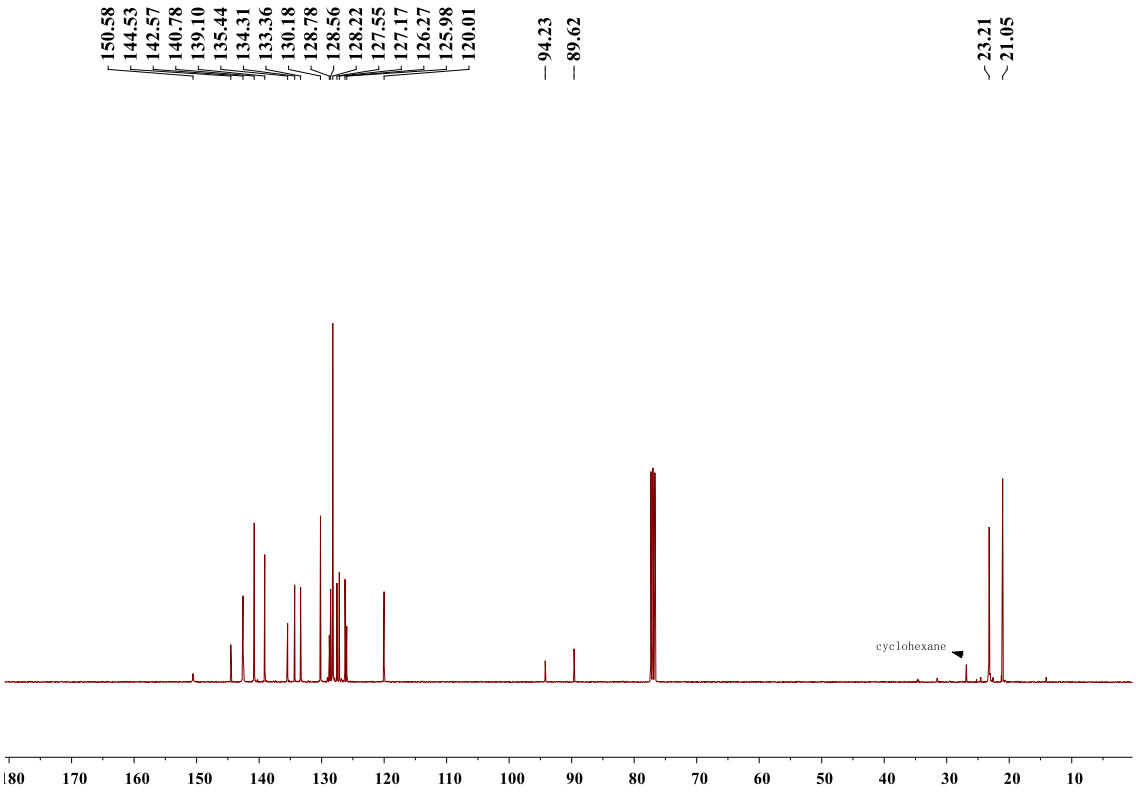


Figure S70: ^{13}C NMR spectrum of compound **3** in $CDCl_3$

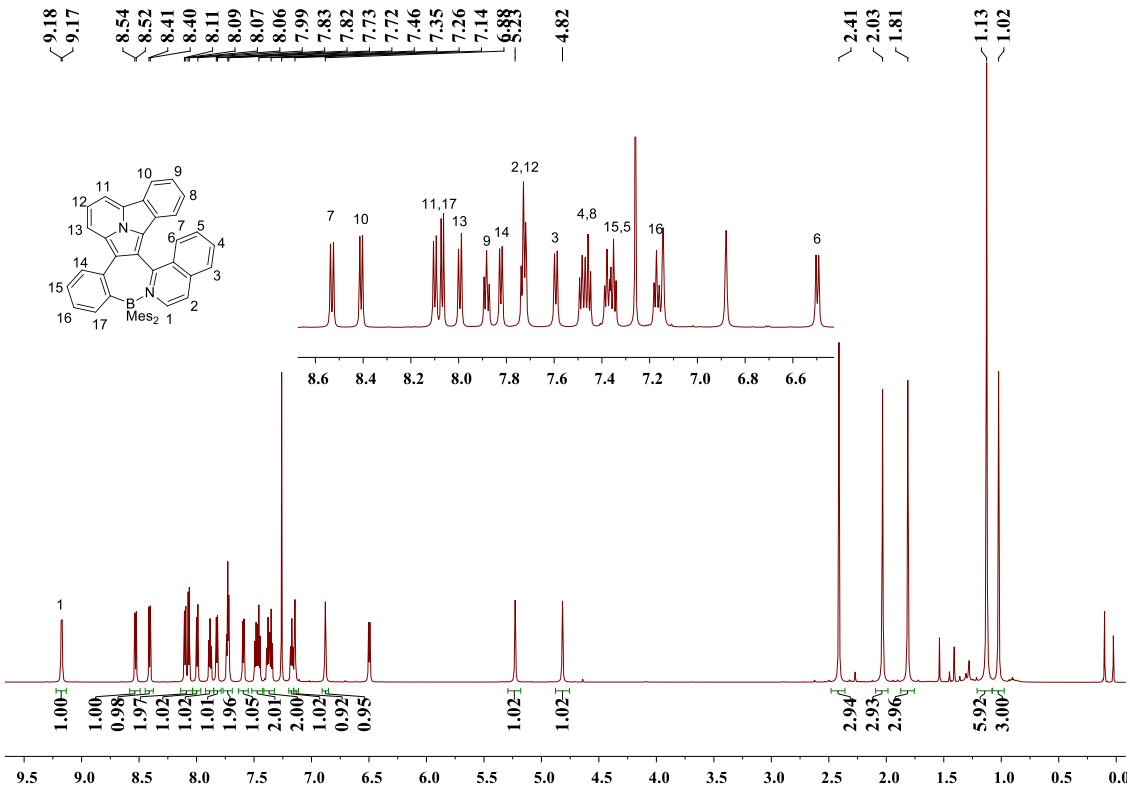


Figure S71: ^{1}H NMR spectrum of compound **3a** in $CDCl_3$

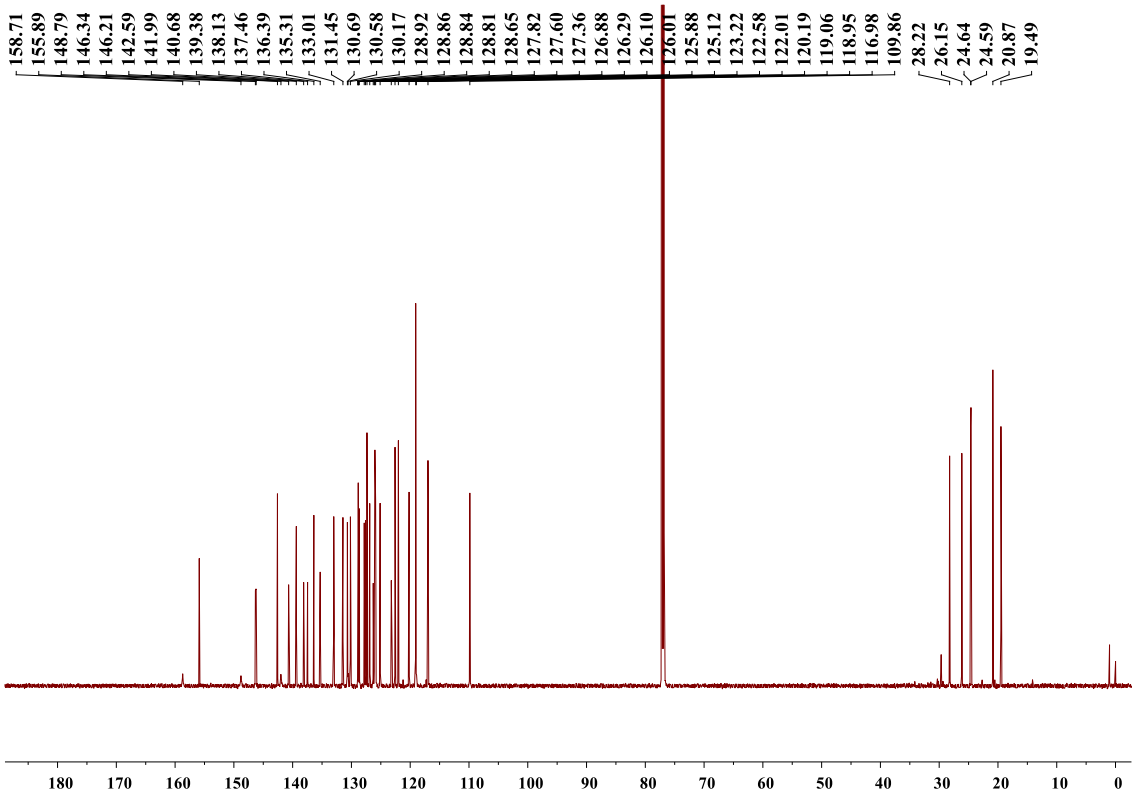


Figure S72: ^{13}C NMR spectrum of compound **3a** in $CDCl_3$

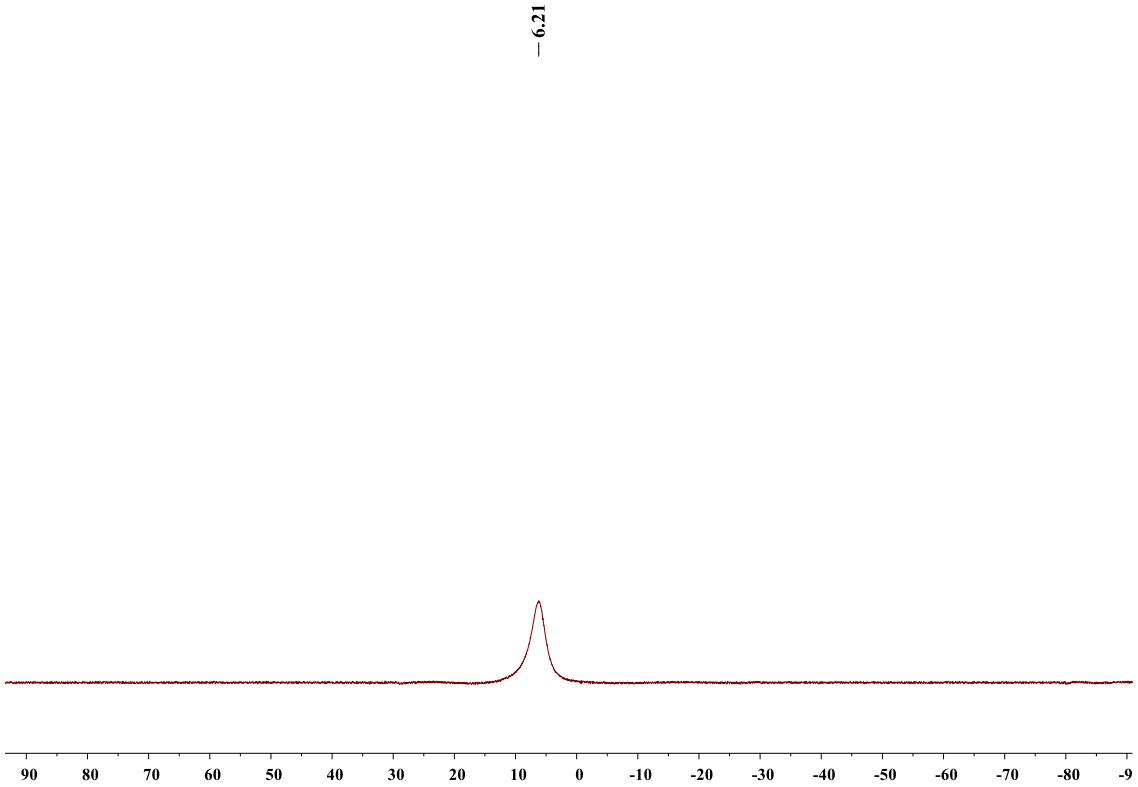


Figure S73: ^{11}B NMR spectrum of compound **3a** in $CDCl_3$

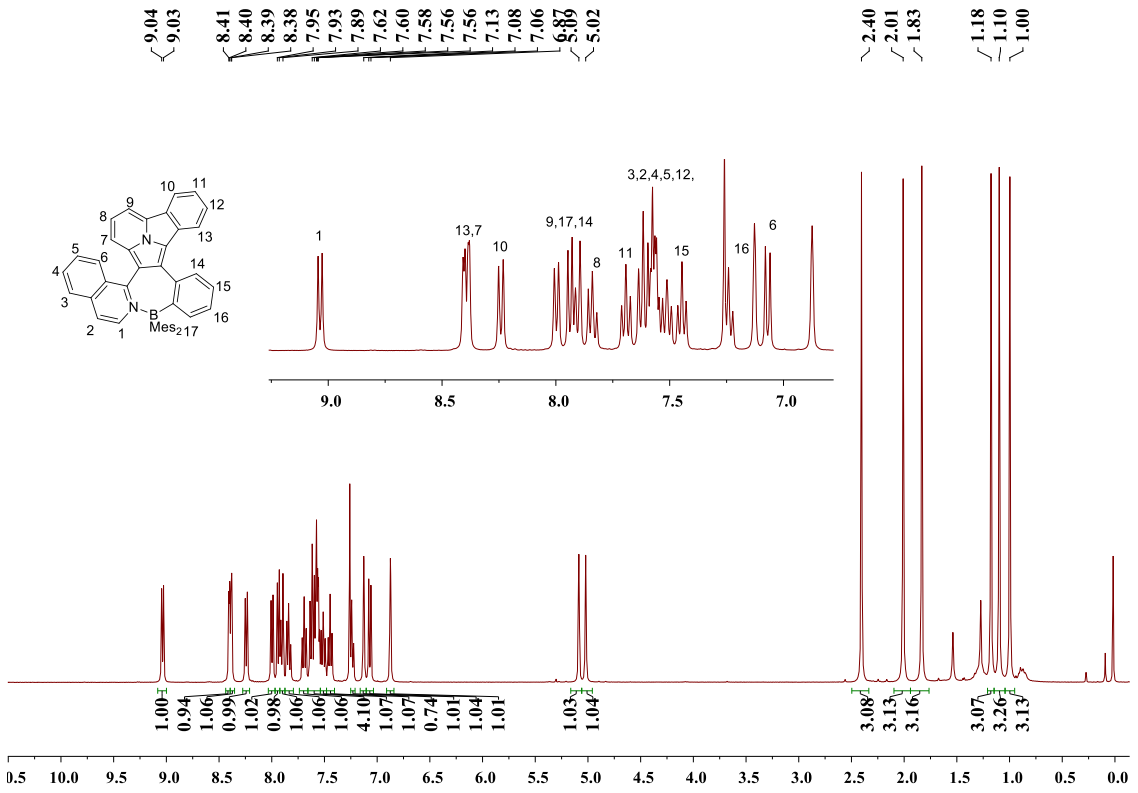


Figure S74: ^{1}H NMR spectrum of compound **3b** in $CDCl_3$

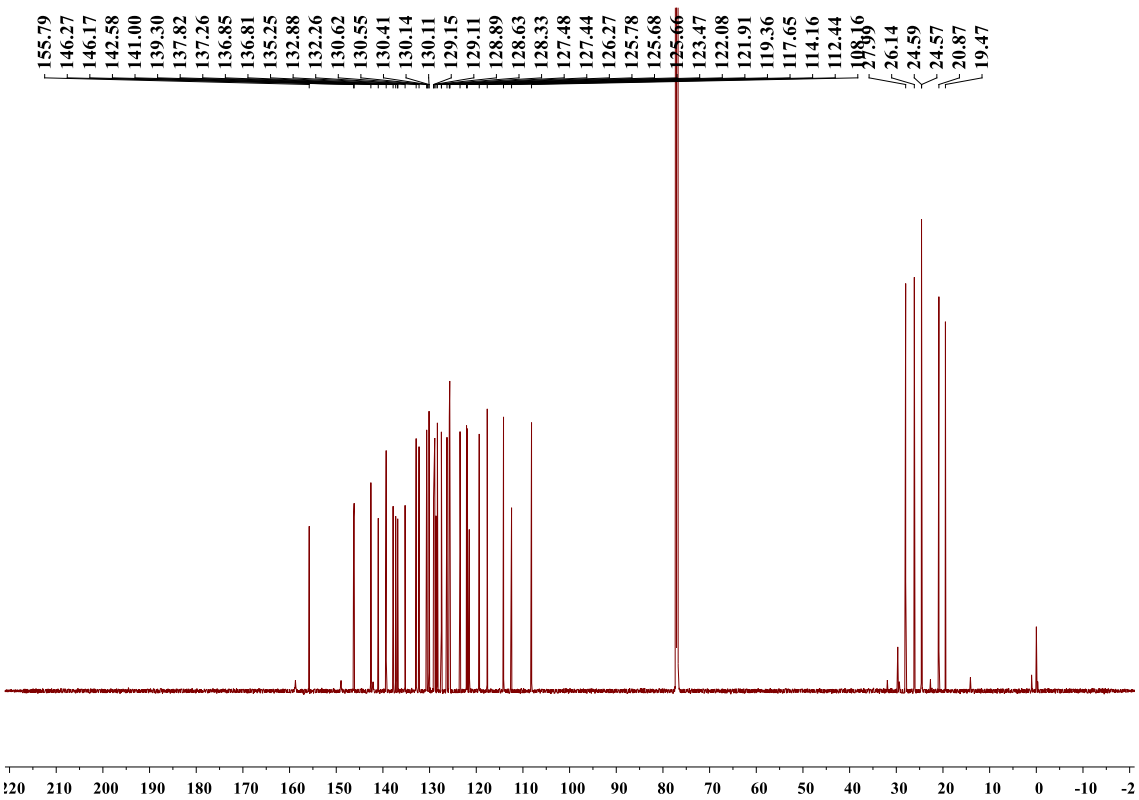


Figure S75: ^{13}C NMR spectrum of compound **3b** in $CDCl_3$

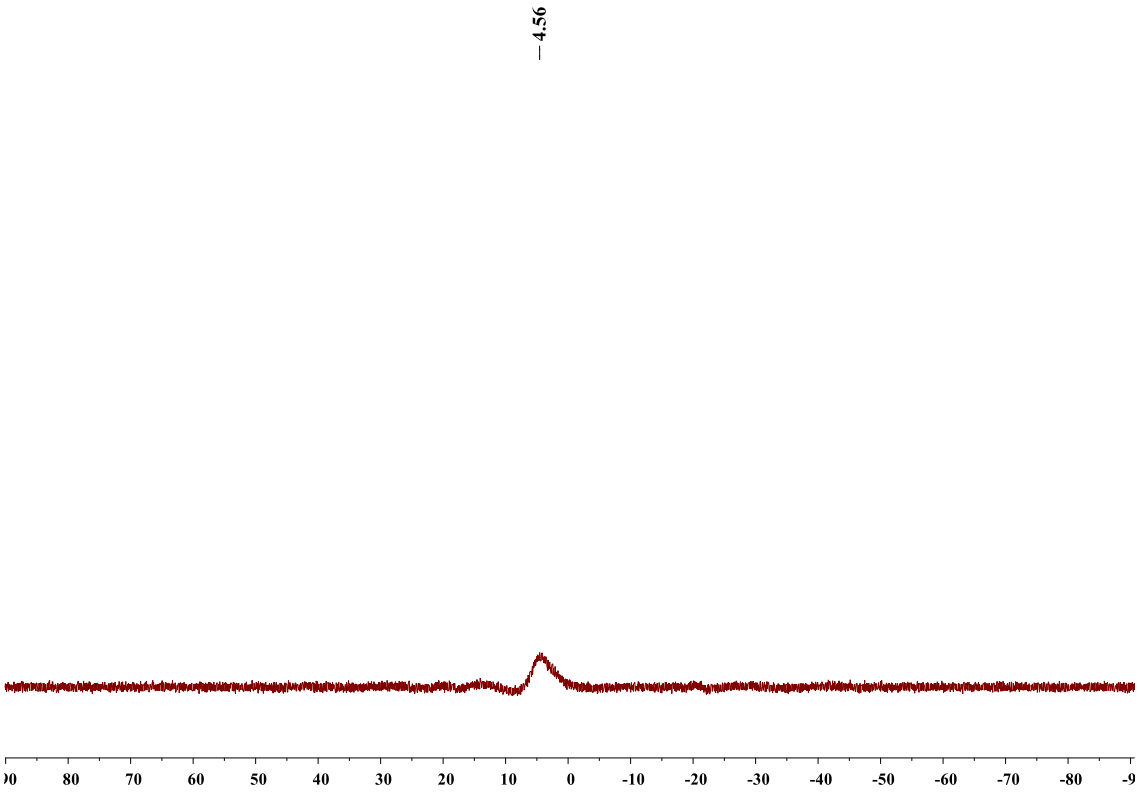


Figure S76: ^{11}B NMR spectrum of compound **3b** in $CDCl_3$

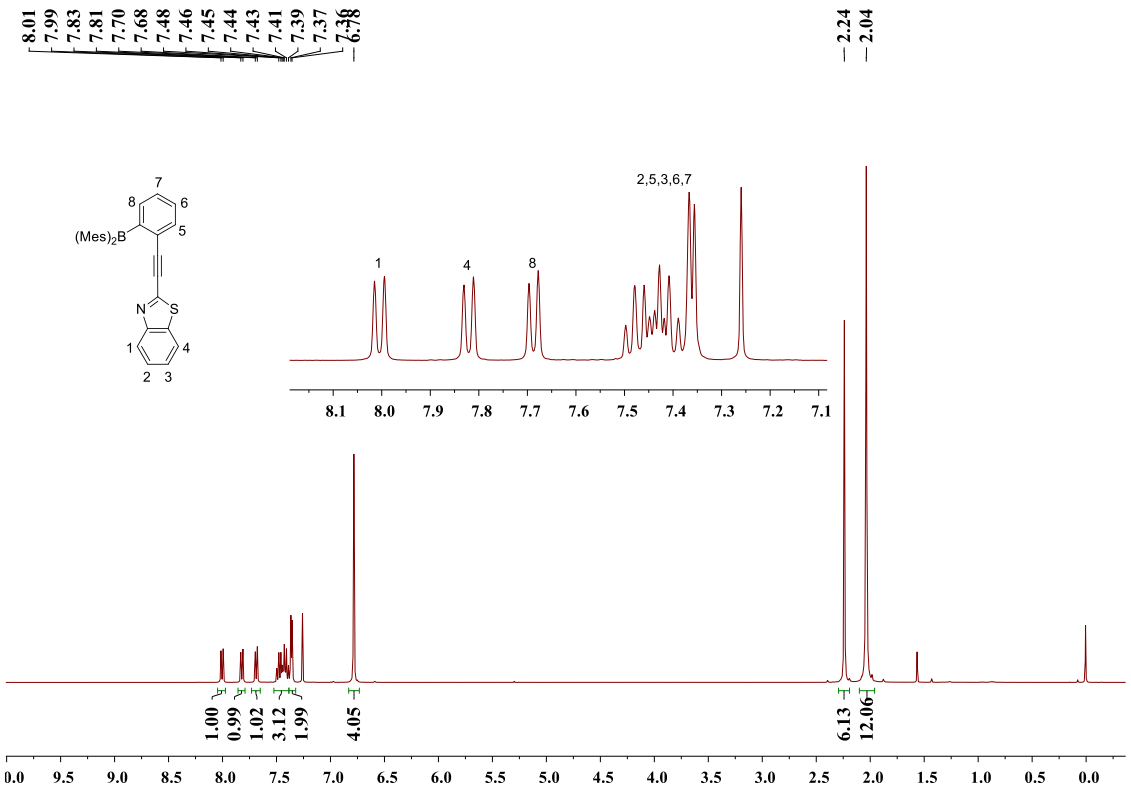


Figure S77: ^{1}H NMR spectrum of compound **4** in $CDCl_3$

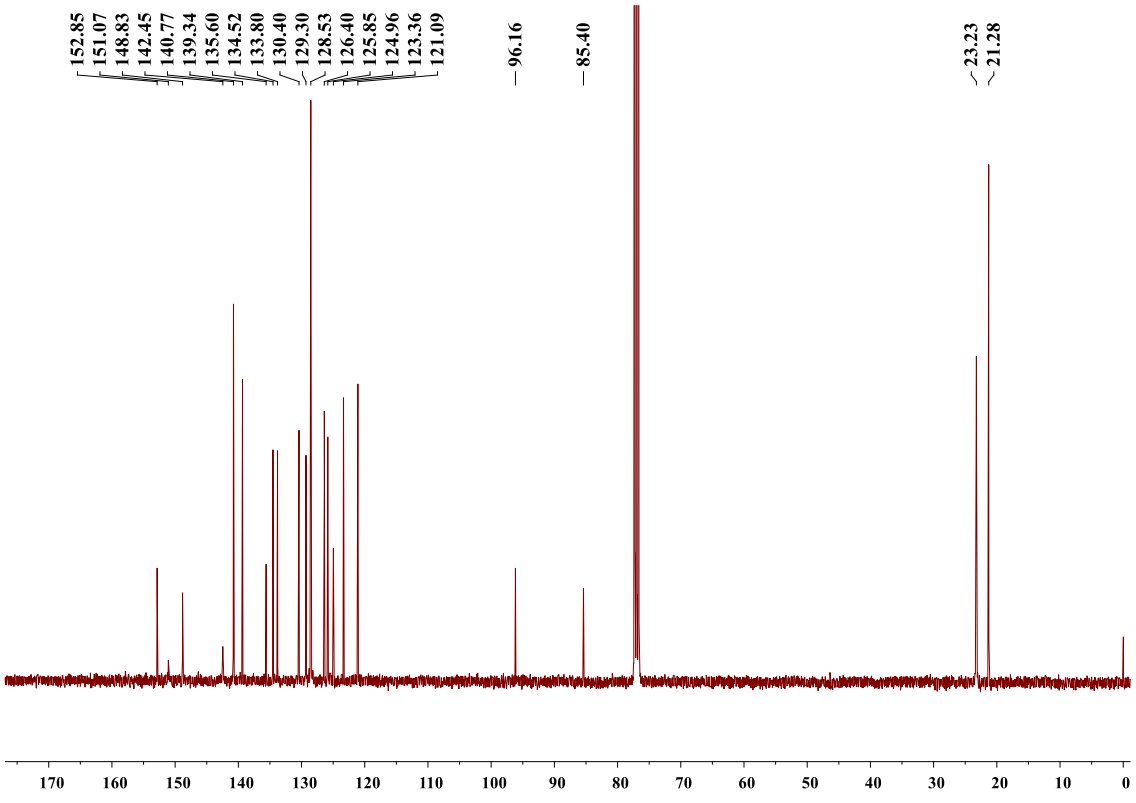


Figure S78: ^{13}C NMR spectrum of compound **4** in $CDCl_3$

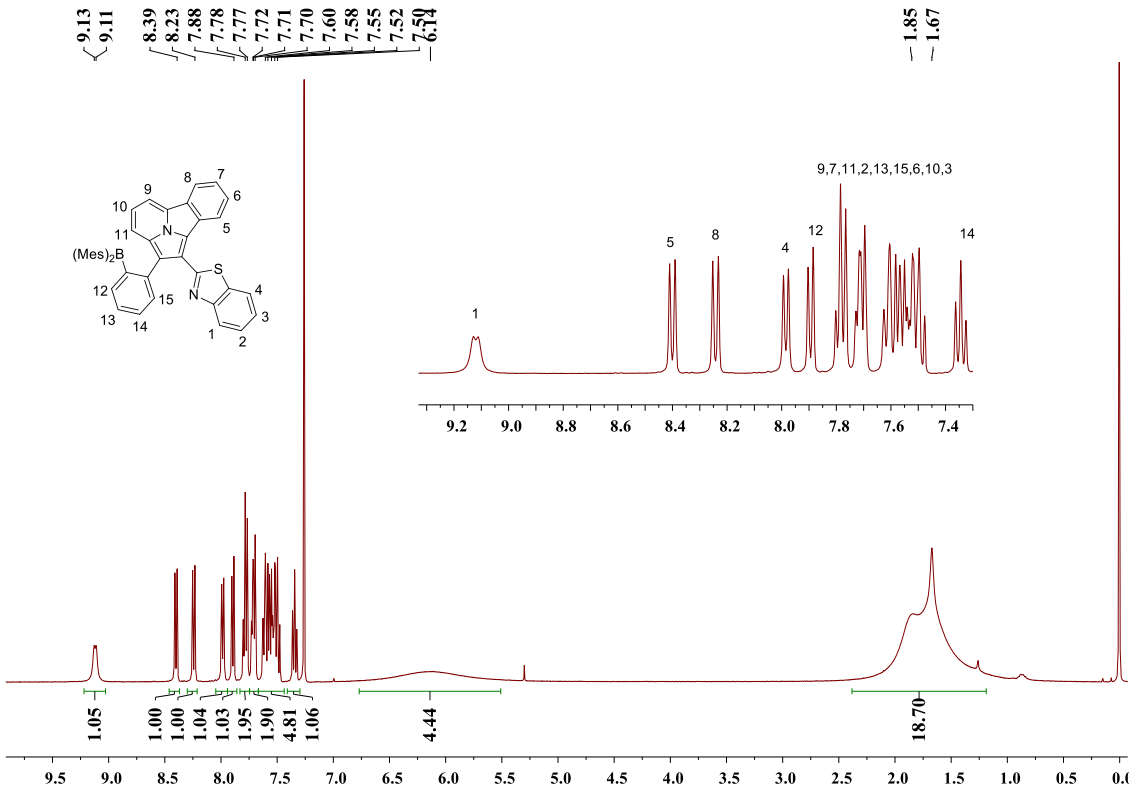


Figure S79: ^{1}H NMR spectrum of compound **4a** in $CDCl_3$

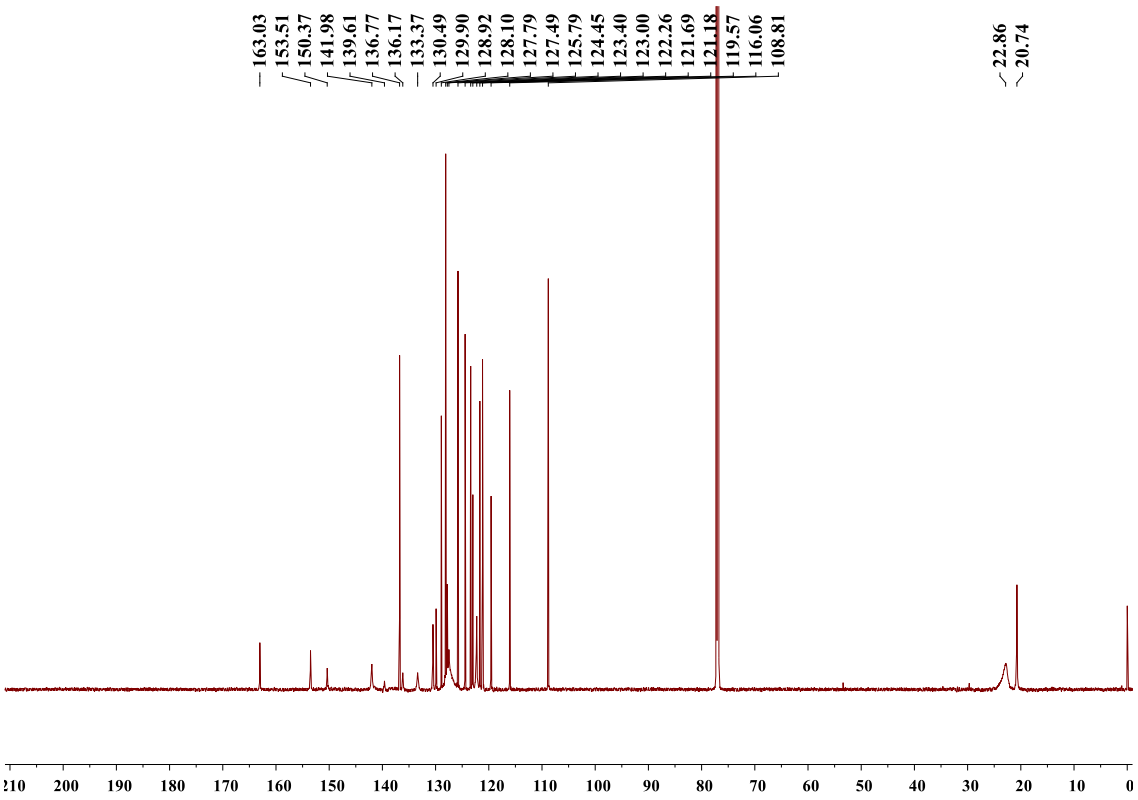


Figure S80: The ^{13}C NMR spectrum of compound **4a** in $CDCl_3$

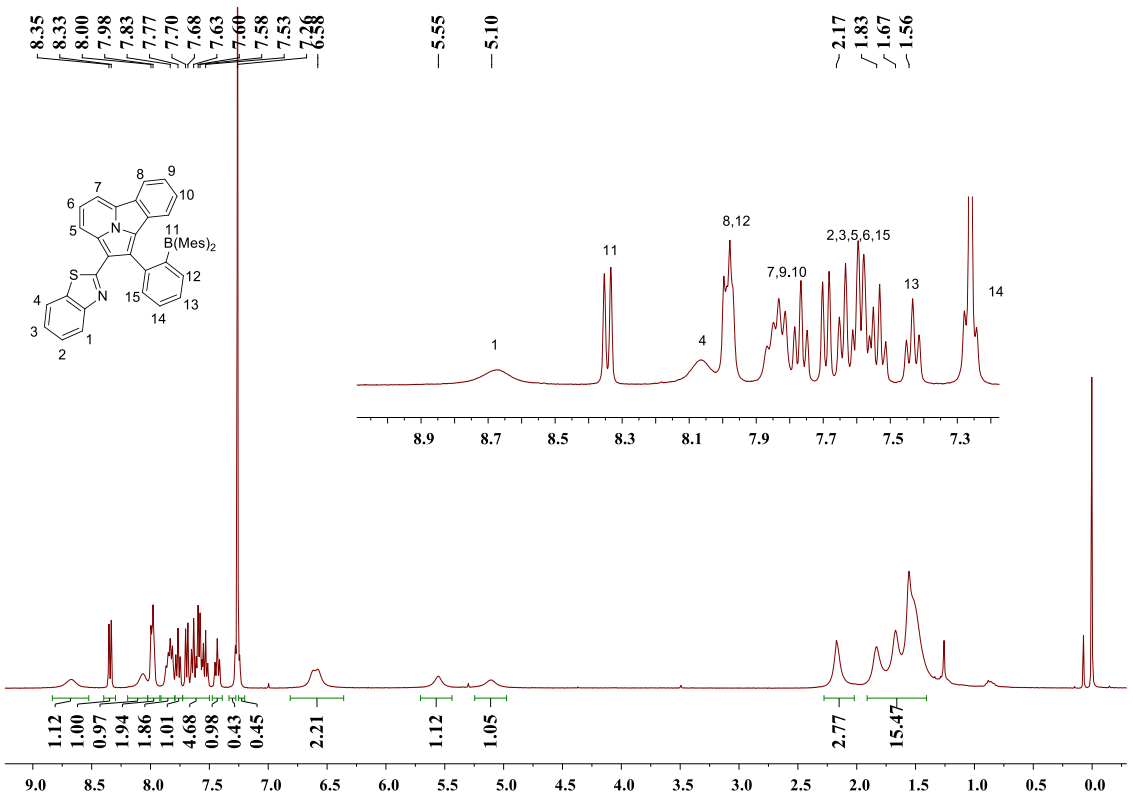


Figure S81: ^{1}H NMR spectrum of compound **4b** in $CDCl_3$

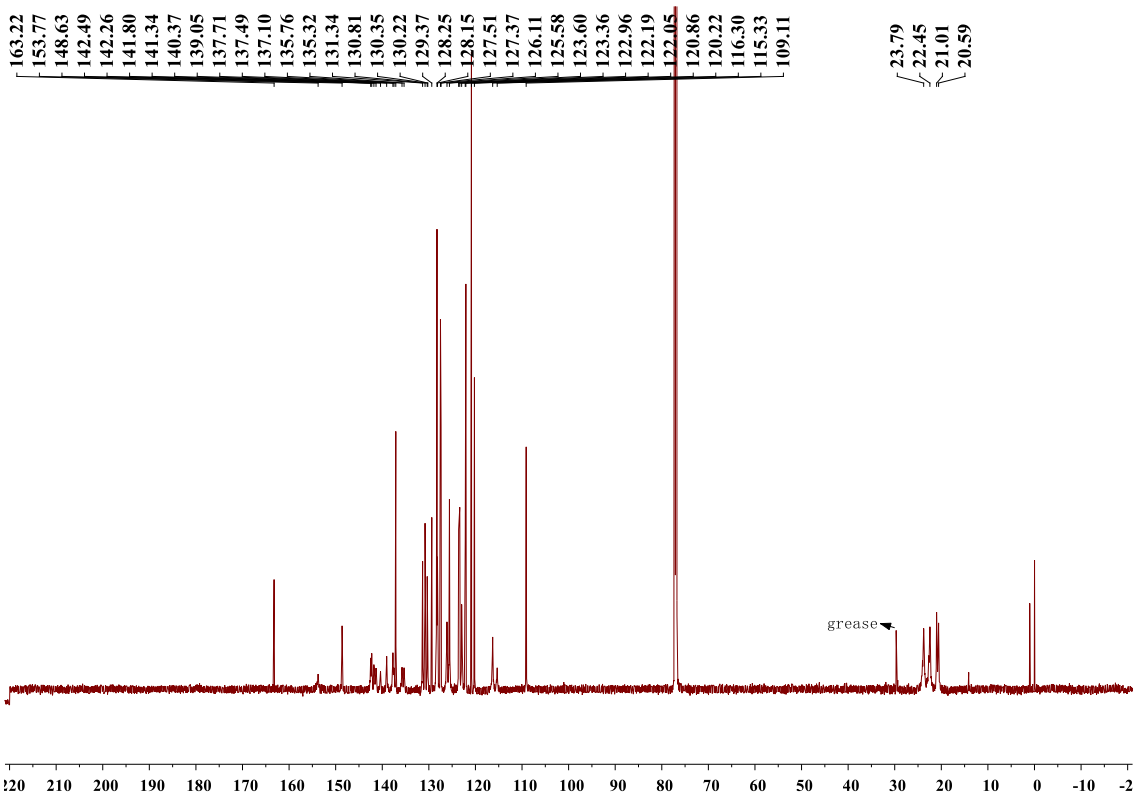


Figure S82: ^{13}C NMR spectrum of compound **4b** in $CDCl_3$

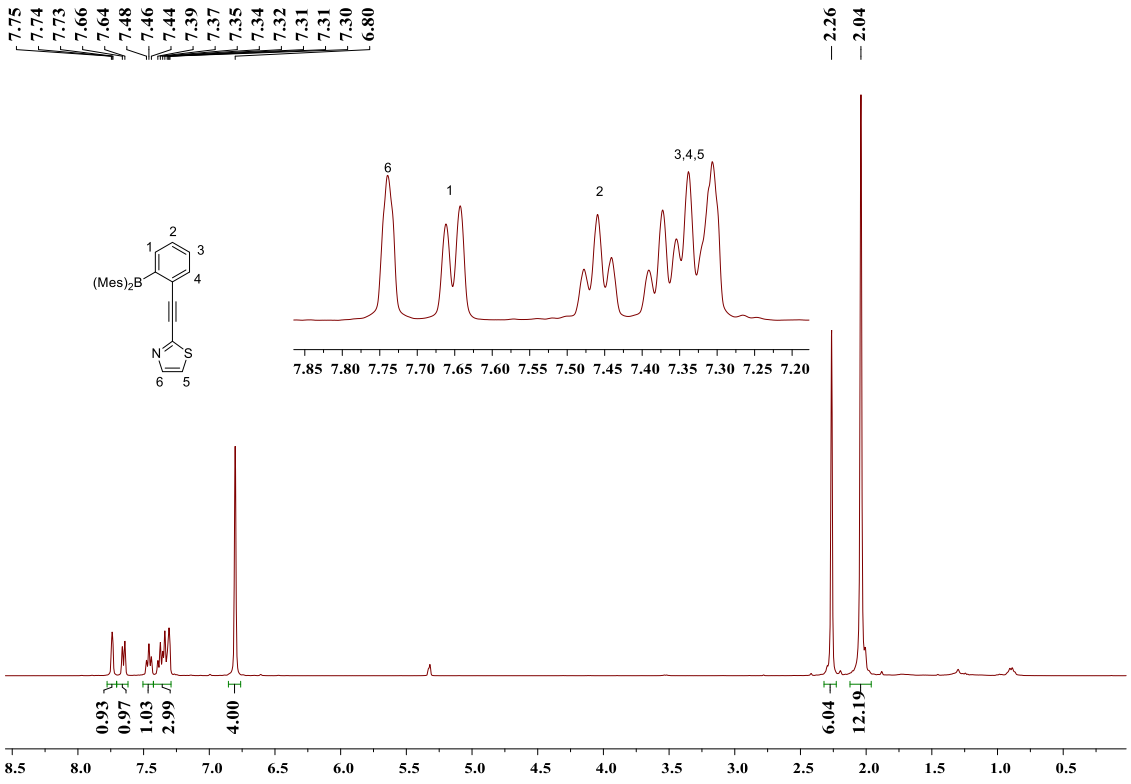


Figure S83: ^{1}H NMR spectrum of compound **5** in CD_2Cl_2

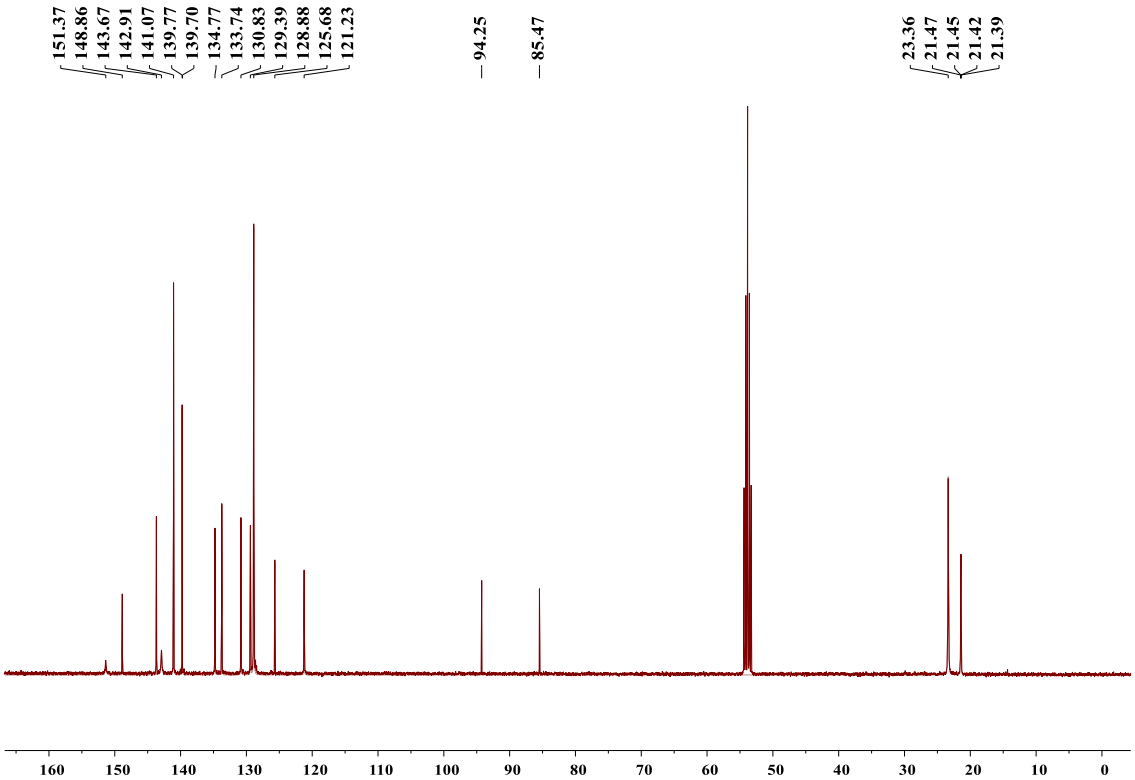


Figure S84: ^{13}C NMR spectrum of compound **5** in CD_2Cl_2

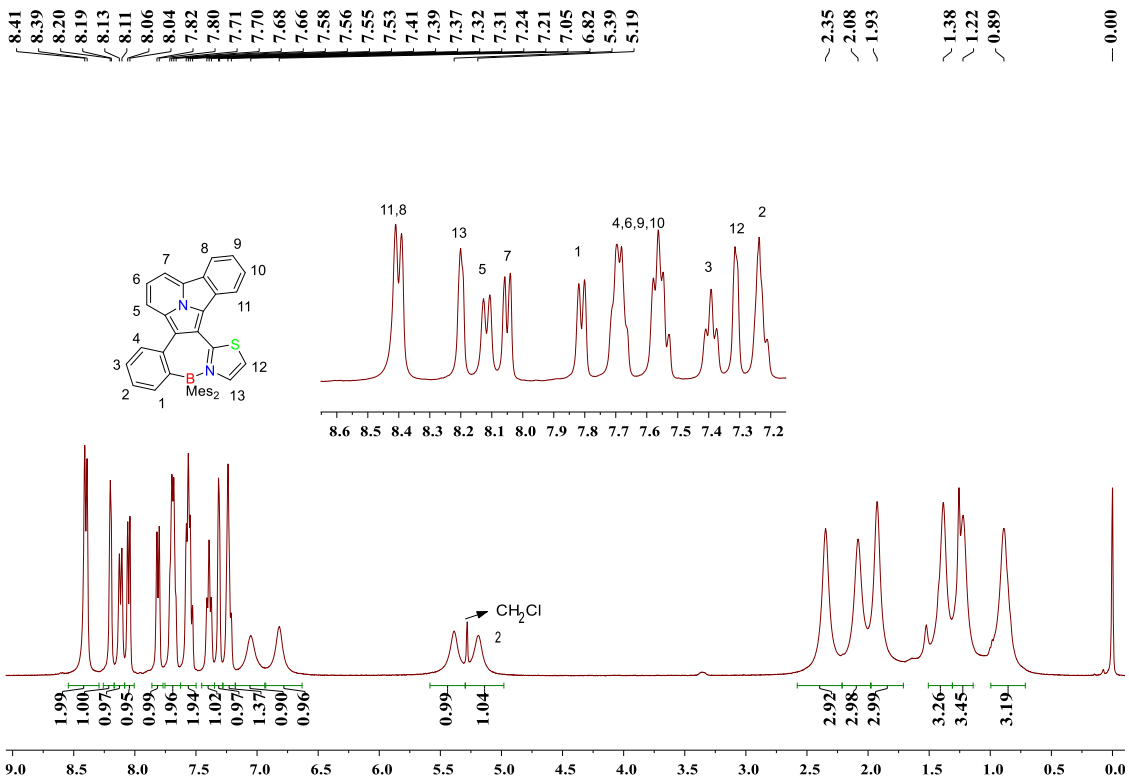


Figure S85: ^{1}H NMR spectrum of compound **5a** in $CDCl_3$

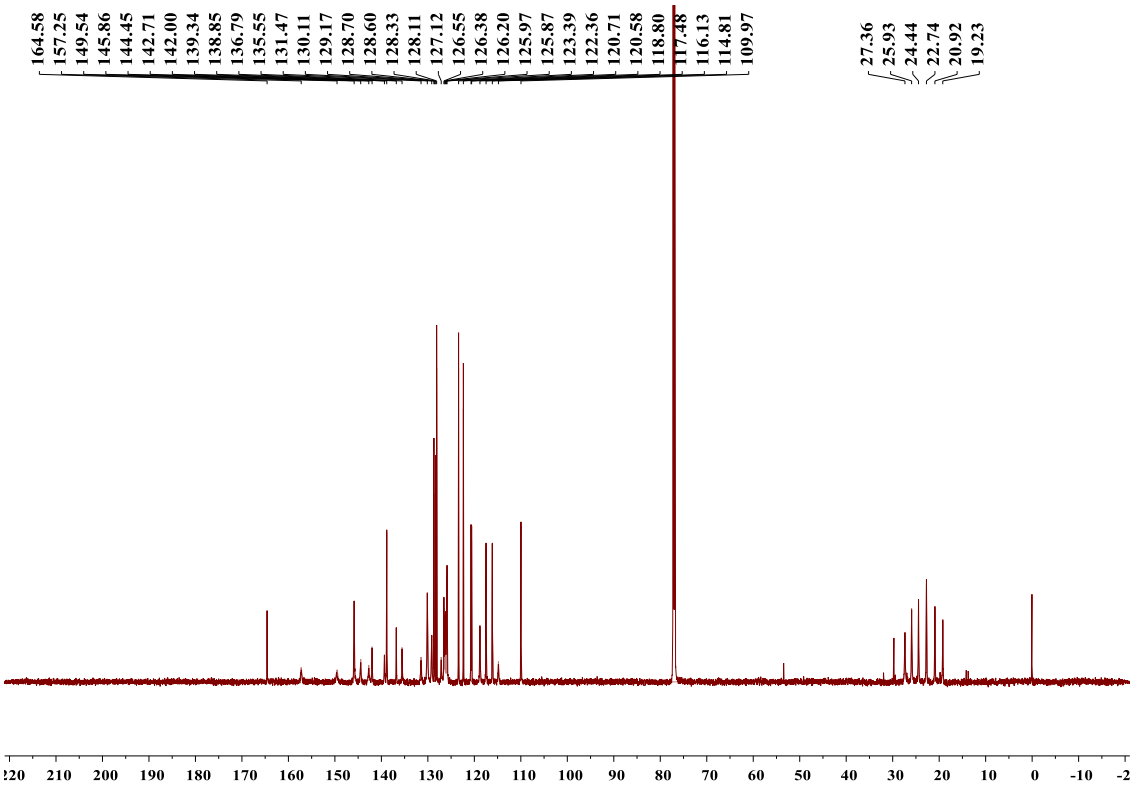


Figure S86: ^{13}C NMR spectrum of compound **5a** in $CDCl_3$

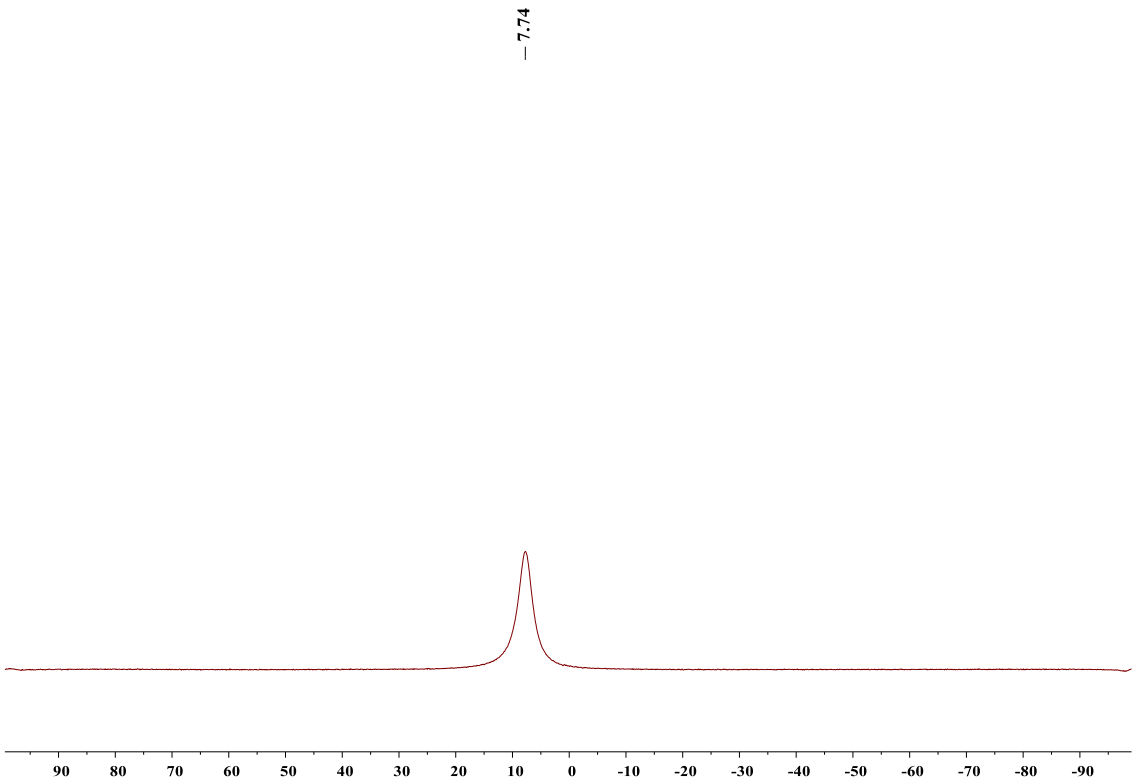


Figure S87: ^{11}B NMR spectrum of compound **5a** in $CDCl_3$

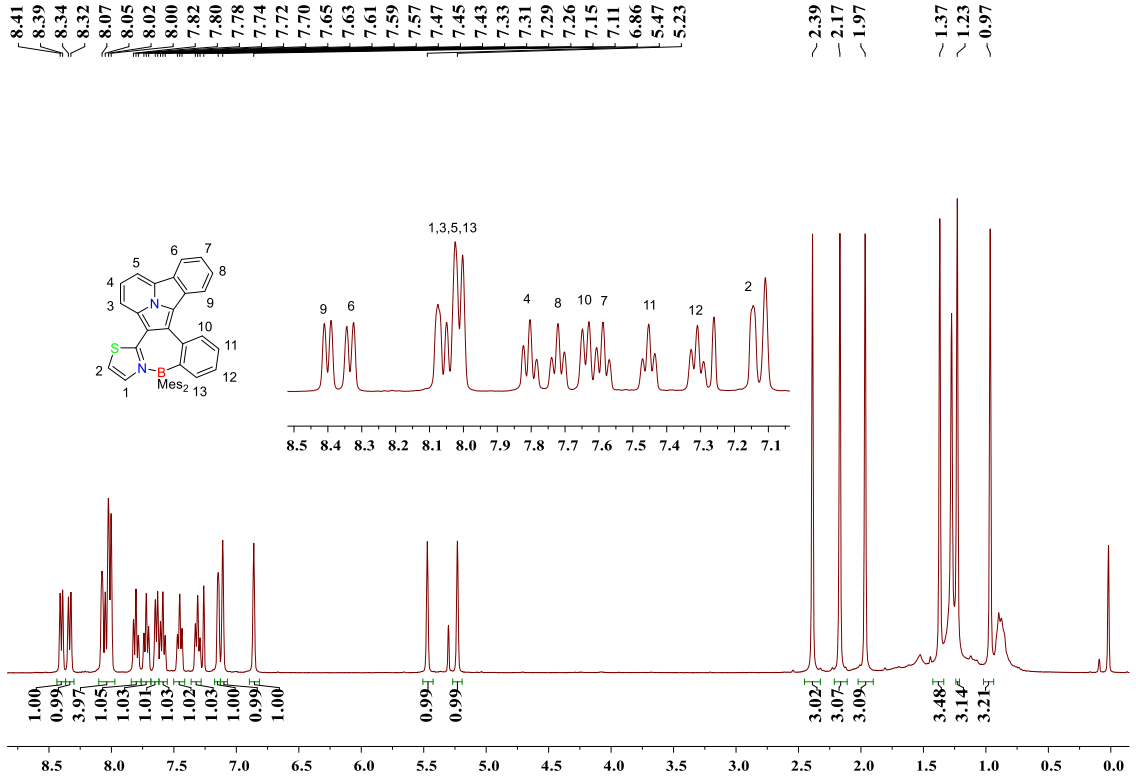


Figure S88: ^{1}H NMR spectrum of compound **5b** in $CDCl_3$

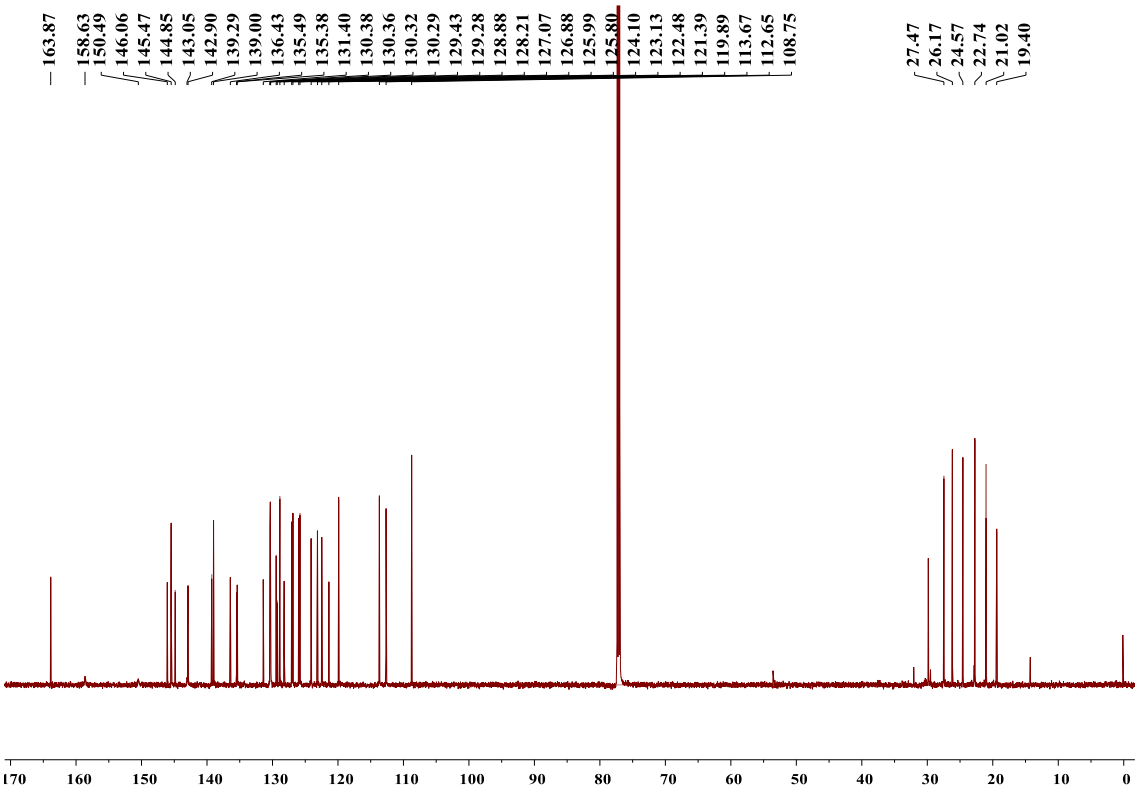


Figure S89: ^{13}C NMR spectrum of compound **5b** in $CDCl_3$

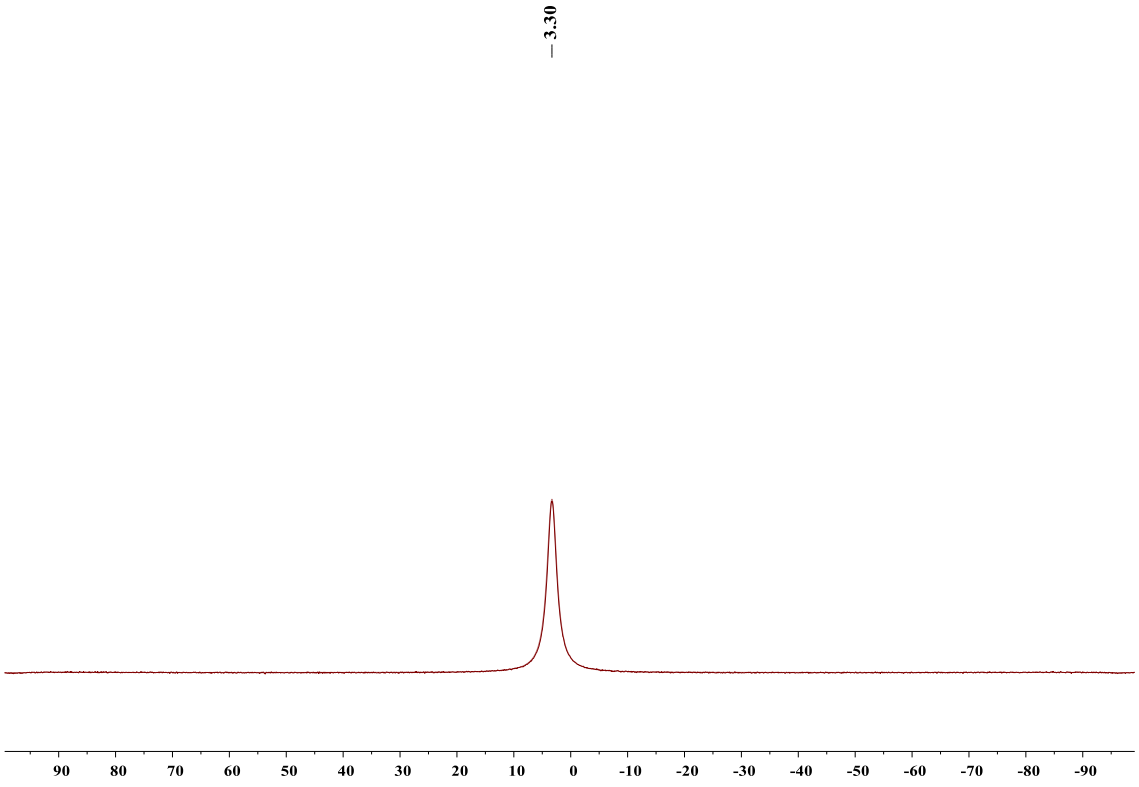


Figure S90: ^{11}B NMR spectrum of compound **5b** in $CDCl_3$

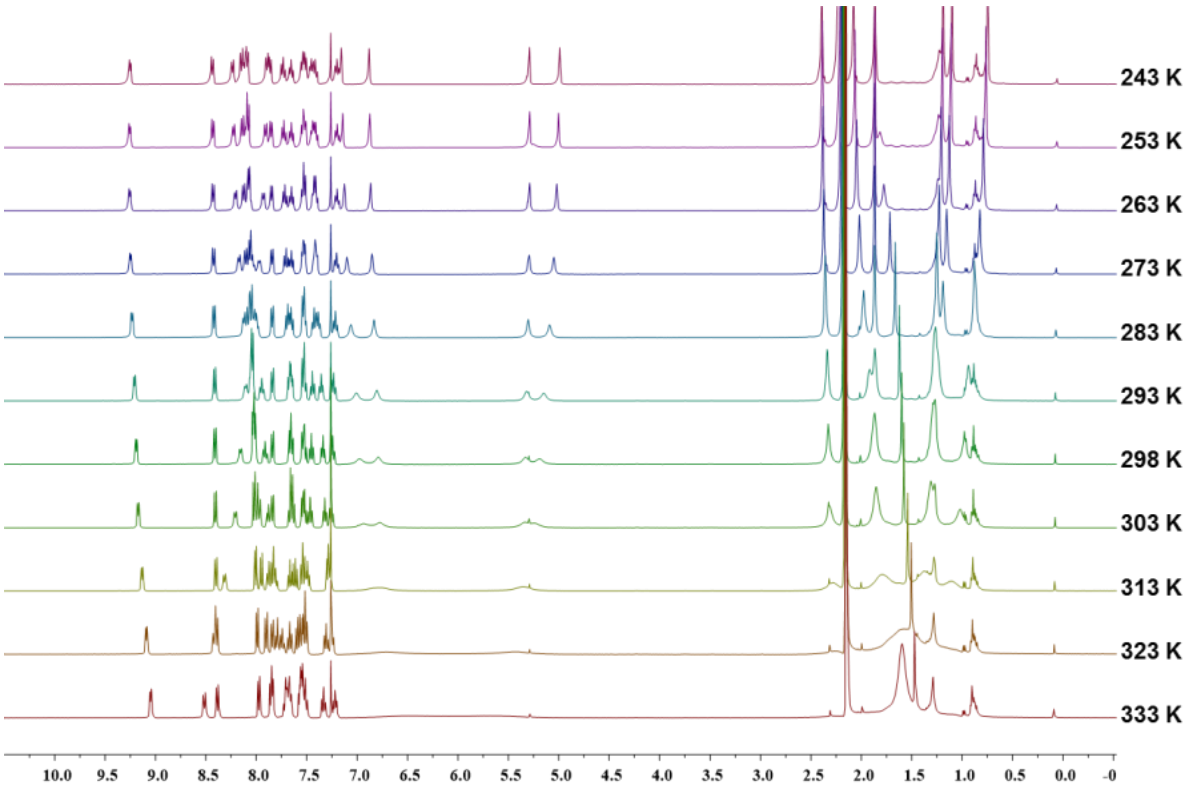


Figure S91: ^{1}H NMR spectra of **2a** (in $CDCl_3$) recorded at different temperatures

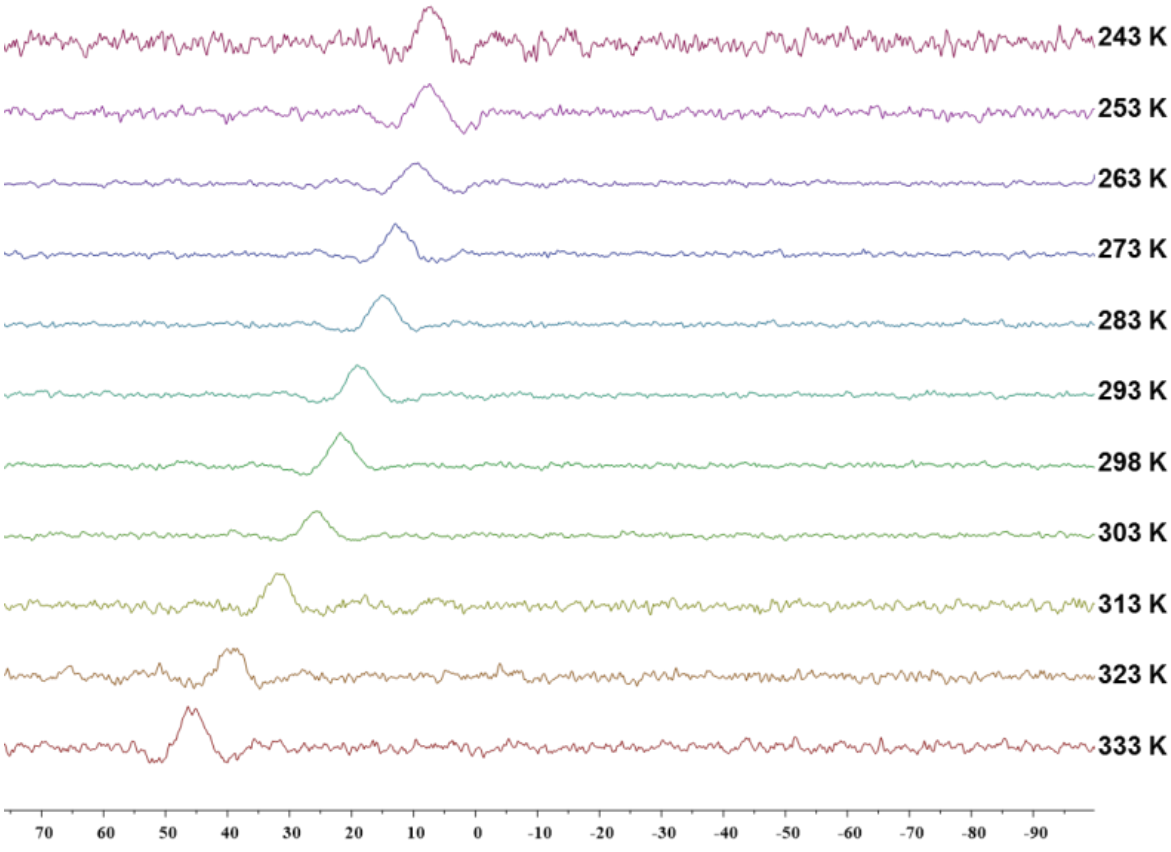


Figure S92: ^{11}B NMR spectral change of **2a** with temperature in $CDCl_3$.

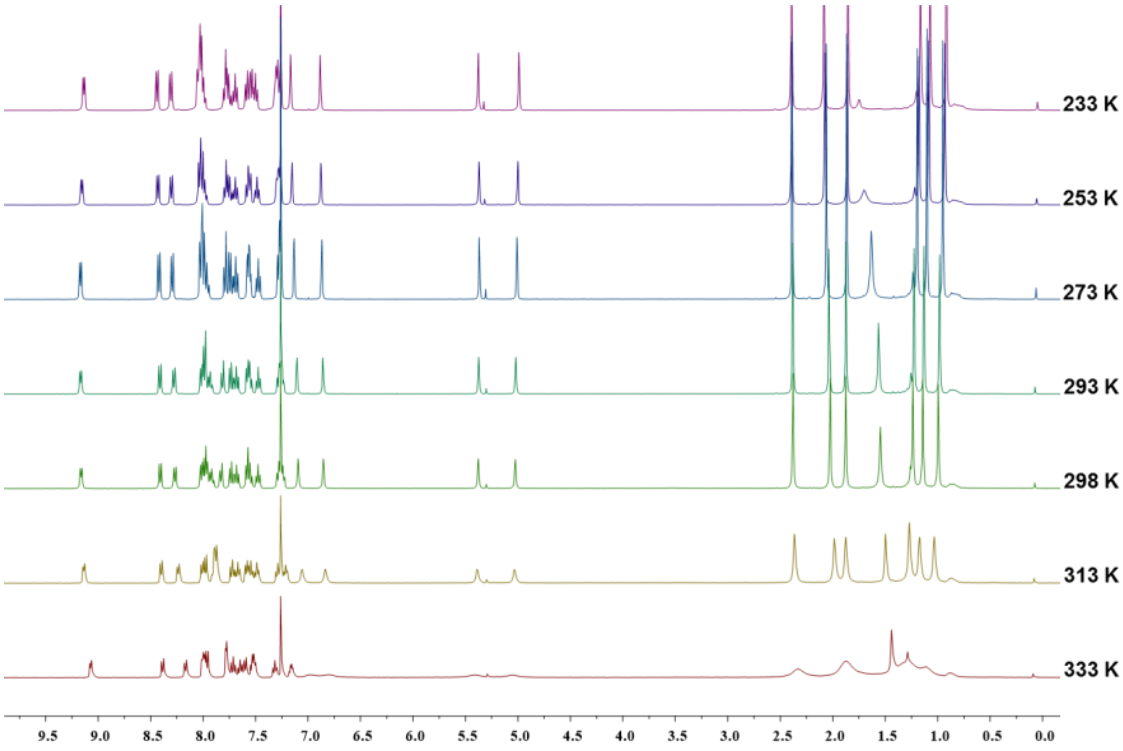


Figure S93: ^{1}H NMR spectra of **2b** (in $CDCl_3$) recorded at different temperatures

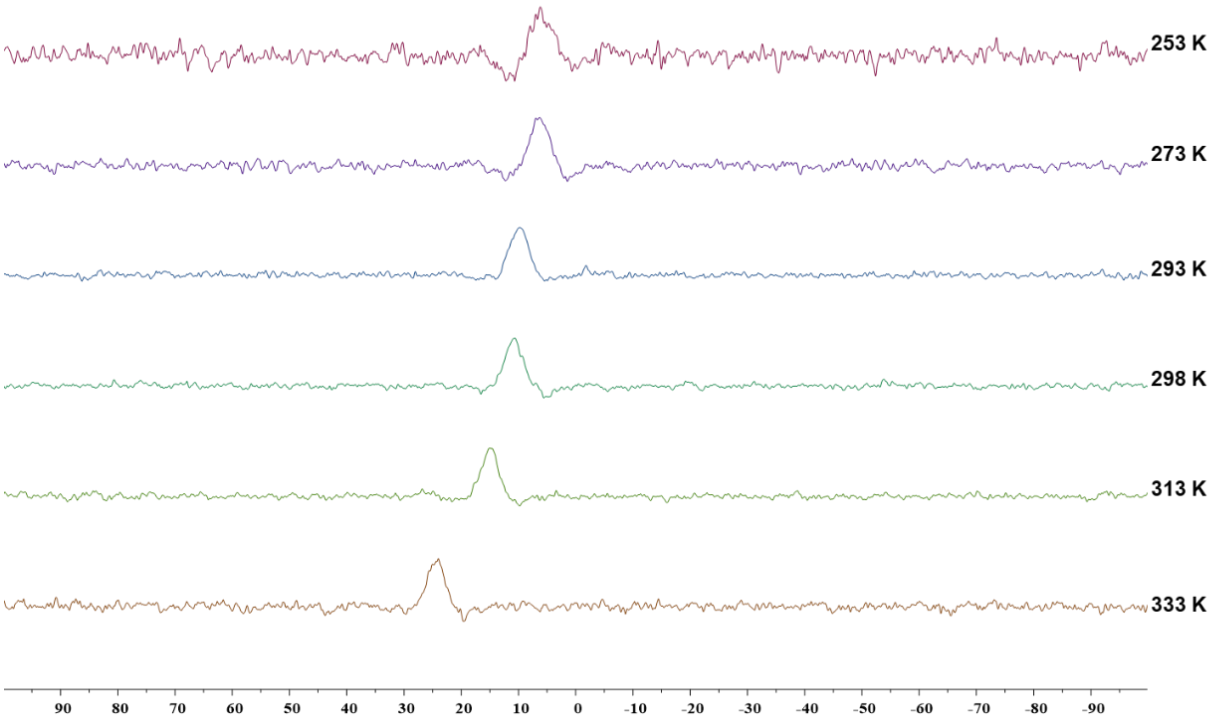


Figure S94: ^{11}B NMR spectral change of **2b** with temperature in $CDCl_3$.

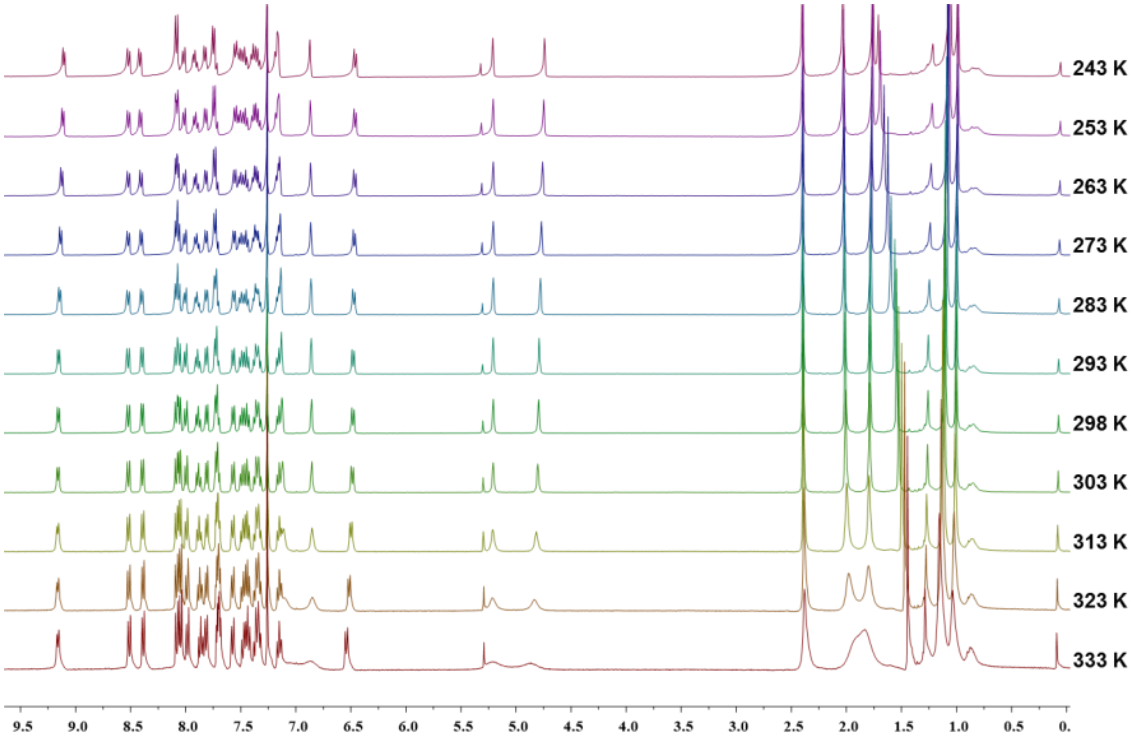


Figure S95: ^{1}H NMR spectra of **3a** (in $CDCl_3$) recorded at different temperatures

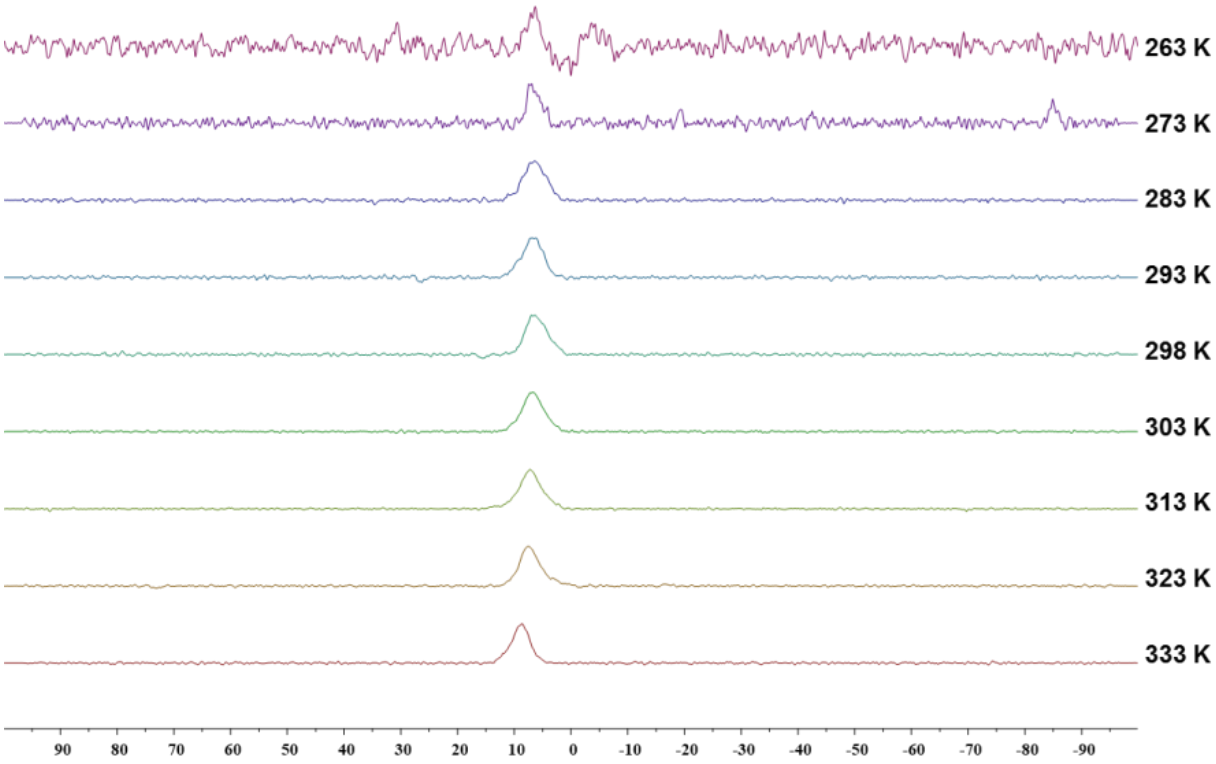


Figure S96: ^{11}B NMR spectral change of **3a** with temperature in $CDCl_3$.

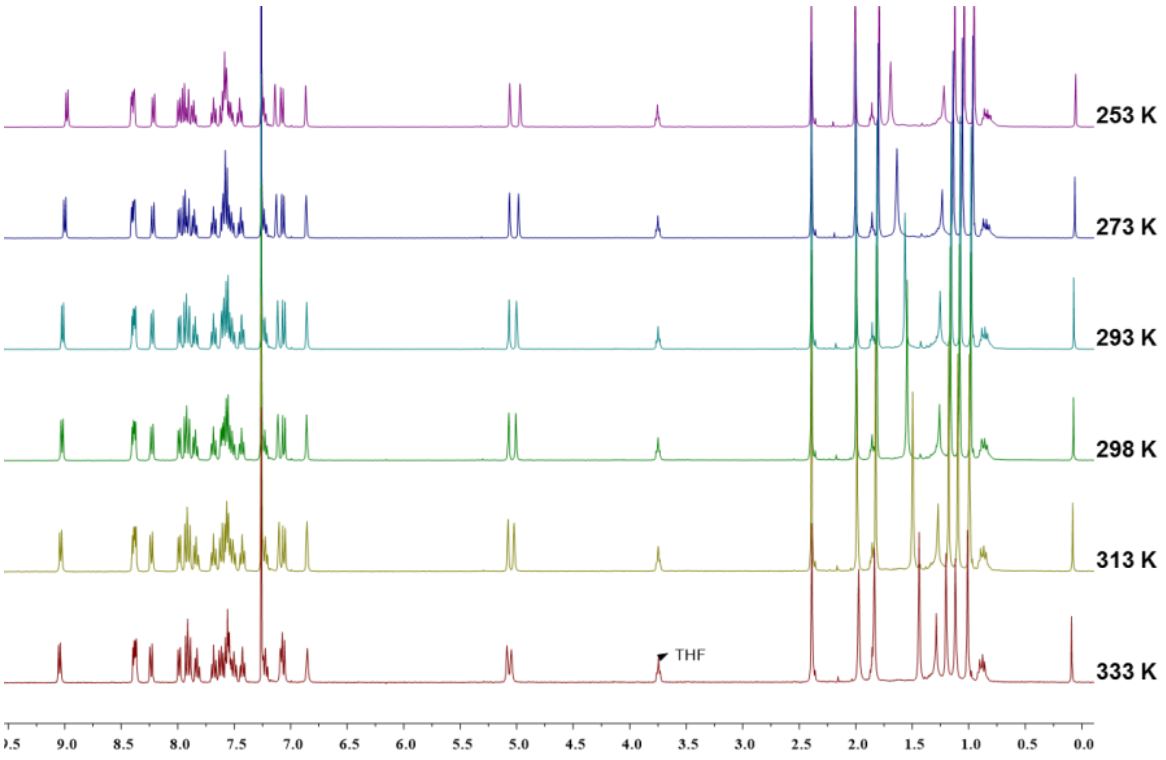


Figure S97: ^{1}H NMR spectra of **3b** (in $CDCl_3$) recorded at different temperatures

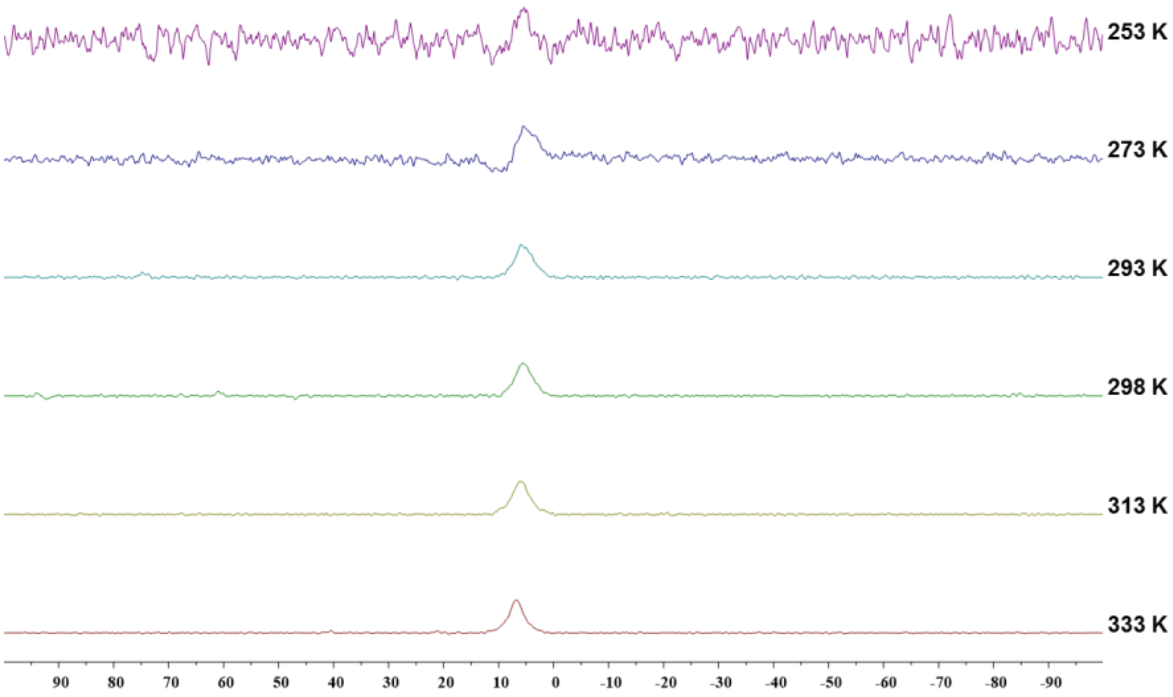


Figure S98: ^{11}B NMR spectral change of **3b** with temperature in $CDCl_3$.

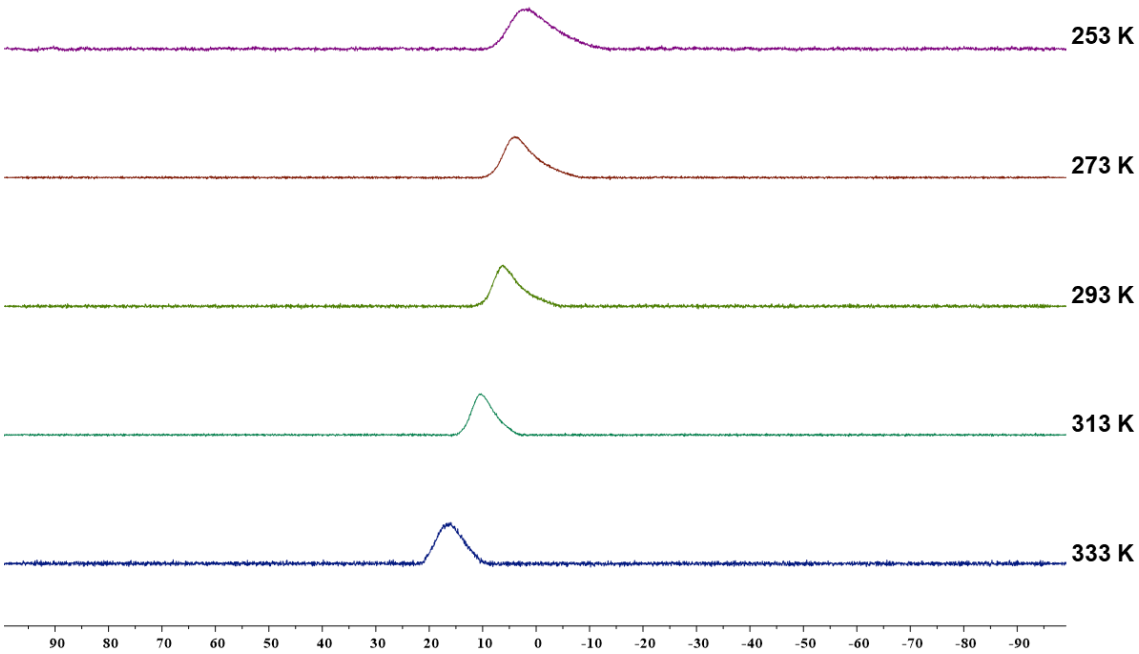


Figure S99: ^{11}B NMR spectral change of **5a** with temperature in $CDCl_3$.

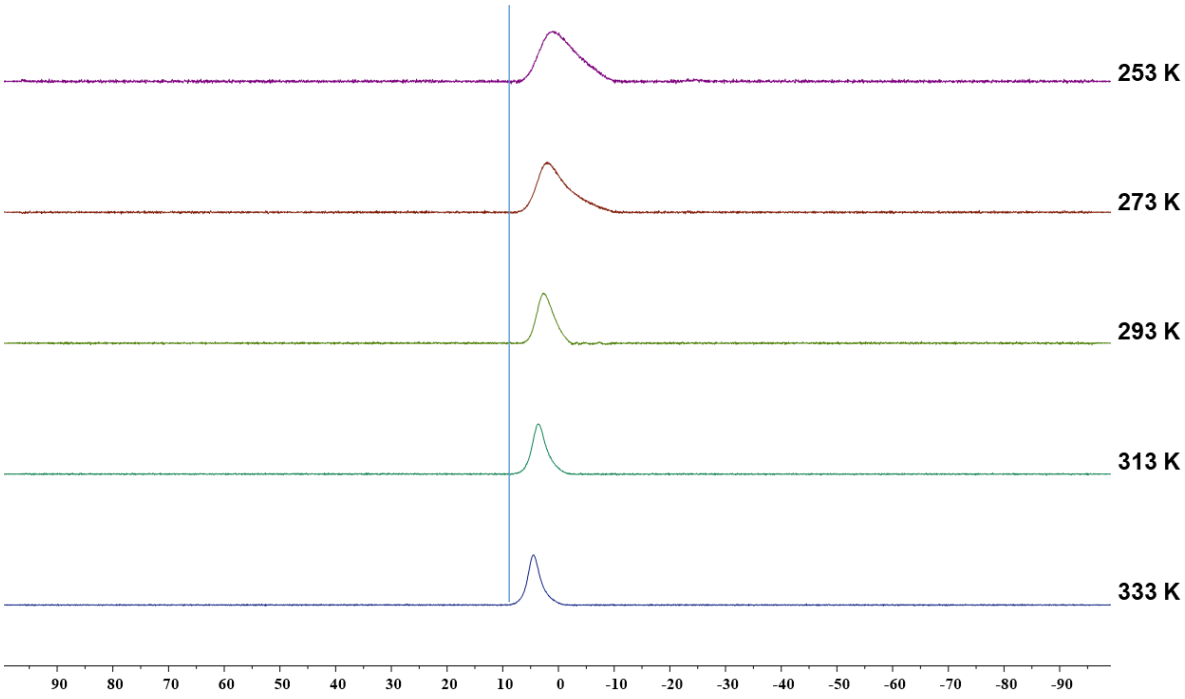


Figure S100: ^{11}B NMR spectral change of **5b** with temperature in $CDCl_3$.

V. X-ray Crystallographic Data

The crystal data were collected on a Bruker D8-Venture diffractometer with Mo-target (λ = 0.71073 Å) at 180 K for all compounds. Data were processed on a PC with the aid of the Bruker SHELXTL software package and corrected for absorption effects. All non-hydrogen atoms were refined anisotropically. The positions of hydrogen atoms were calculated and refined isotropically. The crystal data were deposited to the Cambridge Crystallographic Data Centre with deposition numbers of CCDC 1839688 (B1a), 1839689 (B1b), 1839690 (B2a), 1839691 (B2b), 1839692(B3b), 1839693 (B3a), 1839694 (B4a), 1839695 (B4b), 1854311(B5a), 1853312(B5b). This data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif].

Table S48. Crystal data and structure refinement for B1a.

Identification code	b1a-sr	
Empirical formula	C43 H37 B N2	
Formula weight	592.55	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.489(3) Å	α= 98.386(18)°.
	b = 12.387(7) Å	β= 100.888(15)°.
	c = 17.400(6) Å	γ = 91.61(3)°.
Volume	1774.6(13) $Å^3$	
Z	2	
Density (calculated)	1.109 Mg/m^3	
Absorption coefficient	0.063 mm^{-1}	
F(000)	628	
Crystal size	0.367 x 0.207 x 0.146 mm^3	
Theta range for data collection	2.413 to 27.203°.	
Index ranges	-10<=h<=10, -15<=k<=15, -21<=l<=22	
Reflections collected	16860	
Independent reflections	7652 [R(int) = 0.0737]	
Completeness to theta = 25.242°	96.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.991 and 0.977	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7652 / 0 / 421	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0767, wR2 = 0.1875	
R indices (all data)	R1 = 0.1322, wR2 = 0.2080	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.408 and -0.289 $e.Å^{-3}$	

Table S49. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for B1a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	1230(4)	7181(2)	5989(2)	26(1)
N(1)	7265(3)	3645(2)	8501(1)	37(1)
N(2)	2891(3)	1950(2)	8410(1)	43(1)
C(1)	2192(3)	6288(2)	6395(1)	27(1)
C(2)	1597(3)	5711(2)	6930(1)	27(1)
C(3)	2509(3)	5005(2)	7346(1)	28(1)
C(4)	4076(3)	4809(2)	7243(1)	28(1)
C(5)	4676(3)	5353(2)	6699(1)	32(1)
C(6)	3768(3)	6076(2)	6293(1)	30(1)
C(7)	5118(3)	4127(2)	7720(1)	30(1)
C(8)	6768(3)	4436(2)	8043(1)	35(1)
C(9)	7929(4)	5270(2)	8084(2)	41(1)
C(10)	9439(4)	5243(3)	8553(2)	50(1)
C(11)	9859(4)	4402(3)	9002(2)	53(1)
C(12)	8748(4)	3575(3)	8985(2)	44(1)
C(13)	8497(4)	2593(3)	9333(2)	48(1)
C(14)	9538(5)	2101(3)	9885(2)	61(1)
C(15)	8986(6)	1182(3)	10111(2)	68(1)
C(16)	7426(5)	732(3)	9819(2)	63(1)
C(17)	6359(4)	1200(3)	9274(2)	51(1)
C(18)	6883(4)	2146(2)	9032(2)	41(1)
C(19)	6110(3)	2871(2)	8506(1)	35(1)
C(20)	4734(3)	3153(2)	8011(1)	32(1)
C(21)	3178(3)	2510(2)	7837(1)	31(1)
C(22)	2106(3)	2456(2)	7122(2)	35(1)
C(23)	678(4)	1848(2)	7009(2)	45(1)
C(24)	365(4)	1294(2)	7596(2)	52(1)
C(25)	1503(4)	1360(3)	8279(2)	52(1)
C(26)	-251(3)	7632(2)	6340(1)	25(1)
C(27)	-115(3)	8045(2)	7151(1)	28(1)
C(28)	1476(3)	8205(2)	7720(2)	38(1)
C(29)	-1467(3)	8378(2)	7447(2)	32(1)
C(30)	-2968(3)	8341(2)	6969(2)	33(1)

C(31)	-4420(4)	8666(3)	7312(2)	47(1)
C(32)	-3092(3)	7984(2)	6166(2)	30(1)
C(33)	-1780(3)	7631(2)	5850(1)	28(1)
C(34)	-2036(4)	7251(2)	4967(2)	39(1)
C(35)	1838(3)	7620(2)	5283(1)	26(1)
C(36)	2243(3)	6908(2)	4646(1)	27(1)
C(37)	1814(4)	5697(2)	4502(2)	41(1)
C(38)	2999(3)	7318(2)	4097(1)	31(1)
C(39)	3363(3)	8422(2)	4140(1)	30(1)
C(40)	4188(4)	8857(2)	3549(2)	45(1)
C(41)	2886(3)	9130(2)	4740(1)	28(1)
C(42)	2116(3)	8750(2)	5294(1)	25(1)
C(43)	1597(3)	9603(2)	5912(2)	34(1)

Table S50. Bond lengths [Å] and angles [°] for B1a.

B(1)-C(1)	1.565(4)	C(13)-C(14)	1.399(4)
B(1)-C(35)	1.578(3)	C(13)-C(18)	1.435(5)
B(1)-C(26)	1.580(3)	C(14)-C(15)	1.357(5)
N(1)-C(19)	1.354(4)	C(15)-C(16)	1.394(6)
N(1)-C(8)	1.377(3)	C(16)-C(17)	1.385(4)
N(1)-C(12)	1.388(4)	C(17)-C(18)	1.392(4)
N(2)-C(25)	1.333(4)	C(18)-C(19)	1.456(4)
N(2)-C(21)	1.348(3)	C(19)-C(20)	1.400(4)
C(1)-C(2)	1.408(3)	C(20)-C(21)	1.480(4)
C(1)-C(6)	1.409(3)	C(21)-C(22)	1.388(4)
C(2)-C(3)	1.377(3)	C(22)-C(23)	1.375(4)
C(3)-C(4)	1.398(3)	C(23)-C(24)	1.373(4)
C(4)-C(5)	1.399(3)	C(24)-C(25)	1.373(5)
C(4)-C(7)	1.468(3)	C(26)-C(27)	1.410(3)
C(5)-C(6)	1.383(3)	C(26)-C(33)	1.412(4)
C(7)-C(8)	1.426(4)	C(27)-C(29)	1.393(3)
C(7)-C(20)	1.427(4)	C(27)-C(28)	1.505(4)
C(8)-C(9)	1.392(4)	C(29)-C(30)	1.379(4)
C(9)-C(10)	1.388(4)	C(30)-C(32)	1.386(4)
C(10)-C(11)	1.406(5)	C(30)-C(31)	1.507(3)
C(11)-C(12)	1.367(5)	C(32)-C(33)	1.387(3)
C(12)-C(13)	1.463(5)	C(33)-C(34)	1.511(3)

C(35)-C(42)	1.410(3)
C(35)-C(36)	1.415(3)
C(36)-C(38)	1.392(3)
C(36)-C(37)	1.507(4)
C(38)-C(39)	1.382(4)
C(39)-C(41)	1.391(3)
C(39)-C(40)	1.501(3)
C(41)-C(42)	1.390(3)
C(42)-C(43)	1.530(3)

C(1)-B(1)-C(35)	118.5(2)
C(1)-B(1)-C(26)	117.7(2)
C(35)-B(1)-C(26)	123.7(2)
C(19)-N(1)-C(8)	114.6(2)
C(19)-N(1)-C(12)	116.6(2)
C(8)-N(1)-C(12)	128.7(3)
C(25)-N(2)-C(21)	117.7(3)
C(2)-C(1)-C(6)	115.9(2)
C(2)-C(1)-B(1)	122.5(2)
C(6)-C(1)-B(1)	121.4(2)
C(3)-C(2)-C(1)	122.3(2)
C(2)-C(3)-C(4)	121.2(2)
C(3)-C(4)-C(5)	117.4(2)
C(3)-C(4)-C(7)	122.5(2)
C(5)-C(4)-C(7)	120.0(2)
C(6)-C(5)-C(4)	121.2(2)
C(5)-C(6)-C(1)	122.0(2)
C(8)-C(7)-C(20)	107.5(2)
C(8)-C(7)-C(4)	122.2(2)
C(20)-C(7)-C(4)	130.1(2)
N(1)-C(8)-C(9)	114.3(3)
N(1)-C(8)-C(7)	104.1(2)
C(9)-C(8)-C(7)	141.4(3)
C(10)-C(9)-C(8)	119.8(3)
C(9)-C(10)-C(11)	122.6(3)
C(12)-C(11)-C(10)	119.4(3)
C(11)-C(12)-N(1)	115.2(3)
C(11)-C(12)-C(13)	142.3(3)
N(1)-C(12)-C(13)	102.4(3)
C(14)-C(13)-C(18)	120.5(3)
C(14)-C(13)-C(12)	130.3(4)
C(18)-C(13)-C(12)	109.2(2)
C(15)-C(14)-C(13)	118.0(4)
C(14)-C(15)-C(16)	122.2(3)
C(17)-C(16)-C(15)	121.5(4)
C(16)-C(17)-C(18)	118.0(4)
C(17)-C(18)-C(13)	119.9(3)
C(17)-C(18)-C(19)	133.4(3)
C(13)-C(18)-C(19)	106.7(3)
N(1)-C(19)-C(20)	105.4(2)
N(1)-C(19)-C(18)	105.2(3)
C(20)-C(19)-C(18)	149.5(3)
C(19)-C(20)-C(7)	108.5(3)
C(19)-C(20)-C(21)	123.6(2)
C(7)-C(20)-C(21)	128.0(2)
N(2)-C(21)-C(22)	122.0(3)
N(2)-C(21)-C(20)	115.6(2)
C(22)-C(21)-C(20)	122.3(2)
C(23)-C(22)-C(21)	118.8(3)
C(24)-C(23)-C(22)	119.4(3)
C(23)-C(24)-C(25)	118.5(3)
N(2)-C(25)-C(24)	123.6(3)
C(27)-C(26)-C(33)	117.1(2)
C(27)-C(26)-B(1)	122.0(2)
C(33)-C(26)-B(1)	120.9(2)
C(29)-C(27)-C(26)	120.3(2)
C(29)-C(27)-C(28)	117.2(2)
C(26)-C(27)-C(28)	122.4(2)
C(30)-C(29)-C(27)	122.3(2)
C(29)-C(30)-C(32)	117.6(2)
C(29)-C(30)-C(31)	121.1(2)
C(32)-C(30)-C(31)	121.4(3)
C(30)-C(32)-C(33)	121.9(2)
C(32)-C(33)-C(26)	120.7(2)
C(32)-C(33)-C(34)	118.0(2)
C(26)-C(33)-C(34)	121.2(2)

C(42)-C(35)-C(36)	117.0(2)	C(38)-C(39)-C(41)	117.5(2)
C(42)-C(35)-B(1)	120.8(2)	C(38)-C(39)-C(40)	121.8(2)
C(36)-C(35)-B(1)	122.1(2)	C(41)-C(39)-C(40)	120.6(2)
C(38)-C(36)-C(35)	120.4(2)	C(42)-C(41)-C(39)	121.8(2)
C(38)-C(36)-C(37)	117.0(2)	C(41)-C(42)-C(35)	120.7(2)
C(35)-C(36)-C(37)	122.5(2)	C(41)-C(42)-C(43)	117.4(2)
C(39)-C(38)-C(36)	122.2(2)	C(35)-C(42)-C(43)	121.9(2)

Table S51. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for B1a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... \ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	21(2)	28(2)	29(1)	3(1)	7(1)	-3(1)
N(1)	30(1)	50(2)	30(1)	3(1)	4(1)	12(1)
N(2)	50(2)	44(2)	39(1)	13(1)	14(1)	5(1)
C(1)	26(2)	26(1)	32(1)	5(1)	10(1)	1(1)
C(2)	21(1)	31(1)	31(1)	5(1)	11(1)	1(1)
C(3)	27(2)	34(2)	28(1)	8(1)	12(1)	4(1)
C(4)	29(2)	31(1)	28(1)	3(1)	12(1)	7(1)
C(5)	26(2)	36(2)	38(1)	9(1)	15(1)	8(1)
C(6)	27(2)	34(2)	34(1)	10(1)	15(1)	5(1)
C(7)	26(2)	39(2)	26(1)	4(1)	10(1)	6(1)
C(8)	35(2)	44(2)	29(1)	3(1)	14(1)	12(1)
C(9)	31(2)	50(2)	44(2)	3(1)	16(1)	3(1)
C(10)	34(2)	69(2)	46(2)	-2(2)	18(2)	0(2)
C(11)	26(2)	84(3)	44(2)	-5(2)	5(1)	10(2)
C(12)	28(2)	69(2)	32(1)	2(1)	4(1)	17(2)
C(13)	46(2)	64(2)	32(2)	4(1)	5(1)	28(2)
C(14)	56(2)	88(3)	36(2)	3(2)	-1(2)	42(2)
C(15)	89(3)	79(3)	39(2)	16(2)	6(2)	50(2)
C(16)	88(3)	60(2)	45(2)	15(2)	11(2)	35(2)
C(17)	73(3)	47(2)	37(2)	10(1)	15(2)	23(2)
C(18)	44(2)	54(2)	27(1)	4(1)	8(1)	22(2)
C(19)	35(2)	40(2)	30(1)	4(1)	7(1)	11(1)
C(20)	36(2)	37(2)	25(1)	5(1)	9(1)	14(1)
C(21)	32(2)	30(2)	30(1)	2(1)	8(1)	6(1)
C(22)	37(2)	32(2)	34(1)	-1(1)	6(1)	4(1)

C(23)	35(2)	35(2)	60(2)	-3(1)	1(2)	5(1)
C(24)	41(2)	40(2)	77(2)	2(2)	21(2)	-3(2)
C(25)	58(2)	44(2)	58(2)	8(1)	25(2)	-4(2)
C(26)	20(1)	27(1)	28(1)	9(1)	6(1)	-1(1)
C(27)	21(1)	33(2)	34(1)	9(1)	9(1)	2(1)
C(28)	26(2)	51(2)	35(1)	1(1)	7(1)	5(1)
C(29)	31(2)	34(2)	36(1)	8(1)	16(1)	3(1)
C(30)	24(2)	31(2)	51(2)	14(1)	17(1)	2(1)
C(31)	28(2)	62(2)	61(2)	20(2)	25(2)	11(2)
C(32)	17(1)	35(2)	42(2)	17(1)	6(1)	0(1)
C(33)	24(2)	28(1)	33(1)	12(1)	6(1)	-1(1)
C(34)	32(2)	48(2)	35(1)	7(1)	1(1)	0(1)
C(35)	21(1)	28(1)	30(1)	4(1)	8(1)	4(1)
C(36)	21(1)	29(1)	30(1)	4(1)	6(1)	0(1)
C(37)	50(2)	31(2)	43(2)	-2(1)	16(1)	-6(1)
C(38)	30(2)	33(2)	31(1)	2(1)	12(1)	7(1)
C(39)	24(2)	37(2)	33(1)	9(1)	10(1)	4(1)
C(40)	46(2)	50(2)	46(2)	11(1)	26(2)	4(2)
C(41)	23(2)	26(1)	38(1)	8(1)	10(1)	1(1)
C(42)	20(1)	29(1)	29(1)	5(1)	9(1)	6(1)
C(43)	33(2)	28(2)	44(2)	4(1)	18(1)	3(1)

Table S52. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for B1a.

	x	y	z	U(eq)
H(2)	530	5813	7008	32
H(3)	2065	4644	7708	34
H(5)	5727	5223	6607	38
H(6)	4219	6440	5935	36
H(9)	7688	5855	7792	49
H(10)	10219	5816	8572	60
H(11)	10907	4409	9315	64
H(14)	10601	2401	10096	73
H(15)	9685	833	10480	82
H(16)	7087	91	9997	76
H(17)	5302	884	9073	61

H(22)	2355	2832	6718	42
H(23)	-85	1813	6529	54
H(24)	-618	873	7532	63
H(25)	1290	965	8680	62
H(28A)	1741	8988	7895	57
H(28B)	2313	7886	7455	57
H(28C)	1409	7846	8179	57
H(29)	-1351	8640	7997	39
H(31A)	-4784	8069	7560	71
H(31B)	-5283	8819	6888	71
H(31C)	-4137	9322	7710	71
H(32)	-4106	7982	5822	36
H(34A)	-3184	7237	4736	58
H(34B)	-1649	6515	4868	58
H(34C)	-1441	7754	4725	58
H(37A)	1215	5482	3959	61
H(37B)	1149	5523	4875	61
H(37C)	2799	5299	4578	61
H(38)	3273	6823	3678	37
H(40A)	5300	8636	3622	67
H(40B)	4184	9657	3627	67
H(40C)	3620	8562	3012	67
H(41)	3092	9895	4771	34
H(43A)	1924	10337	5831	51
H(43B)	2108	9482	6444	51
H(43C)	427	9539	5857	51

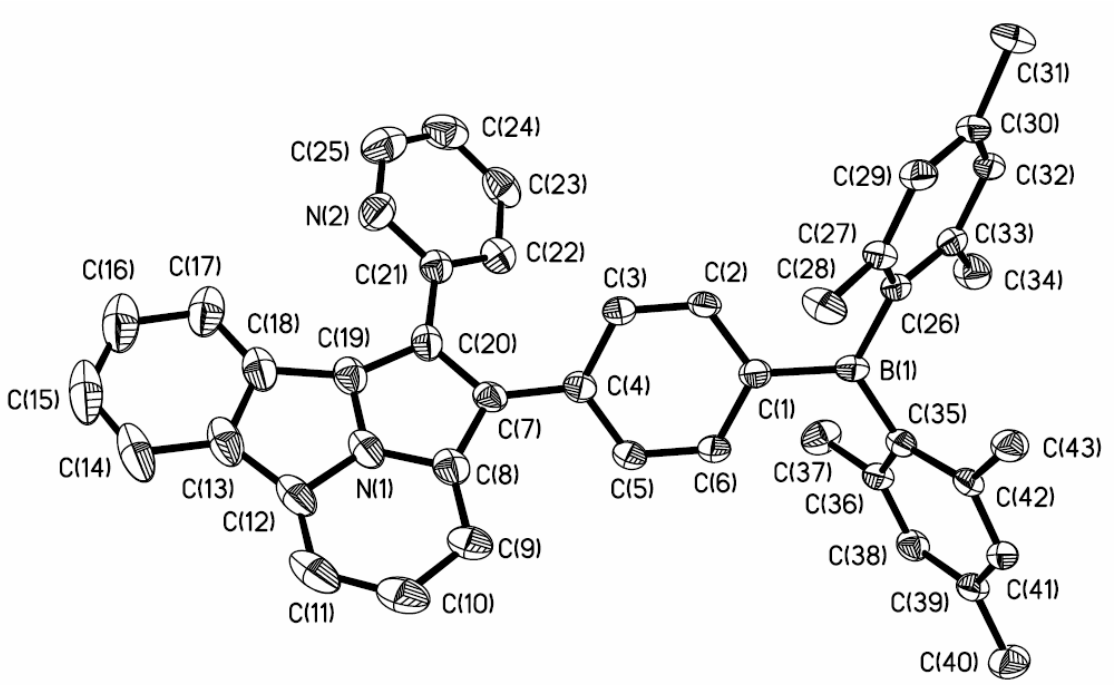


Figure S101. A diagram showing the structure of **B1a** with labeling schemes and 35% thermal ellipsoids. H atoms are omitted for clarity.

Table S53. Crystal data and structure refinement for B1b.

Identification code	b1b-sr	
Empirical formula	C43 H38 B N2	
Formula weight	593.56	
Temperature	179(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.1887(14) Å	α= 81.008(6)°.
	b = 13.353(2) Å	β= 83.598(6)°.
	c = 15.493(2) Å	γ = 78.061(6)°.
Volume	1631.5(5) $Å^3$	
Z	2	
Density (calculated)	1.208 Mg/m^3	
Absorption coefficient	0.069 mm^{-1}	
F(000)	630	
Crystal size	0.293 x 0.204 x 0.138 mm^3	
Theta range for data collection	2.199 to 27.202°.	
Index ranges	-10<=h<=10, -17<=k<=17, -18<=l<=19	
Reflections collected	19378	
Independent reflections	7207 [R(int) = 0.1340]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.991 and 0.980	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7207 / 0 / 423	
Goodness-of-fit on F^2	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.1223, wR2 = 0.2965	
R indices (all data)	R1 = 0.2006, wR2 = 0.3284	
Extinction coefficient	0.028(6)	
Largest diff. peak and hole	0.502 and -0.389 $e.Å^{-3}$	

Table S54. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for B1b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	3637(7)	1275(4)	2941(3)	31(1)
N(1)	10175(5)	5062(3)	1584(2)	33(1)
N(2)	7095(6)	6040(4)	3785(3)	58(1)
C(1)	4913(6)	2017(3)	2684(3)	31(1)
C(2)	5685(6)	2326(3)	3334(3)	32(1)
C(3)	6738(6)	3029(3)	3134(3)	30(1)
C(4)	7018(6)	3486(3)	2274(3)	27(1)
C(5)	6286(6)	3174(3)	1616(3)	31(1)
C(6)	5264(6)	2447(4)	1824(3)	36(1)
C(7)	8078(6)	4277(3)	2081(3)	29(1)
C(8)	9490(6)	4247(3)	1483(3)	30(1)
C(9)	10607(6)	3766(3)	808(3)	30(1)
C(10)	10607(6)	2906(4)	396(3)	34(1)
C(11)	11855(7)	2651(4)	-246(4)	44(1)
C(12)	13083(7)	3238(4)	-511(3)	46(1)
C(13)	13107(6)	4085(4)	-123(3)	40(1)
C(14)	11886(6)	4354(3)	553(3)	31(1)
C(15)	11581(6)	5200(4)	1069(3)	34(1)
C(16)	12235(7)	6025(4)	1195(4)	44(1)
C(17)	11445(7)	6654(4)	1830(4)	48(1)
C(18)	10000(7)	6471(4)	2331(4)	44(1)
C(19)	9321(6)	5624(3)	2213(3)	33(1)
C(20)	7964(6)	5137(3)	2547(3)	32(1)
C(21)	6622(6)	5540(3)	3194(3)	34(1)
C(22)	4983(6)	5443(4)	3180(3)	41(1)
C(23)	3794(8)	5865(4)	3795(4)	53(2)
C(24)	4267(9)	6366(5)	4399(4)	60(2)
C(25)	5909(9)	6445(5)	4355(4)	66(2)
C(26)	2645(6)	1291(3)	3877(3)	31(1)
C(27)	2672(6)	386(3)	4476(3)	32(1)
C(28)	1764(6)	423(4)	5295(3)	36(1)
C(29)	843(7)	1332(4)	5538(3)	39(1)
C(30)	801(6)	2229(4)	4948(3)	37(1)

C(31)	1709(6)	2233(4)	4132(3)	32(1)
C(32)	1563(7)	3254(4)	3535(4)	47(1)
C(33)	3711(7)	-635(4)	4281(3)	42(1)
C(34)	-146(7)	1351(5)	6426(3)	50(1)
C(35)	3327(6)	597(3)	2260(3)	29(1)
C(36)	1725(6)	650(3)	2005(3)	30(1)
C(37)	1504(7)	100(4)	1355(3)	38(1)
C(38)	2810(7)	-530(4)	942(3)	38(1)
C(39)	4375(7)	-612(4)	1214(3)	42(1)
C(40)	4678(6)	-89(4)	1858(3)	39(1)
C(41)	6435(7)	-282(5)	2163(4)	54(2)
C(42)	207(6)	1319(4)	2399(3)	40(1)
C(43)	2544(9)	-1101(5)	220(4)	62(2)

Table S55. Bond lengths [Å] and angles [°] for B1b.

B(1)-C(1)	1.563(7)	C(12)-C(13)	1.365(7)
B(1)-C(35)	1.566(7)	C(13)-C(14)	1.401(7)
B(1)-C(26)	1.583(7)	C(14)-C(15)	1.448(6)
N(1)-C(15)	1.354(6)	C(15)-C(16)	1.369(7)
N(1)-C(8)	1.360(6)	C(16)-C(17)	1.409(7)
N(1)-C(19)	1.364(6)	C(17)-C(18)	1.385(8)
N(2)-C(25)	1.325(7)	C(18)-C(19)	1.404(7)
N(2)-C(21)	1.347(6)	C(19)-C(20)	1.411(7)
C(1)-C(6)	1.389(6)	C(20)-C(21)	1.476(7)
C(1)-C(2)	1.402(6)	C(21)-C(22)	1.377(7)
C(2)-C(3)	1.380(6)	C(22)-C(23)	1.382(7)
C(3)-C(4)	1.391(6)	C(23)-C(24)	1.363(8)
C(4)-C(5)	1.395(6)	C(24)-C(25)	1.363(9)
C(4)-C(7)	1.477(6)	C(26)-C(27)	1.402(6)
C(5)-C(6)	1.387(6)	C(26)-C(31)	1.419(6)
C(7)-C(8)	1.397(6)	C(27)-C(28)	1.399(7)
C(7)-C(20)	1.432(6)	C(27)-C(33)	1.505(7)
C(8)-C(9)	1.447(6)	C(28)-C(29)	1.373(7)
C(9)-C(10)	1.399(6)	C(29)-C(30)	1.385(7)
C(9)-C(14)	1.421(6)	C(29)-C(34)	1.518(7)
C(10)-C(11)	1.374(7)	C(30)-C(31)	1.394(7)
C(11)-C(12)	1.388(8)	C(31)-C(32)	1.514(7)

C(35)-C(36)	1.396(6)	C(13)-C(12)-C(11)	120.6(5)
C(35)-C(40)	1.434(6)	C(12)-C(13)-C(14)	119.4(5)
C(36)-C(37)	1.383(6)	C(13)-C(14)-C(9)	119.8(4)
C(36)-C(42)	1.503(7)	C(13)-C(14)-C(15)	131.8(5)
C(37)-C(38)	1.380(7)	C(9)-C(14)-C(15)	108.3(4)
C(38)-C(39)	1.371(7)	N(1)-C(15)-C(16)	115.3(4)
C(38)-C(43)	1.508(7)	N(1)-C(15)-C(14)	103.3(4)
C(39)-C(40)	1.374(7)	C(16)-C(15)-C(14)	141.4(5)
C(40)-C(41)	1.524(7)	C(15)-C(16)-C(17)	119.7(5)
		C(18)-C(17)-C(16)	121.9(5)
C(1)-B(1)-C(35)	119.6(4)	C(17)-C(18)-C(19)	119.1(5)
C(1)-B(1)-C(26)	117.4(4)	N(1)-C(19)-C(18)	114.7(5)
C(35)-B(1)-C(26)	122.9(4)	N(1)-C(19)-C(20)	105.6(4)
C(15)-N(1)-C(8)	117.1(4)	C(18)-C(19)-C(20)	139.7(4)
C(15)-N(1)-C(19)	129.4(4)	C(19)-C(20)-C(7)	107.1(4)
C(8)-N(1)-C(19)	113.5(4)	C(19)-C(20)-C(21)	124.2(4)
C(25)-N(2)-C(21)	117.0(5)	C(7)-C(20)-C(21)	128.4(4)
C(6)-C(1)-C(2)	116.9(4)	N(2)-C(21)-C(22)	122.0(5)
C(6)-C(1)-B(1)	122.7(4)	N(2)-C(21)-C(20)	115.5(5)
C(2)-C(1)-B(1)	120.3(4)	C(22)-C(21)-C(20)	122.6(4)
C(3)-C(2)-C(1)	121.8(4)	C(21)-C(22)-C(23)	118.9(5)
C(2)-C(3)-C(4)	120.5(4)	C(24)-C(23)-C(22)	119.4(6)
C(3)-C(4)-C(5)	118.4(4)	C(23)-C(24)-C(25)	117.9(5)
C(3)-C(4)-C(7)	119.7(4)	N(2)-C(25)-C(24)	124.8(5)
C(5)-C(4)-C(7)	121.9(4)	C(27)-C(26)-C(31)	118.3(4)
C(6)-C(5)-C(4)	120.3(4)	C(27)-C(26)-B(1)	121.3(4)
C(5)-C(6)-C(1)	121.9(4)	C(31)-C(26)-B(1)	120.3(4)
C(8)-C(7)-C(20)	107.9(4)	C(28)-C(27)-C(26)	120.0(4)
C(8)-C(7)-C(4)	125.7(4)	C(28)-C(27)-C(33)	118.1(4)
C(20)-C(7)-C(4)	125.9(4)	C(26)-C(27)-C(33)	121.9(4)
N(1)-C(8)-C(7)	105.9(4)	C(29)-C(28)-C(27)	121.7(5)
N(1)-C(8)-C(9)	103.6(4)	C(28)-C(29)-C(30)	118.7(5)
C(7)-C(8)-C(9)	150.6(4)	C(28)-C(29)-C(34)	120.7(5)
C(10)-C(9)-C(14)	119.5(4)	C(30)-C(29)-C(34)	120.5(5)
C(10)-C(9)-C(8)	132.8(4)	C(29)-C(30)-C(31)	121.6(5)
C(14)-C(9)-C(8)	107.7(4)	C(30)-C(31)-C(26)	119.6(4)
C(11)-C(10)-C(9)	118.7(5)	C(30)-C(31)-C(32)	117.3(4)
C(10)-C(11)-C(12)	121.9(5)	C(26)-C(31)-C(32)	123.0(4)

C(36)-C(35)-C(40)	117.1(4)
C(36)-C(35)-B(1)	121.3(4)
C(40)-C(35)-B(1)	121.5(4)
C(37)-C(36)-C(35)	120.1(4)
C(37)-C(36)-C(42)	118.0(4)
C(35)-C(36)-C(42)	121.9(4)
C(38)-C(37)-C(36)	122.9(5)
C(39)-C(38)-C(37)	117.1(4)
C(39)-C(38)-C(43)	121.0(5)
C(37)-C(38)-C(43)	121.9(5)
C(38)-C(39)-C(40)	122.9(5)
C(39)-C(40)-C(35)	119.8(5)
C(39)-C(40)-C(41)	119.4(5)
C(35)-C(40)-C(41)	120.7(4)

Table S56. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for B1b. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	26(3)	30(3)	35(3)	2(2)	-11(2)	-2(2)
N(1)	36(2)	30(2)	35(2)	-9(2)	1(2)	-10(2)
N(2)	52(3)	73(3)	57(3)	-40(3)	3(2)	-14(3)
C(1)	30(3)	33(2)	30(2)	-7(2)	3(2)	-9(2)
C(2)	33(3)	36(2)	27(2)	-2(2)	-1(2)	-9(2)
C(3)	24(2)	38(2)	25(2)	-6(2)	-3(2)	-2(2)
C(4)	25(2)	28(2)	27(2)	-8(2)	4(2)	-4(2)
C(5)	37(3)	36(2)	22(2)	-3(2)	-1(2)	-14(2)
C(6)	42(3)	43(3)	29(3)	-9(2)	-4(2)	-19(2)
C(7)	31(3)	28(2)	31(2)	-9(2)	-3(2)	-9(2)
C(8)	34(3)	26(2)	34(3)	-4(2)	-5(2)	-10(2)
C(9)	28(3)	32(2)	27(2)	-1(2)	-3(2)	-3(2)
C(10)	34(3)	35(2)	33(3)	-9(2)	1(2)	-3(2)
C(11)	44(3)	38(3)	49(3)	-13(2)	-1(3)	-3(2)
C(12)	37(3)	50(3)	42(3)	-4(2)	9(2)	4(3)
C(13)	30(3)	43(3)	43(3)	-2(2)	4(2)	-3(2)
C(14)	27(3)	30(2)	35(3)	-1(2)	-5(2)	-2(2)
C(15)	30(3)	36(3)	36(3)	-2(2)	-2(2)	-12(2)
C(16)	36(3)	46(3)	54(3)	-8(2)	6(2)	-21(2)
C(17)	51(4)	39(3)	61(4)	-17(3)	3(3)	-23(3)
C(18)	52(3)	37(3)	50(3)	-15(2)	-9(3)	-16(3)
C(19)	36(3)	35(2)	30(2)	-14(2)	-3(2)	-6(2)
C(20)	31(3)	33(2)	33(3)	-9(2)	-1(2)	-8(2)
C(21)	39(3)	33(2)	31(3)	-10(2)	-5(2)	-2(2)
C(22)	34(3)	46(3)	43(3)	-15(2)	-9(2)	-1(2)
C(23)	41(3)	56(3)	59(4)	-20(3)	4(3)	3(3)
C(24)	59(4)	65(4)	51(4)	-27(3)	11(3)	4(3)
C(25)	60(4)	85(5)	64(4)	-51(4)	7(3)	-12(4)
C(26)	31(3)	34(2)	31(2)	-6(2)	-6(2)	-12(2)

C(27)	32(3)	34(2)	32(3)	-5(2)	-7(2)	-10(2)
C(28)	41(3)	35(3)	36(3)	0(2)	-9(2)	-16(2)
C(29)	40(3)	52(3)	30(3)	-8(2)	1(2)	-22(3)
C(30)	32(3)	41(3)	41(3)	-12(2)	-3(2)	-11(2)
C(31)	31(3)	36(3)	33(3)	-4(2)	-2(2)	-11(2)
C(32)	51(4)	32(3)	56(3)	-8(2)	-3(3)	-4(2)
C(33)	43(3)	39(3)	44(3)	-3(2)	-6(2)	-6(2)
C(34)	49(4)	64(4)	38(3)	-9(3)	1(3)	-17(3)
C(35)	25(2)	30(2)	33(3)	-4(2)	0(2)	-5(2)
C(36)	31(3)	27(2)	33(3)	-2(2)	-2(2)	-9(2)
C(37)	38(3)	39(3)	41(3)	0(2)	-13(2)	-13(2)
C(38)	50(3)	36(3)	32(3)	-9(2)	-1(2)	-16(2)
C(39)	41(3)	42(3)	42(3)	-17(2)	1(2)	-3(2)
C(40)	31(3)	41(3)	44(3)	-13(2)	-2(2)	-3(2)
C(41)	32(3)	62(4)	68(4)	-22(3)	-10(3)	1(3)
C(42)	33(3)	46(3)	45(3)	-5(2)	-11(2)	-8(2)
C(43)	84(5)	65(4)	43(3)	-23(3)	-8(3)	-19(4)

Table S57. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for B1b.

	x	y	z	U(eq)
H(2)	5478	2044	3929	38
H(3)	7276	3202	3588	35
H(5)	6488	3460	1022	37
H(6)	4789	2237	1366	43
H(10)	9761	2505	558	41
H(11)	11879	2057	-517	53
H(12)	13914	3049	-967	55
H(13)	13945	4487	-310	48
H(16)	13218	6173	855	53
H(17)	11917	7220	1917	57
H(18)	9477	6913	2748	53
H(22)	4676	5092	2753	49
H(23)	2657	5805	3798	63

H(24)	3478	6652	4835	72
H(25)	6225	6818	4763	80
H(28)	1786	-197	5693	43
H(30)	138	2857	5104	45
H(32A)	480	3695	3675	70
H(32B)	1645	3131	2923	70
H(32C)	2469	3598	3622	70
H(33A)	4867	-680	4417	64
H(33B)	3695	-692	3659	64
H(33C)	3247	-1199	4641	64
H(34A)	-589	713	6587	75
H(34B)	-1077	1947	6397	75
H(34C)	588	1406	6867	75
H(37)	405	159	1185	45
H(39)	5291	-1050	946	50
H(41A)	7232	-651	1745	81
H(41B)	6460	-699	2743	81
H(41C)	6745	381	2198	81
H(42A)	-789	1256	2131	61
H(42B)	346	2041	2291	61
H(42C)	75	1098	3032	61
H(43A)	3299	-1777	263	92
H(43B)	2780	-701	-350	92
H(43C)	1381	-1198	276	92

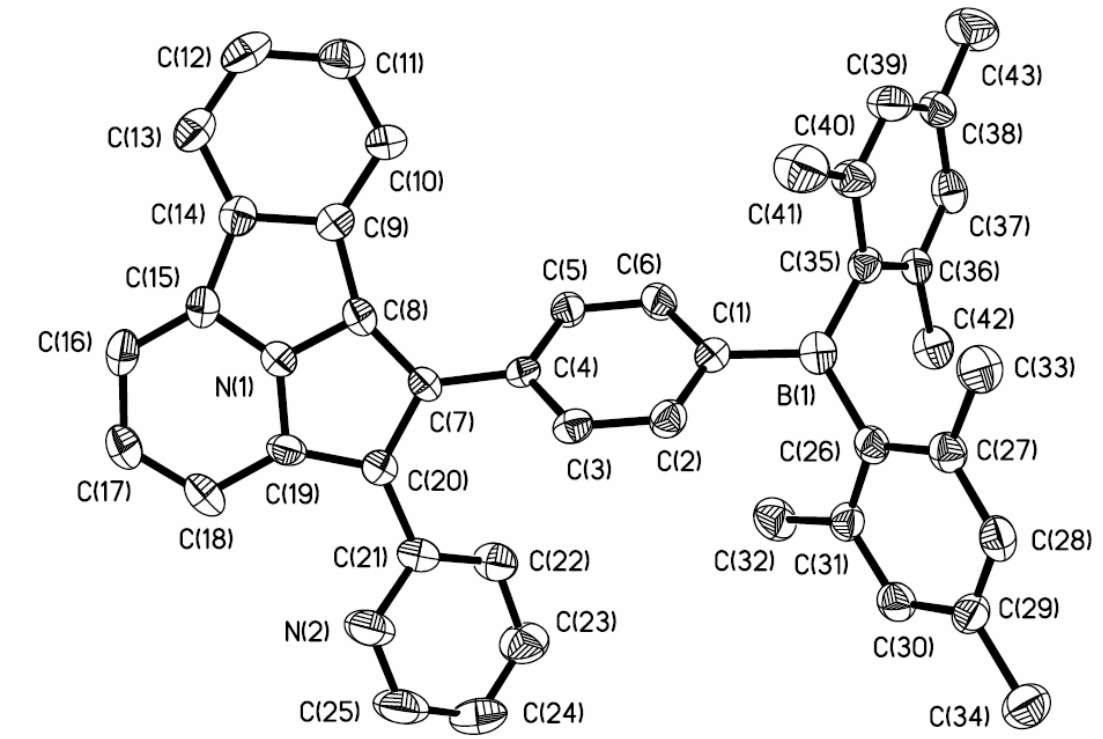


Figure S102. A diagram showing the structure of **B1b** with labeling schemes and 35% thermal ellipsoids. H atoms are omitted for clarity.

Table S58. Crystal data and structure refinement for B2a.

Identification code	b2a-sr	
Empirical formula	C43 H37 B N2	
Formula weight	592.55	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.196(3) Å	α= 74.441(9)°.
	b = 14.091(4) Å	β= 87.034(9)°.
	c = 14.197(4) Å	γ = 75.138(8)°.
Volume	1712.7(9) $Å^3$	
Z	2	
Density (calculated)	1.149 Mg/m^3	
Absorption coefficient	0.066 mm^{-1}	
F(000)	628	
Crystal size	0.190 x 0.080 x 0.035 mm^3	
Theta range for data collection	2.756 to 27.193°.	
Index ranges	-11<=h<=11, -18<=k<=18, -18<=l<=18	
Reflections collected	18842	
Independent reflections	7536 [R(int) = 0.1783]	
Completeness to theta = 25.242°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.998 and 0.988	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7536 / 0 / 422	
Goodness-of-fit on F^2	0.912	
Final R indices [I>2sigma(I)]	R1 = 0.0939, wR2 = 0.1719	
R indices (all data)	R1 = 0.2364, wR2 = 0.2128	
Extinction coefficient	0.0111(19)	
Largest diff. peak and hole	0.286 and -0.272 $e.Å^{-3}$	

Table S59. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for B2a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	5180(3)	8194(2)	6842(2)	22(1)
C(1)	4422(4)	9035(3)	7115(3)	27(1)
B(1)	7114(4)	7798(3)	6901(3)	24(1)
N(2)	5517(3)	5121(2)	6215(2)	28(1)
C(2)	2879(4)	9348(3)	7122(3)	31(1)
C(3)	2036(4)	8781(3)	6864(3)	32(1)
C(4)	2779(4)	7911(3)	6611(3)	28(1)
C(5)	4349(4)	7622(3)	6604(3)	22(1)
C(7)	4637(4)	5773(3)	6687(3)	26(1)
C(6)	5069(4)	6692(3)	6335(3)	25(1)
C(8)	3839(4)	5151(3)	7388(3)	29(1)
C(9)	2856(4)	5356(3)	8137(3)	33(1)
C(10)	2289(5)	4588(4)	8703(3)	42(1)
C(12)	3700(5)	3383(3)	7845(3)	44(1)
C(11)	2690(5)	3623(4)	8550(3)	49(1)
C(13)	4280(5)	4153(3)	7260(3)	34(1)
C(14)	5403(4)	4134(3)	6507(3)	34(1)
C(15)	6377(5)	3482(3)	6061(3)	43(1)
C(18)	6514(4)	5548(3)	5587(3)	27(1)
C(17)	7510(4)	4853(3)	5156(3)	36(1)
C(16)	7417(5)	3859(4)	5394(3)	46(1)
C(19)	6226(4)	6555(3)	5653(3)	23(1)
C(20)	7111(4)	7270(3)	5208(3)	28(1)
C(21)	7629(5)	7286(3)	4262(3)	37(1)
C(22)	8671(5)	7820(4)	3859(3)	46(1)
C(23)	9192(4)	8367(3)	4381(3)	39(1)
C(24)	8645(4)	8370(3)	5305(3)	32(1)
C(25)	7587(4)	7835(3)	5763(3)	24(1)
C(26)	7726(4)	8631(3)	7302(3)	25(1)
C(27)	8670(4)	8353(3)	8149(3)	28(1)
C(28)	9333(5)	7275(3)	8743(3)	40(1)

C(29)	9115(4)	9086(3)	8480(3)	36(1)
C(30)	8715(5)	10101(3)	8021(3)	38(1)
C(31)	9198(5)	10883(4)	8395(4)	62(2)
C(32)	7857(5)	10386(3)	7172(3)	40(1)
C(33)	7384(4)	9690(3)	6808(3)	31(1)
C(34)	6449(5)	10154(3)	5859(3)	40(1)
C(35)	7410(4)	6631(3)	7603(3)	21(1)
C(36)	6539(4)	6368(3)	8440(3)	25(1)
C(37)	5518(4)	7159(3)	8878(3)	38(1)
C(38)	6616(4)	5363(3)	8917(3)	32(1)
C(39)	7551(4)	4550(3)	8636(3)	31(1)
C(40)	7538(5)	3459(3)	9128(3)	48(1)
C(41)	8519(4)	4799(3)	7892(3)	32(1)
C(42)	8485(4)	5794(3)	7397(3)	22(1)
C(43)	9755(4)	5914(3)	6669(3)	30(1)

Table S60. Bond lengths [Å] and angles [°] for B2a.

N(1)-C(1)	1.355(4)	C(8)-C(13)	1.419(5)
N(1)-C(5)	1.355(4)	C(9)-C(10)	1.366(6)
N(1)-B(1)	1.721(5)	C(10)-C(11)	1.387(6)
C(1)-C(2)	1.374(5)	C(12)-C(11)	1.380(6)
B(1)-C(35)	1.640(6)	C(12)-C(13)	1.385(6)
B(1)-C(25)	1.642(6)	C(13)-C(14)	1.448(6)
B(1)-C(26)	1.659(6)	C(14)-C(15)	1.371(5)
N(2)-C(7)	1.357(4)	C(15)-C(16)	1.411(6)
N(2)-C(14)	1.369(5)	C(18)-C(19)	1.402(5)
N(2)-C(18)	1.382(5)	C(18)-C(17)	1.406(5)
C(2)-C(3)	1.370(5)	C(17)-C(16)	1.374(6)
C(3)-C(4)	1.370(5)	C(19)-C(20)	1.450(5)
C(4)-C(5)	1.397(5)	C(20)-C(21)	1.398(5)
C(5)-C(6)	1.449(5)	C(20)-C(25)	1.413(5)
C(7)-C(6)	1.408(5)	C(21)-C(22)	1.376(6)
C(7)-C(8)	1.443(6)	C(22)-C(23)	1.380(6)
C(6)-C(19)	1.412(5)	C(23)-C(24)	1.381(5)
C(8)-C(9)	1.401(5)	C(24)-C(25)	1.409(5)

C(26)-C(27)	1.425(5)
C(26)-C(33)	1.428(5)
C(27)-C(29)	1.397(5)
C(27)-C(28)	1.511(5)
C(29)-C(30)	1.364(6)
C(30)-C(32)	1.383(6)
C(30)-C(31)	1.511(6)
C(32)-C(33)	1.390(5)
C(33)-C(34)	1.530(5)
C(35)-C(36)	1.418(5)
C(35)-C(42)	1.418(5)
C(36)-C(38)	1.381(5)
C(36)-C(37)	1.512(5)
C(38)-C(39)	1.384(5)
C(39)-C(41)	1.377(5)
C(39)-C(40)	1.512(6)
C(41)-C(42)	1.382(5)
C(42)-C(43)	1.531(5)

C(1)-N(1)-C(5)	117.1(3)
C(1)-N(1)-B(1)	121.8(3)
C(5)-N(1)-B(1)	120.9(3)
N(1)-C(1)-C(2)	123.4(4)
C(35)-B(1)-C(25)	112.5(3)
C(35)-B(1)-C(26)	117.7(3)
C(25)-B(1)-C(26)	111.8(3)
C(35)-B(1)-N(1)	102.4(3)
C(25)-B(1)-N(1)	103.7(3)
C(26)-B(1)-N(1)	107.2(3)
C(7)-N(2)-C(14)	116.2(4)
C(7)-N(2)-C(18)	113.1(3)
C(14)-N(2)-C(18)	130.2(3)
C(3)-C(2)-C(1)	119.6(3)
C(4)-C(3)-C(2)	118.1(3)
C(3)-C(4)-C(5)	120.8(4)
N(1)-C(5)-C(4)	121.0(3)
N(1)-C(5)-C(6)	120.8(3)
C(4)-C(5)-C(6)	118.2(3)
N(2)-C(7)-C(6)	105.2(3)
N(2)-C(7)-C(8)	104.3(3)
C(6)-C(7)-C(8)	149.8(3)
C(7)-C(6)-C(19)	108.6(3)
C(7)-C(6)-C(5)	123.9(3)
C(19)-C(6)-C(5)	127.4(4)
C(9)-C(8)-C(13)	120.1(4)
C(9)-C(8)-C(7)	132.1(4)
C(13)-C(8)-C(7)	107.7(3)
C(10)-C(9)-C(8)	118.5(4)
C(9)-C(10)-C(11)	121.0(4)
C(11)-C(12)-C(13)	117.8(4)
C(12)-C(11)-C(10)	122.1(5)
C(12)-C(13)-C(8)	120.5(4)
C(12)-C(13)-C(14)	131.0(4)
C(8)-C(13)-C(14)	108.4(4)
N(2)-C(14)-C(15)	114.6(4)
N(2)-C(14)-C(13)	103.4(3)
C(15)-C(14)-C(13)	141.9(5)
C(14)-C(15)-C(16)	118.9(4)
N(2)-C(18)-C(19)	105.4(3)
N(2)-C(18)-C(17)	113.4(4)
C(19)-C(18)-C(17)	141.1(4)
C(16)-C(17)-C(18)	119.1(4)
C(17)-C(16)-C(15)	123.7(4)
C(18)-C(19)-C(6)	107.7(3)
C(18)-C(19)-C(20)	125.5(3)
C(6)-C(19)-C(20)	126.3(3)
C(21)-C(20)-C(25)	121.2(4)
C(21)-C(20)-C(19)	117.9(4)
C(25)-C(20)-C(19)	120.4(3)
C(22)-C(21)-C(20)	120.8(4)
C(21)-C(22)-C(23)	120.0(4)
C(22)-C(23)-C(24)	118.9(4)

C(23)-C(24)-C(25)	124.0(4)
C(24)-C(25)-C(20)	115.1(3)
C(24)-C(25)-B(1)	120.6(3)
C(20)-C(25)-B(1)	124.0(4)
C(27)-C(26)-C(33)	114.2(4)
C(27)-C(26)-B(1)	123.3(3)
C(33)-C(26)-B(1)	122.5(3)
C(29)-C(27)-C(26)	121.3(4)
C(29)-C(27)-C(28)	113.6(4)
C(26)-C(27)-C(28)	125.0(3)
C(30)-C(29)-C(27)	123.4(4)
C(29)-C(30)-C(32)	116.4(4)
C(29)-C(30)-C(31)	122.6(4)
C(32)-C(30)-C(31)	120.9(4)
C(30)-C(32)-C(33)	122.6(4)
C(32)-C(33)-C(26)	121.9(4)
C(32)-C(33)-C(34)	114.7(4)
C(26)-C(33)-C(34)	123.3(4)
C(36)-C(35)-C(42)	114.3(3)
C(36)-C(35)-B(1)	122.2(3)
C(42)-C(35)-B(1)	123.3(3)
C(38)-C(36)-C(35)	121.2(3)
C(38)-C(36)-C(37)	116.4(4)
C(35)-C(36)-C(37)	122.4(4)
C(36)-C(38)-C(39)	123.4(4)
C(41)-C(39)-C(38)	115.5(4)
C(41)-C(39)-C(40)	122.1(4)
C(38)-C(39)-C(40)	122.3(4)
C(39)-C(41)-C(42)	122.8(4)
C(41)-C(42)-C(35)	121.9(4)
C(41)-C(42)-C(43)	114.7(3)
C(35)-C(42)-C(43)	123.2(4)

Table S61. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for B2a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	13(2)	30(2)	24(2)	-12(2)	1(1)	-4(2)
C(1)	19(2)	36(2)	31(2)	-14(2)	2(2)	-8(2)
B(1)	11(2)	35(3)	30(3)	-17(2)	2(2)	-4(2)
N(2)	26(2)	28(2)	30(2)	-12(2)	-6(2)	-3(2)
C(2)	25(2)	34(2)	36(2)	-19(2)	4(2)	0(2)
C(3)	15(2)	46(3)	36(2)	-16(2)	-4(2)	0(2)
C(4)	15(2)	39(3)	34(2)	-16(2)	1(2)	-7(2)
C(5)	15(2)	33(2)	22(2)	-11(2)	2(2)	-7(2)
C(7)	20(2)	32(2)	29(2)	-15(2)	-1(2)	-4(2)
C(6)	15(2)	37(3)	26(2)	-15(2)	0(2)	-6(2)
C(8)	25(2)	35(3)	29(2)	-11(2)	-12(2)	-8(2)
C(9)	25(2)	46(3)	30(2)	-11(2)	-7(2)	-9(2)
C(10)	38(3)	56(3)	34(3)	-4(2)	-9(2)	-21(3)
C(12)	55(3)	38(3)	37(3)	-6(2)	-19(3)	-10(3)
C(11)	56(3)	56(3)	35(3)	7(2)	-15(3)	-30(3)
C(13)	36(3)	38(3)	29(2)	-7(2)	-16(2)	-9(2)
C(14)	32(2)	35(3)	35(2)	-12(2)	-21(2)	-2(2)
C(15)	45(3)	33(3)	50(3)	-17(2)	-18(3)	4(2)
C(18)	16(2)	38(3)	30(2)	-14(2)	-8(2)	-7(2)
C(17)	27(2)	47(3)	34(3)	-24(2)	-7(2)	7(2)
C(16)	37(3)	51(3)	49(3)	-32(3)	-10(2)	14(3)
C(19)	15(2)	33(2)	22(2)	-12(2)	-2(2)	-4(2)
C(20)	18(2)	39(3)	24(2)	-11(2)	-6(2)	1(2)
C(21)	29(2)	53(3)	25(2)	-16(2)	-2(2)	1(2)
C(22)	42(3)	62(3)	26(2)	-10(2)	8(2)	-3(3)
C(23)	22(2)	52(3)	35(3)	-5(2)	6(2)	-7(2)
C(24)	21(2)	41(3)	31(2)	-8(2)	-2(2)	-5(2)
C(25)	9(2)	29(2)	29(2)	-5(2)	-1(2)	2(2)
C(26)	15(2)	35(3)	27(2)	-10(2)	2(2)	-9(2)
C(27)	22(2)	35(3)	33(2)	-17(2)	5(2)	-10(2)
C(28)	32(2)	50(3)	42(3)	-20(2)	-17(2)	-7(2)
C(29)	23(2)	54(3)	38(3)	-20(2)	2(2)	-17(2)

C(30)	29(2)	46(3)	51(3)	-28(3)	13(2)	-20(2)
C(31)	58(3)	65(4)	85(4)	-42(3)	17(3)	-34(3)
C(32)	37(3)	27(3)	61(3)	-17(2)	10(3)	-12(2)
C(33)	23(2)	27(3)	39(3)	-8(2)	7(2)	-5(2)
C(34)	38(3)	31(3)	41(3)	1(2)	-1(2)	-3(2)
C(35)	15(2)	29(2)	23(2)	-12(2)	-1(2)	-8(2)
C(36)	17(2)	36(3)	20(2)	-6(2)	-4(2)	-6(2)
C(37)	28(2)	61(3)	24(2)	-15(2)	5(2)	-5(2)
C(38)	22(2)	52(3)	22(2)	-2(2)	-4(2)	-19(2)
C(39)	27(2)	33(3)	29(2)	-1(2)	-11(2)	-9(2)
C(40)	47(3)	41(3)	54(3)	0(2)	-13(3)	-19(2)
C(41)	29(2)	34(3)	33(2)	-14(2)	-6(2)	-2(2)
C(42)	17(2)	27(2)	27(2)	-9(2)	-4(2)	-9(2)
C(43)	16(2)	43(3)	32(2)	-15(2)	1(2)	-3(2)

Table S62. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for B2a.

	x	y	z	U(eq)
H(1A)	4987	9429	7312	33
H(2A)	2399	9953	7304	38
H(3A)	968	8984	6860	39
H(4A)	2219	7500	6438	34
H(9A)	2589	6014	8248	40
H(10A)	1611	4717	9208	51
H(12A)	3988	2713	7764	53
H(11A)	2254	3111	8944	59
H(15A)	6352	2789	6198	52
H(17A)	8238	5067	4706	44
H(16A)	8091	3399	5092	56
H(21A)	7257	6924	3893	44
H(22A)	9032	7813	3221	55
H(23A)	9915	8735	4110	46
H(24A)	9004	8756	5653	38
H(28A)	10126	7268	9182	60
H(28B)	9761	6849	8303	60
H(28C)	8543	7007	9130	60

H(29A)	9728	8866	9055	43
H(31A)	8846	10847	9065	93
H(31B)	8764	11565	7973	93
H(31C)	10299	10745	8391	93
H(32A)	7580	11085	6823	48
H(34A)	5574	10685	5955	60
H(34B)	6108	9622	5677	60
H(34C)	7067	10452	5336	60
H(37A)	5522	6896	9591	58
H(37B)	4491	7314	8620	58
H(37C)	5877	7780	8708	58
H(38A)	5994	5223	9466	38
H(40A)	8485	3004	9003	72
H(40B)	6695	3295	8867	72
H(40C)	7425	3370	9835	72
H(41A)	9240	4265	7711	38
H(43A)	10606	5313	6854	45
H(43B)	10079	6523	6677	45
H(43C)	9393	5984	6011	45

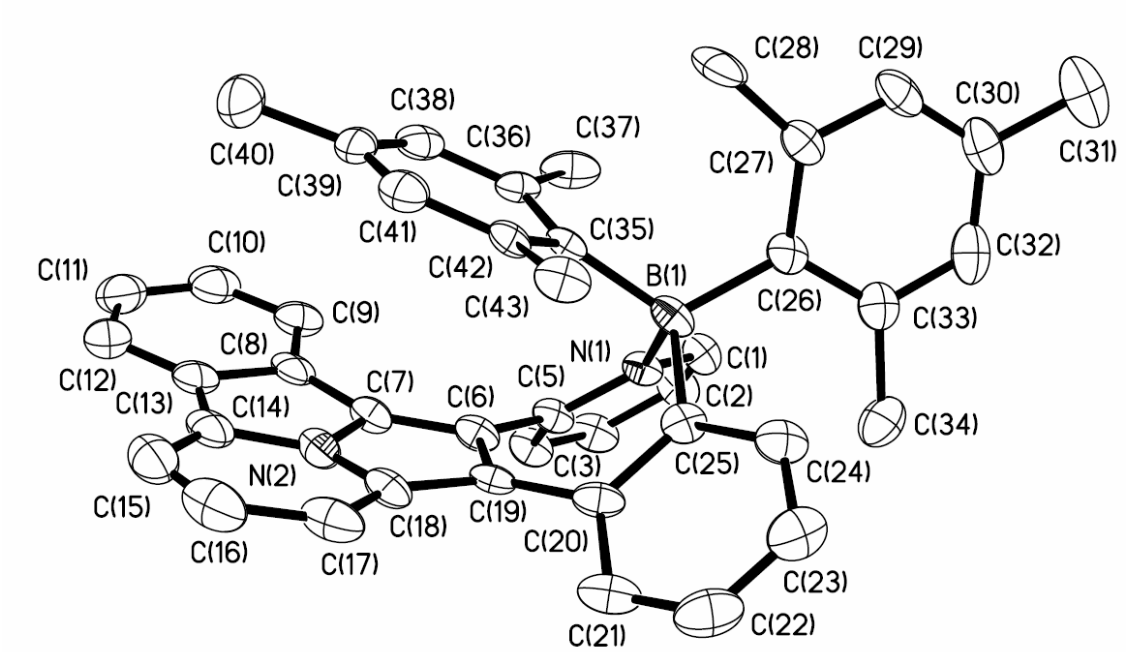


Figure S103. A diagram showing the crystal structure of **B2a** with labeling schemes and 35% thermal ellipsoids. H atoms are omitted for clarity.

Table S63. Crystal data and structure refinement for b2b.

Identification code	b2b	
Empirical formula	C86 H74 B2 N4	
Formula weight	1185.11	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.296(6) Å	α= 111.16(2)°.
	b = 18.788(10) Å	β= 90.63(2)°.
	c = 19.886(11) Å	γ = 97.62(2)°.
Volume	3204(3) $Å^3$	
Z	2	
Density (calculated)	1.229 Mg/m^3	
Absorption coefficient	0.070 mm^{-1}	
F(000)	1256	
Crystal size	0.326 x 0.320 x 0.200 mm^3	
Theta range for data collection	2.201 to 27.327°.	
Index ranges	-12<=h<=12, -24<=k<=22, -25<=l<=25	
Reflections collected	38712	
Independent reflections	14058 [R(int) = 0.0822]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.986 and 0.977	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14058 / 0 / 841	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0724, wR2 = 0.1592	
R indices (all data)	R1 = 0.1357, wR2 = 0.1855	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.546 and -0.364 $e.Å^{-3}$	

Table S64. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for b2b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	9838(2)	6533(1)	9701(1)	24(1)
N(2)	9546(2)	9133(1)	10705(1)	37(1)
N(3)	5513(2)	3612(1)	5906(1)	21(1)
N(4)	5453(2)	1018(1)	4596(1)	24(1)
B(1)	8171(3)	6408(2)	9264(2)	21(1)
B(2)	3660(3)	3398(2)	5707(2)	23(1)
C(1)	8409(3)	6828(2)	8667(1)	24(1)
C(2)	7925(3)	6428(2)	7945(1)	30(1)
C(3)	7934(3)	6784(2)	7439(2)	40(1)
C(4)	8478(3)	7565(2)	7658(2)	41(1)
C(5)	8952(3)	7984(2)	8368(2)	38(1)
C(6)	8911(3)	7637(2)	8880(2)	30(1)
C(7)	9303(3)	8140(2)	9640(2)	29(1)
C(8)	10068(3)	7957(2)	10151(2)	28(1)
C(9)	10640(3)	7251(2)	10056(1)	26(1)
C(10)	12018(3)	7318(2)	10376(2)	32(1)
C(11)	12579(3)	6687(2)	10378(2)	34(1)
C(12)	11727(3)	5966(2)	10056(2)	30(1)
C(13)	10401(3)	5916(2)	9725(1)	25(1)
C(14)	8989(3)	8910(2)	10016(2)	31(1)
C(15)	8189(3)	9507(2)	10008(2)	38(1)
C(16)	7377(3)	9624(2)	9486(2)	50(1)
C(17)	6721(4)	10271(2)	9659(2)	62(1)
C(18)	6863(4)	10826(2)	10371(3)	68(1)
C(19)	7669(4)	10735(2)	10912(2)	57(1)
C(20)	8327(3)	10080(2)	10727(2)	43(1)
C(21)	9215(3)	9822(2)	11189(2)	42(1)
C(22)	9725(4)	10037(2)	11905(2)	51(1)
C(23)	10498(4)	9520(2)	12079(2)	54(1)
C(24)	10738(3)	8821(2)	11584(2)	41(1)
C(25)	10226(3)	8600(2)	10839(2)	34(1)
C(26)	7191(2)	6908(1)	9911(1)	22(1)
C(27)	7392(3)	6980(2)	10644(1)	27(1)

C(28)	6839(3)	7550(2)	11203(2)	34(1)
C(29)	6064(3)	8072(2)	11076(2)	36(1)
C(30)	5715(3)	7945(2)	10362(2)	33(1)
C(31)	6205(3)	7361(1)	9780(1)	25(1)
C(32)	5557(3)	7239(2)	9038(2)	37(1)
C(33)	8149(3)	6433(2)	10870(2)	37(1)
C(34)	5566(4)	8729(2)	11689(2)	59(1)
C(35)	7666(3)	5462(1)	8844(1)	21(1)
C(36)	8554(3)	4998(2)	8339(1)	23(1)
C(37)	8160(3)	4201(2)	7991(1)	28(1)
C(38)	6881(3)	3801(2)	8099(1)	28(1)
C(39)	5978(3)	4245(1)	8567(1)	24(1)
C(40)	6326(3)	5050(1)	8925(1)	22(1)
C(41)	5144(3)	5439(2)	9364(2)	28(1)
C(42)	9988(3)	5317(2)	8121(2)	32(1)
C(43)	6461(3)	2935(2)	7710(2)	43(1)
C(44)	3049(2)	2862(1)	6171(1)	22(1)
C(45)	1930(3)	3064(2)	6636(1)	28(1)
C(46)	1750(3)	1901(2)	6888(1)	31(1)
C(47)	1290(3)	2597(2)	6986(1)	32(1)
C(48)	2832(3)	1673(2)	6432(1)	27(1)
C(49)	3466(2)	2140(1)	6074(1)	22(1)
C(50)	4487(3)	1820(1)	5531(1)	22(1)
C(51)	5736(2)	2234(1)	5380(1)	22(1)
C(52)	6358(3)	3044(1)	5732(1)	22(1)
C(53)	7865(3)	3234(2)	5855(1)	26(1)
C(54)	8533(3)	3993(2)	6127(1)	30(1)
C(55)	7676(3)	4566(2)	6288(1)	29(1)
C(56)	6200(3)	4357(2)	6174(1)	26(1)
C(57)	4324(3)	1047(2)	5028(1)	24(1)
C(58)	3422(3)	296(2)	4682(1)	26(1)
C(59)	2113(3)	-40(2)	4844(2)	32(1)
C(60)	1504(3)	-780(2)	4384(2)	38(1)
C(61)	2171(3)	-1195(2)	3772(2)	44(1)
C(62)	3461(3)	-878(2)	3598(2)	39(1)
C(63)	4086(3)	-133(2)	4046(2)	29(1)
C(64)	5405(3)	355(2)	3995(1)	28(1)
C(65)	6481(3)	362(2)	3539(2)	38(1)

C(66)	7488(3)	1043(2)	3703(2)	40(1)
C(67)	7424(3)	1717(2)	4296(2)	32(1)
C(68)	6345(3)	1716(1)	4778(1)	24(1)
C(69)	3541(3)	2884(2)	4817(1)	23(1)
C(70)	2575(3)	2181(2)	4474(1)	29(1)
C(71)	2766(3)	1672(2)	3775(2)	40(1)
C(72)	3845(4)	1838(2)	3362(2)	44(1)
C(73)	4640(3)	2570(2)	3654(2)	42(1)
C(74)	4500(3)	3090(2)	4354(2)	31(1)
C(75)	1246(3)	1937(2)	4811(2)	42(1)
C(76)	4084(4)	1267(2)	2616(2)	70(1)
C(77)	5367(3)	3895(2)	4567(2)	47(1)
C(78)	3032(3)	4229(2)	6009(1)	26(1)
C(79)	2139(3)	4471(2)	5571(2)	34(1)
C(80)	1659(3)	5186(2)	5858(2)	40(1)
C(81)	1980(3)	5699(2)	6562(2)	41(1)
C(82)	2796(3)	5463(2)	7006(2)	37(1)
C(83)	3293(3)	4745(2)	6748(2)	30(1)
C(84)	4116(3)	4586(2)	7332(2)	35(1)
C(85)	1639(4)	3989(2)	4784(2)	53(1)
C(86)	1498(4)	6483(2)	6844(2)	63(1)

Table S65. Bond lengths [Å] and angles [°] for b2b.

N(1)-C(13)	1.351(3)	B(1)-C(35)	1.665(4)
N(1)-C(9)	1.381(3)	B(2)-C(78)	1.646(4)
N(1)-B(1)	1.713(3)	B(2)-C(44)	1.650(4)
N(2)-C(25)	1.352(3)	B(2)-C(69)	1.676(4)
N(2)-C(14)	1.354(4)	C(1)-C(2)	1.394(4)
N(2)-C(21)	1.382(4)	C(1)-C(6)	1.431(4)
N(3)-C(52)	1.355(3)	C(2)-C(3)	1.393(4)
N(3)-C(56)	1.367(3)	C(3)-C(4)	1.392(4)
N(3)-B(2)	1.724(3)	C(4)-C(5)	1.377(4)
N(4)-C(57)	1.358(3)	C(5)-C(6)	1.393(4)
N(4)-C(64)	1.375(3)	C(6)-C(7)	1.474(4)
N(4)-C(68)	1.379(3)	C(7)-C(8)	1.399(4)
B(1)-C(1)	1.650(4)	C(7)-C(14)	1.439(4)
B(1)-C(26)	1.658(4)	C(8)-C(9)	1.444(4)

C(8)-C(25)	1.452(4)	C(46)-C(48)	1.368(4)
C(9)-C(10)	1.394(4)	C(46)-C(47)	1.377(4)
C(10)-C(11)	1.358(4)	C(48)-C(49)	1.396(3)
C(11)-C(12)	1.396(4)	C(49)-C(50)	1.461(3)
C(12)-C(13)	1.367(4)	C(50)-C(51)	1.407(3)
C(14)-C(15)	1.431(4)	C(50)-C(57)	1.422(4)
C(15)-C(16)	1.374(4)	C(51)-C(68)	1.422(4)
C(15)-C(20)	1.437(4)	C(51)-C(52)	1.458(4)
C(16)-C(17)	1.366(5)	C(52)-C(53)	1.395(3)
C(17)-C(18)	1.416(6)	C(53)-C(54)	1.383(4)
C(18)-C(19)	1.378(5)	C(54)-C(55)	1.372(4)
C(19)-C(20)	1.379(4)	C(55)-C(56)	1.369(4)
C(20)-C(21)	1.475(5)	C(57)-C(58)	1.462(4)
C(21)-C(22)	1.389(5)	C(58)-C(59)	1.392(4)
C(22)-C(23)	1.416(5)	C(58)-C(63)	1.430(4)
C(23)-C(24)	1.374(5)	C(59)-C(60)	1.396(4)
C(24)-C(25)	1.444(4)	C(60)-C(61)	1.391(4)
C(26)-C(31)	1.412(3)	C(61)-C(62)	1.372(4)
C(26)-C(27)	1.422(4)	C(62)-C(63)	1.402(4)
C(27)-C(28)	1.395(4)	C(63)-C(64)	1.458(4)
C(27)-C(33)	1.507(4)	C(64)-C(65)	1.359(4)
C(28)-C(29)	1.379(4)	C(65)-C(66)	1.413(4)
C(29)-C(30)	1.381(4)	C(66)-C(67)	1.394(4)
C(29)-C(34)	1.518(4)	C(67)-C(68)	1.395(4)
C(30)-C(31)	1.406(4)	C(69)-C(74)	1.406(4)
C(31)-C(32)	1.513(4)	C(69)-C(70)	1.428(4)
C(35)-C(40)	1.420(3)	C(70)-C(71)	1.403(4)
C(35)-C(36)	1.423(3)	C(70)-C(75)	1.507(4)
C(36)-C(37)	1.399(4)	C(71)-C(72)	1.378(4)
C(36)-C(42)	1.520(3)	C(72)-C(73)	1.384(5)
C(37)-C(38)	1.383(4)	C(72)-C(76)	1.524(5)
C(38)-C(39)	1.382(4)	C(73)-C(74)	1.401(4)
C(38)-C(43)	1.522(4)	C(74)-C(77)	1.524(4)
C(39)-C(40)	1.409(4)	C(78)-C(79)	1.423(4)
C(40)-C(41)	1.509(3)	C(78)-C(83)	1.436(4)
C(44)-C(45)	1.397(3)	C(79)-C(80)	1.393(4)
C(44)-C(49)	1.408(3)	C(79)-C(85)	1.527(5)
C(45)-C(47)	1.385(4)	C(80)-C(81)	1.384(5)

C(81)-C(82)	1.381(4)	C(1)-C(6)-C(7)	122.5(2)
C(81)-C(86)	1.507(4)	C(8)-C(7)-C(14)	105.4(2)
C(82)-C(83)	1.404(4)	C(8)-C(7)-C(6)	126.3(2)
C(83)-C(84)	1.521(4)	C(14)-C(7)-C(6)	128.3(2)
		C(7)-C(8)-C(9)	128.2(3)
C(13)-N(1)-C(9)	117.2(2)	C(7)-C(8)-C(25)	109.7(2)
C(13)-N(1)-B(1)	119.9(2)	C(9)-C(8)-C(25)	122.1(2)
C(9)-N(1)-B(1)	122.86(19)	N(1)-C(9)-C(10)	120.4(2)
C(25)-N(2)-C(14)	114.2(2)	N(1)-C(9)-C(8)	122.2(2)
C(25)-N(2)-C(21)	128.6(3)	C(10)-C(9)-C(8)	117.2(2)
C(14)-N(2)-C(21)	116.8(3)	C(11)-C(10)-C(9)	121.3(3)
C(52)-N(3)-C(56)	117.5(2)	C(10)-C(11)-C(12)	118.0(3)
C(52)-N(3)-B(2)	120.8(2)	C(13)-C(12)-C(11)	119.4(2)
C(56)-N(3)-B(2)	121.37(19)	N(1)-C(13)-C(12)	123.5(2)
C(57)-N(4)-C(64)	116.2(2)	N(2)-C(14)-C(15)	105.4(3)
C(57)-N(4)-C(68)	112.9(2)	N(2)-C(14)-C(7)	106.9(2)
C(64)-N(4)-C(68)	130.0(2)	C(15)-C(14)-C(7)	147.0(3)
C(1)-B(1)-C(26)	109.15(19)	C(16)-C(15)-C(14)	134.2(3)
C(1)-B(1)-C(35)	110.0(2)	C(16)-C(15)-C(20)	118.4(3)
C(26)-B(1)-C(35)	119.7(2)	C(14)-C(15)-C(20)	107.4(3)
C(1)-B(1)-N(1)	106.44(18)	C(17)-C(16)-C(15)	119.8(4)
C(26)-B(1)-N(1)	103.31(19)	C(16)-C(17)-C(18)	121.0(4)
C(35)-B(1)-N(1)	107.28(18)	C(19)-C(18)-C(17)	121.3(3)
C(78)-B(2)-C(44)	110.2(2)	C(18)-C(19)-C(20)	116.9(4)
C(78)-B(2)-C(69)	119.6(2)	C(19)-C(20)-C(15)	122.6(3)
C(44)-B(2)-C(69)	111.6(2)	C(19)-C(20)-C(21)	129.0(3)
C(78)-B(2)-N(3)	106.1(2)	C(15)-C(20)-C(21)	108.4(3)
C(44)-B(2)-N(3)	105.50(18)	N(2)-C(21)-C(22)	117.2(3)
C(69)-B(2)-N(3)	102.47(18)	N(2)-C(21)-C(20)	102.0(3)
C(2)-C(1)-C(6)	117.2(2)	C(22)-C(21)-C(20)	140.7(3)
C(2)-C(1)-B(1)	120.4(2)	C(21)-C(22)-C(23)	117.1(3)
C(6)-C(1)-B(1)	121.7(2)	C(24)-C(23)-C(22)	123.6(3)
C(3)-C(2)-C(1)	122.6(3)	C(23)-C(24)-C(25)	119.4(3)
C(4)-C(3)-C(2)	118.8(3)	N(2)-C(25)-C(24)	113.9(3)
C(5)-C(4)-C(3)	120.5(3)	N(2)-C(25)-C(8)	103.8(2)
C(4)-C(5)-C(6)	121.0(3)	C(24)-C(25)-C(8)	142.1(3)
C(5)-C(6)-C(1)	119.8(3)	C(31)-C(26)-C(27)	115.4(2)
C(5)-C(6)-C(7)	117.6(3)	C(31)-C(26)-B(1)	121.4(2)

C(27)-C(26)-B(1)	122.9(2)	C(57)-C(50)-C(49)	125.5(2)
C(28)-C(27)-C(26)	121.6(2)	C(50)-C(51)-C(68)	107.4(2)
C(28)-C(27)-C(33)	115.4(2)	C(50)-C(51)-C(52)	129.8(2)
C(26)-C(27)-C(33)	123.0(2)	C(68)-C(51)-C(52)	122.8(2)
C(29)-C(28)-C(27)	122.0(3)	N(3)-C(52)-C(53)	119.7(2)
C(28)-C(29)-C(30)	116.4(2)	N(3)-C(52)-C(51)	121.5(2)
C(28)-C(29)-C(34)	121.8(3)	C(53)-C(52)-C(51)	118.7(2)
C(30)-C(29)-C(34)	121.7(3)	C(54)-C(53)-C(52)	121.6(2)
C(29)-C(30)-C(31)	123.2(3)	C(55)-C(54)-C(53)	118.4(2)
C(30)-C(31)-C(26)	120.0(2)	C(56)-C(55)-C(54)	118.2(2)
C(30)-C(31)-C(32)	115.9(2)	N(3)-C(56)-C(55)	124.5(2)
C(26)-C(31)-C(32)	124.0(2)	N(4)-C(57)-C(50)	105.6(2)
C(40)-C(35)-C(36)	114.0(2)	N(4)-C(57)-C(58)	103.8(2)
C(40)-C(35)-B(1)	124.6(2)	C(50)-C(57)-C(58)	149.6(2)
C(36)-C(35)-B(1)	121.4(2)	C(59)-C(58)-C(63)	118.2(2)
C(37)-C(36)-C(35)	122.2(2)	C(59)-C(58)-C(57)	133.2(3)
C(37)-C(36)-C(42)	114.1(2)	C(63)-C(58)-C(57)	108.6(2)
C(35)-C(36)-C(42)	123.8(2)	C(58)-C(59)-C(60)	119.0(3)
C(38)-C(37)-C(36)	123.3(2)	C(61)-C(60)-C(59)	122.2(3)
C(39)-C(38)-C(37)	115.4(2)	C(62)-C(61)-C(60)	120.1(3)
C(39)-C(38)-C(43)	122.0(2)	C(61)-C(62)-C(63)	118.8(3)
C(37)-C(38)-C(43)	122.6(2)	C(62)-C(63)-C(58)	121.6(2)
C(38)-C(39)-C(40)	123.2(2)	C(62)-C(63)-C(64)	131.5(3)
C(39)-C(40)-C(35)	121.8(2)	C(58)-C(63)-C(64)	106.9(2)
C(39)-C(40)-C(41)	115.1(2)	C(65)-C(64)-N(4)	115.4(2)
C(35)-C(40)-C(41)	123.0(2)	C(65)-C(64)-C(63)	140.1(3)
C(45)-C(44)-C(49)	114.9(2)	N(4)-C(64)-C(63)	104.5(2)
C(45)-C(44)-B(2)	120.8(2)	C(64)-C(65)-C(66)	118.3(3)
C(49)-C(44)-B(2)	123.9(2)	C(67)-C(66)-C(65)	123.8(3)
C(47)-C(45)-C(44)	122.9(2)	C(66)-C(67)-C(68)	118.7(3)
C(48)-C(46)-C(47)	119.0(2)	N(4)-C(68)-C(67)	113.6(2)
C(46)-C(47)-C(45)	120.4(2)	N(4)-C(68)-C(51)	105.7(2)
C(46)-C(48)-C(49)	120.5(2)	C(67)-C(68)-C(51)	140.3(2)
C(48)-C(49)-C(44)	122.2(2)	C(74)-C(69)-C(70)	114.3(2)
C(48)-C(49)-C(50)	117.5(2)	C(74)-C(69)-B(2)	121.2(2)
C(44)-C(49)-C(50)	120.0(2)	C(70)-C(69)-B(2)	124.3(2)
C(51)-C(50)-C(57)	108.4(2)	C(71)-C(70)-C(69)	121.9(3)
C(51)-C(50)-C(49)	126.0(2)	C(71)-C(70)-C(75)	114.5(3)

C(69)-C(70)-C(75)	123.6(3)	C(80)-C(79)-C(78)	119.9(3)
C(72)-C(71)-C(70)	122.2(3)	C(80)-C(79)-C(85)	116.0(3)
C(71)-C(72)-C(73)	115.6(3)	C(78)-C(79)-C(85)	124.1(3)
C(71)-C(72)-C(76)	121.8(3)	C(81)-C(80)-C(79)	124.5(3)
C(73)-C(72)-C(76)	122.6(3)	C(82)-C(81)-C(80)	116.7(3)
C(72)-C(73)-C(74)	123.7(3)	C(82)-C(81)-C(86)	120.4(3)
C(73)-C(74)-C(69)	121.0(3)	C(80)-C(81)-C(86)	123.0(3)
C(73)-C(74)-C(77)	116.8(3)	C(81)-C(82)-C(83)	121.3(3)
C(69)-C(74)-C(77)	122.1(3)	C(82)-C(83)-C(78)	122.3(3)
C(79)-C(78)-C(83)	115.2(2)	C(82)-C(83)-C(84)	112.8(3)
C(79)-C(78)-B(2)	122.9(2)	C(78)-C(83)-C(84)	124.9(2)
C(83)-C(78)-B(2)	121.9(2)		

Table S66. Anisotropic displacement parameters ($Å^2x\ 10^3$) for b2b. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	19(1)	22(1)	31(1)	10(1)	4(1)	5(1)
N(2)	35(1)	29(1)	44(2)	12(1)	1(1)	-3(1)
N(3)	18(1)	22(1)	23(1)	10(1)	4(1)	4(1)
N(4)	20(1)	24(1)	27(1)	6(1)	2(1)	5(1)
B(1)	16(1)	20(2)	25(2)	8(1)	0(1)	4(1)
B(2)	14(1)	28(2)	29(2)	14(1)	0(1)	2(1)
C(1)	20(1)	26(2)	33(2)	14(1)	10(1)	11(1)
C(2)	35(2)	28(2)	31(2)	13(1)	9(1)	14(1)
C(3)	48(2)	52(2)	29(2)	17(2)	10(1)	28(2)
C(4)	46(2)	49(2)	51(2)	37(2)	18(2)	26(2)
C(5)	35(2)	39(2)	52(2)	30(2)	9(1)	10(1)
C(6)	21(1)	32(2)	48(2)	26(2)	9(1)	10(1)
C(7)	25(1)	19(1)	43(2)	13(1)	6(1)	-1(1)
C(8)	22(1)	20(1)	40(2)	11(1)	3(1)	-1(1)
C(9)	24(1)	23(1)	31(2)	11(1)	4(1)	-1(1)
C(10)	24(1)	30(2)	39(2)	10(1)	-1(1)	-5(1)
C(11)	23(1)	43(2)	38(2)	18(2)	-1(1)	4(1)
C(12)	25(1)	32(2)	38(2)	16(1)	1(1)	9(1)
C(13)	22(1)	21(1)	34(2)	12(1)	4(1)	4(1)
C(14)	23(1)	28(2)	50(2)	22(1)	8(1)	3(1)

C(15)	32(2)	28(2)	58(2)	21(2)	8(1)	3(1)
C(16)	42(2)	47(2)	72(2)	36(2)	-2(2)	7(2)
C(17)	59(2)	44(2)	91(3)	28(2)	-1(2)	23(2)
C(18)	56(2)	45(2)	108(4)	27(3)	5(2)	26(2)
C(19)	52(2)	38(2)	80(3)	16(2)	10(2)	15(2)
C(20)	34(2)	30(2)	57(2)	8(2)	12(2)	-2(1)
C(21)	36(2)	12(2)	64(2)	0(2)	19(2)	-1(1)
C(22)	52(2)	40(2)	56(2)	13(2)	3(2)	0(2)
C(23)	61(2)	50(2)	44(2)	12(2)	-3(2)	-5(2)
C(24)	44(2)	28(2)	46(2)	9(2)	-1(2)	-1(1)
C(25)	27(1)	27(2)	47(2)	16(2)	3(1)	-2(1)
C(26)	19(1)	16(1)	28(1)	7(1)	2(1)	0(1)
C(27)	20(1)	28(2)	29(2)	8(1)	2(1)	-1(1)
C(28)	28(1)	38(2)	26(2)	2(1)	2(1)	-2(1)
C(29)	31(2)	25(2)	36(2)	-5(1)	12(1)	-2(1)
C(30)	24(1)	22(2)	53(2)	11(1)	12(1)	6(1)
C(31)	21(1)	21(1)	34(2)	10(1)	5(1)	3(1)
C(32)	26(1)	46(2)	48(2)	24(2)	6(1)	16(1)
C(33)	31(2)	55(2)	34(2)	26(2)	5(1)	7(1)
C(34)	58(2)	41(2)	57(2)	-9(2)	18(2)	8(2)
C(35)	23(1)	21(1)	22(1)	11(1)	2(1)	6(1)
C(36)	23(1)	25(1)	24(1)	11(1)	4(1)	7(1)
C(37)	34(1)	26(2)	25(1)	7(1)	7(1)	14(1)
C(38)	35(2)	23(2)	26(1)	10(1)	-1(1)	3(1)
C(39)	22(1)	24(1)	25(1)	10(1)	-1(1)	-2(1)
C(40)	22(1)	26(1)	22(1)	13(1)	1(1)	4(1)
C(41)	21(1)	24(2)	38(2)	10(1)	7(1)	-1(1)
C(42)	30(1)	32(2)	37(2)	14(1)	14(1)	11(1)
C(43)	53(2)	25(2)	43(2)	5(1)	7(2)	1(1)
C(44)	16(1)	25(1)	23(1)	8(1)	-1(1)	0(1)
C(45)	23(1)	33(2)	28(2)	13(1)	3(1)	3(1)
C(46)	31(1)	36(2)	27(2)	17(1)	3(1)	-5(1)
C(47)	27(1)	38(2)	28(2)	9(1)	10(1)	4(1)
C(48)	28(1)	29(2)	27(1)	12(1)	0(1)	2(1)
C(49)	20(1)	23(1)	22(1)	9(1)	-2(1)	0(1)
C(50)	21(1)	21(1)	25(1)	10(1)	-2(1)	4(1)
C(51)	16(1)	24(1)	26(1)	10(1)	0(1)	5(1)
C(52)	20(1)	26(1)	21(1)	10(1)	3(1)	4(1)

C(53)	17(1)	31(2)	31(2)	11(1)	1(1)	3(1)
C(54)	18(1)	37(2)	32(2)	12(1)	0(1)	0(1)
C(55)	26(1)	25(2)	32(2)	9(1)	2(1)	-3(1)
C(56)	26(1)	24(2)	29(1)	10(1)	4(1)	5(1)
C(57)	19(1)	26(2)	31(2)	14(1)	-1(1)	3(1)
C(58)	22(1)	25(2)	34(2)	12(1)	-4(1)	4(1)
C(59)	26(1)	29(2)	43(2)	15(1)	1(1)	5(1)
C(60)	29(2)	30(2)	53(2)	14(2)	0(1)	-3(1)
C(61)	38(2)	24(2)	59(2)	2(2)	-5(2)	-2(1)
C(62)	32(2)	28(2)	43(2)	-2(1)	-1(1)	3(1)
C(63)	23(1)	28(2)	35(2)	9(1)	-4(1)	5(1)
C(64)	26(1)	23(2)	29(2)	2(1)	-3(1)	5(1)
C(65)	34(2)	36(2)	33(2)	0(1)	4(1)	6(1)
C(66)	29(2)	46(2)	36(2)	7(2)	12(1)	5(1)
C(67)	22(1)	34(2)	38(2)	11(1)	5(1)	4(1)
C(68)	19(1)	21(1)	30(1)	7(1)	-2(1)	1(1)
C(69)	19(1)	30(2)	25(1)	13(1)	0(1)	6(1)
C(70)	25(1)	36(2)	29(2)	16(1)	-6(1)	5(1)
C(71)	46(2)	38(2)	32(2)	9(2)	-15(1)	5(1)
C(72)	49(2)	56(2)	28(2)	12(2)	-3(2)	23(2)
C(73)	32(2)	70(2)	30(2)	23(2)	5(1)	14(2)
C(74)	23(1)	46(2)	30(2)	20(1)	0(1)	5(1)
C(75)	25(1)	55(2)	46(2)	22(2)	-10(1)	-12(1)
C(76)	81(3)	91(3)	32(2)	8(2)	-2(2)	42(2)
C(77)	42(2)	67(2)	43(2)	37(2)	2(2)	-8(2)
C(78)	19(1)	33(2)	35(2)	20(1)	9(1)	7(1)
C(79)	23(1)	42(2)	48(2)	27(2)	7(1)	10(1)
C(80)	23(1)	44(2)	69(2)	37(2)	9(2)	13(1)
C(81)	28(2)	35(2)	71(2)	29(2)	22(2)	12(1)
C(82)	33(2)	32(2)	47(2)	13(2)	18(1)	7(1)
C(83)	25(1)	30(2)	40(2)	17(1)	13(1)	8(1)
C(84)	36(2)	36(2)	32(2)	11(1)	5(1)	8(1)
C(85)	49(2)	72(3)	52(2)	32(2)	-9(2)	29(2)
C(86)	47(2)	43(2)	109(3)	32(2)	25(2)	22(2)

Table S67. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for b2b.

	x	y	z	U(eq)

H(2A)	7575	5892	7792	36
H(3A)	7576	6498	6954	48
H(4A)	8522	7811	7316	50
H(5A)	9312	8518	8509	45
H(10A)	12574	7815	10598	39
H(11A)	13523	6735	10591	41
H(12A)	12066	5516	10068	36
H(13A)	9845	5419	9500	30
H(16A)	7271	9256	9006	59
H(17A)	6162	10350	9295	75
H(18A)	6394	11270	10478	82
H(19A)	7767	11106	11391	69
H(22A)	9561	10511	12261	61
H(23A)	10871	9663	12563	65
H(24A)	11237	8487	11732	50
H(28A)	7001	7581	11686	41
H(30A)	5114	8269	10258	40
H(32A)	4521	7288	9066	56
H(32B)	5673	6722	8702	56
H(32C)	6059	7627	8866	56
H(33A)	7708	6371	11294	56
H(33B)	9182	6641	10989	56
H(33C)	8048	5930	10473	56
H(34A)	5854	8698	12152	89
H(34B)	4505	8691	11641	89
H(34C)	6016	9223	11670	89
H(37A)	8804	3921	7665	33
H(39A)	5078	3996	8652	28
H(41A)	4288	5055	9316	43
H(41B)	4880	5832	9188	43
H(41C)	5496	5684	9873	43
H(42A)	9927	5206	7600	48
H(42B)	10773	5074	8240	48
H(42C)	10188	5876	8382	48
H(43A)	6598	2799	7193	64
H(43B)	5439	2785	7778	64

H(43C)	7075	2662	7907	64
H(45A)	1594	3542	6716	33
H(46A)	1321	1584	7133	37
H(47A)	529	2758	7295	38
H(48A)	3154	1193	6359	33
H(53A)	8446	2832	5749	32
H(54A)	9562	4115	6200	35
H(55A)	8095	5094	6474	35
H(56A)	5613	4757	6289	31
H(59A)	1640	229	5262	38
H(60A)	605	-1006	4493	46
H(61A)	1731	-1700	3474	53
H(62A)	3922	-1159	3180	46
H(65A)	6554	-80	3121	45
H(66A)	8254	1042	3390	47
H(67A)	8101	2168	4371	39
H(71A)	2131	1196	3580	48
H(73A)	5319	2728	3364	51
H(75A)	478	1652	4432	63
H(75B)	904	2396	5153	63
H(75C)	1493	1606	5066	63
H(76A)	4198	1536	2275	104
H(76B)	3245	858	2452	104
H(76C)	4964	1040	2642	104
H(77A)	5370	4060	4152	71
H(77B)	6369	3886	4719	71
H(77C)	4919	4257	4967	71
H(80A)	1072	5332	5550	48
H(82A)	3026	5794	7495	45
H(84A)	4935	4999	7543	52
H(84B)	4482	4091	7118	52
H(84C)	3462	4564	7709	52
H(85A)	959	4250	4609	80
H(85B)	1155	3480	4750	80
H(85C)	2484	3929	4489	80
H(86A)	1750	6750	6510	95
H(86B)	1987	6786	7320	95
H(86C)	442	6424	6885	95

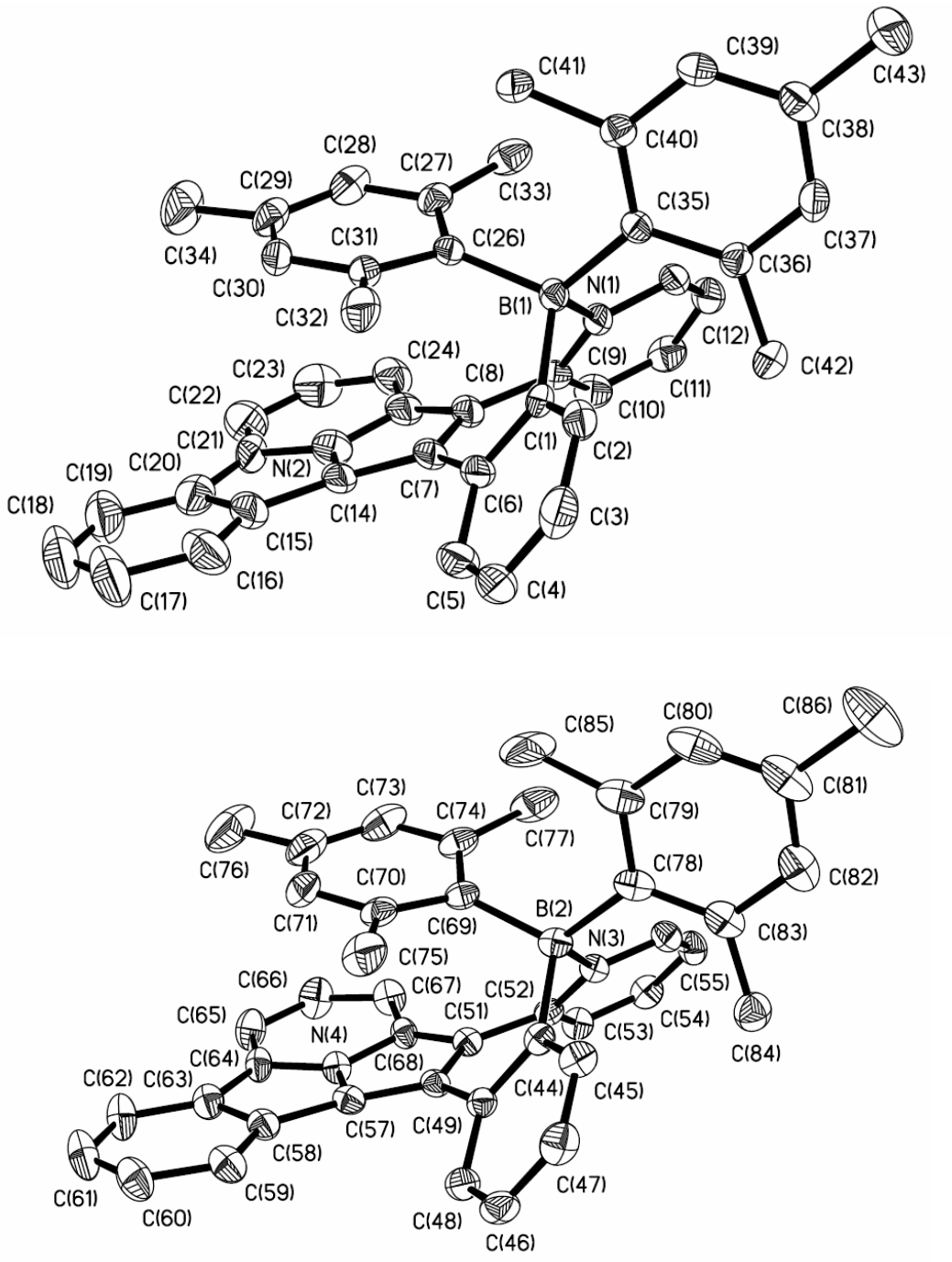


Figure S104. A diagram showing the structures of the two independent molecules in the crystal lattice of **B2b** with labeling schemes, 35% thermal ellipsoids. H atoms are omitted for clarity.

Table S68. Crystal data and structure refinement for b3a.

Identification code	b3a-sr	
Empirical formula	C6.96 H5.78 B0.15 N0.30	
Formula weight	95.20	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.873(19) Å	α= 86.66(4)°.
	b = 16.28(2) Å	β= 80.14(4)°.
	c = 17.74(3) Å	γ = 72.27(4)°.
Volume	3759(9) $Å^3$	
Z	27	
Density (calculated)	1.135 Mg/m^3	
Absorption coefficient	0.065 mm^{-1}	
F(000)	1360	
Crystal size	0.160 x 0.150 x 0.120 mm^3	
Theta range for data collection	2.214 to 27.103°.	
Index ranges	-17<=h<=17, -20<=k<=20, -22<=l<=20	
Reflections collected	36686	
Independent reflections	16022 [R(int) = 0.1446]	
Completeness to theta = 25.242°	97.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.992 and 0.990	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16022 / 0 / 914	
Goodness-of-fit on F^2	0.853	
Final R indices [I>2sigma(I)]	R1 = 0.0807, wR2 = 0.1706	
R indices (all data)	R1 = 0.2272, wR2 = 0.2107	
Extinction coefficient	0.0079(7)	
Largest diff. peak and hole	0.308 and -0.274 $e.Å^{-3}$	

Table S69. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for b3a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	6511(2)	5533(2)	7928(2)	36(1)
N(2)	6179(2)	7478(2)	6018(2)	37(1)
N(3)	7668(2)	10684(2)	1197(2)	34(1)
N(4)	6936(2)	11315(2)	3728(2)	32(1)
B(1)	6724(3)	4794(3)	7226(2)	35(1)
B(2)	7795(3)	9633(3)	1499(2)	31(1)
C(1)	5593(3)	4936(2)	6976(2)	34(1)
C(2)	5129(3)	4270(2)	6983(2)	44(1)
C(3)	4220(3)	4373(3)	6720(2)	55(1)
C(4)	3734(3)	5144(3)	6429(2)	57(1)
C(5)	4170(3)	5811(3)	6383(2)	45(1)
C(6)	5079(3)	5723(2)	6650(2)	36(1)
C(7)	5529(2)	6442(2)	6541(2)	31(1)
C(8)	5636(3)	6928(2)	5860(2)	36(1)
C(9)	5470(3)	6956(3)	5101(2)	47(1)
C(10)	5858(3)	7508(3)	4584(2)	51(1)
C(11)	6440(3)	8008(2)	4779(2)	51(1)
C(12)	6630(3)	8005(2)	5517(2)	40(1)
C(13)	7196(3)	8309(2)	5984(2)	41(1)
C(14)	7822(3)	8853(3)	5819(3)	56(1)
C(15)	8287(3)	9042(3)	6378(3)	69(1)
C(16)	8149(3)	8688(3)	7109(3)	61(1)
C(17)	7557(3)	8135(2)	7295(2)	48(1)
C(18)	7061(3)	7940(2)	6736(2)	38(1)
C(19)	6409(2)	7398(2)	6729(2)	33(1)
C(20)	5997(3)	6734(2)	7069(2)	33(1)
C(21)	6128(2)	6401(2)	7833(2)	35(1)
C(22)	5911(3)	6991(2)	8464(2)	37(1)
C(23)	5418(3)	7889(2)	8385(2)	38(1)
C(24)	5222(3)	8434(3)	8991(2)	49(1)
C(25)	5449(3)	8132(3)	9701(3)	59(1)
C(26)	5916(3)	7262(3)	9801(2)	62(1)
C(27)	6156(3)	6682(3)	9179(2)	48(1)

C(28)	6631(3)	5790(3)	9238(2)	58(1)
C(29)	6776(3)	5266(3)	8632(2)	51(1)
C(30)	7087(3)	3808(2)	7602(2)	38(1)
C(31)	6437(3)	3500(2)	8187(2)	38(1)
C(32)	5461(3)	4079(2)	8654(2)	48(1)
C(33)	6636(3)	2628(2)	8392(2)	43(1)
C(34)	7474(3)	1999(2)	8029(2)	41(1)
C(35)	7641(3)	1050(2)	8210(2)	54(1)
C(36)	8145(3)	2291(2)	7502(2)	46(1)
C(37)	7992(3)	3159(2)	7292(2)	42(1)
C(38)	8864(3)	3337(3)	6734(2)	64(1)
C(39)	7492(3)	5063(2)	6516(2)	39(1)
C(40)	7443(3)	4889(2)	5748(2)	45(1)
C(41)	6882(3)	4271(3)	5537(2)	60(1)
C(42)	7963(3)	5246(3)	5127(2)	54(1)
C(43)	8549(3)	5771(3)	5222(3)	59(1)
C(44)	9072(4)	6169(3)	4548(3)	95(2)
C(45)	8680(3)	5877(3)	5954(3)	58(1)
C(46)	8190(3)	5519(2)	6597(2)	46(1)
C(47)	8520(3)	5618(3)	7356(3)	69(1)
C(48)	6624(3)	9609(2)	1845(2)	31(1)
C(49)	6199(3)	9001(2)	1587(2)	42(1)
C(50)	5264(3)	8900(3)	1916(2)	51(1)
C(51)	4676(3)	9445(3)	2508(2)	55(1)
C(52)	5055(3)	10051(2)	2784(2)	43(1)
C(53)	6012(3)	10128(2)	2470(2)	34(1)
C(54)	6419(2)	10714(2)	2844(2)	30(1)
C(55)	6372(2)	10772(2)	3639(2)	30(1)
C(56)	6016(3)	10419(2)	4331(2)	42(1)
C(57)	6276(3)	10614(3)	5006(2)	50(1)
C(58)	6896(3)	11143(3)	5039(2)	47(1)
C(59)	7264(3)	11502(2)	4371(2)	39(1)
C(60)	7943(3)	12014(2)	4087(2)	40(1)
C(61)	8508(3)	12386(3)	4462(2)	52(1)
C(62)	9110(3)	12834(3)	4046(3)	66(1)
C(63)	9153(3)	12917(3)	3255(3)	59(1)
C(64)	8606(3)	12556(2)	2864(2)	46(1)
C(65)	7990(3)	12089(2)	3279(2)	33(1)

C(66)	7338(3)	11620(2)	3061(2)	35(1)
C(67)	7013(2)	11242(2)	2490(2)	30(1)
C(68)	7264(2)	11376(2)	1667(2)	32(1)
C(69)	7125(2)	12237(2)	1376(2)	32(1)
C(70)	6623(2)	12977(2)	1846(2)	38(1)
C(71)	6505(3)	13791(3)	1547(2)	51(1)
C(72)	6834(3)	13918(3)	772(3)	69(1)
C(73)	7298(3)	13218(3)	305(2)	60(1)
C(74)	7450(3)	12369(3)	598(2)	41(1)
C(75)	7939(3)	11631(3)	144(2)	46(1)
C(76)	8032(3)	10829(3)	443(2)	42(1)
C(77)	8274(3)	8998(2)	737(2)	35(1)
C(78)	9195(3)	8303(2)	671(2)	39(1)
C(79)	9910(3)	8093(2)	1265(2)	51(1)
C(80)	9516(3)	7765(3)	33(2)	48(1)
C(81)	8983(3)	7814(3)	-546(2)	52(1)
C(82)	9340(4)	7190(3)	-1221(3)	83(2)
C(83)	8093(3)	8492(3)	-510(2)	48(1)
C(84)	7742(3)	9057(2)	111(2)	38(1)
C(85)	6767(3)	9756(2)	33(2)	46(1)
C(86)	8471(2)	9499(2)	2197(2)	29(1)
C(87)	9197(3)	9943(2)	2248(2)	38(1)
C(88)	9617(3)	10446(2)	1589(2)	51(1)
C(89)	9629(3)	9896(3)	2907(2)	46(1)
C(90)	9410(3)	9388(3)	3525(2)	48(1)
C(91)	9891(3)	9365(3)	4229(2)	80(2)
C(92)	8785(3)	8896(3)	3445(2)	44(1)
C(93)	8331(2)	8926(2)	2816(2)	33(1)
C(94)	7737(3)	8270(2)	2788(2)	51(1)

Table S70. Bond lengths [Å] and angles [°] for b3a.

N(1)-C(21)	1.361(5)	N(3)-C(76)	1.379(5)
N(1)-C(29)	1.370(5)	N(3)-B(2)	1.728(5)
N(1)-B(1)	1.709(5)	N(4)-C(66)	1.354(5)
N(2)-C(19)	1.343(4)	N(4)-C(55)	1.377(4)
N(2)-C(8)	1.400(5)	N(4)-C(59)	1.379(5)
N(2)-C(12)	1.401(5)	B(1)-C(39)	1.635(6)
N(3)-C(68)	1.358(4)	B(1)-C(1)	1.648(6)

B(1)-C(30)	1.665(6)	C(37)-C(38)	1.516(5)
B(2)-C(86)	1.644(5)	C(39)-C(46)	1.417(5)
B(2)-C(48)	1.648(5)	C(39)-C(40)	1.424(5)
B(2)-C(77)	1.665(5)	C(40)-C(42)	1.407(5)
C(1)-C(6)	1.409(5)	C(40)-C(41)	1.543(5)
C(1)-C(2)	1.417(5)	C(42)-C(43)	1.381(6)
C(2)-C(3)	1.379(5)	C(43)-C(45)	1.369(6)
C(3)-C(4)	1.350(6)	C(43)-C(44)	1.508(6)
C(4)-C(5)	1.386(5)	C(45)-C(46)	1.415(6)
C(5)-C(6)	1.385(5)	C(46)-C(47)	1.527(6)
C(6)-C(7)	1.475(5)	C(48)-C(53)	1.419(5)
C(7)-C(20)	1.405(5)	C(48)-C(49)	1.426(5)
C(7)-C(8)	1.415(5)	C(49)-C(50)	1.382(5)
C(8)-C(9)	1.401(5)	C(50)-C(51)	1.388(5)
C(9)-C(10)	1.403(5)	C(51)-C(52)	1.397(5)
C(10)-C(11)	1.401(5)	C(52)-C(53)	1.389(5)
C(11)-C(12)	1.378(5)	C(53)-C(54)	1.482(5)
C(12)-C(13)	1.434(5)	C(54)-C(55)	1.409(5)
C(13)-C(14)	1.405(5)	C(54)-C(67)	1.416(5)
C(13)-C(18)	1.437(5)	C(55)-C(56)	1.402(5)
C(14)-C(15)	1.367(6)	C(56)-C(57)	1.388(5)
C(15)-C(16)	1.394(6)	C(57)-C(58)	1.401(5)
C(16)-C(17)	1.385(5)	C(58)-C(59)	1.378(5)
C(17)-C(18)	1.399(5)	C(59)-C(60)	1.450(5)
C(18)-C(19)	1.446(5)	C(60)-C(61)	1.393(5)
C(19)-C(20)	1.428(5)	C(60)-C(65)	1.424(5)
C(20)-C(21)	1.450(5)	C(61)-C(62)	1.369(6)
C(21)-C(22)	1.449(5)	C(62)-C(63)	1.394(6)
C(22)-C(27)	1.395(5)	C(63)-C(64)	1.378(5)
C(22)-C(23)	1.422(5)	C(64)-C(65)	1.402(5)
C(23)-C(24)	1.372(5)	C(65)-C(66)	1.458(5)
C(24)-C(25)	1.378(6)	C(66)-C(67)	1.416(5)
C(25)-C(26)	1.380(6)	C(67)-C(68)	1.461(5)
C(26)-C(27)	1.423(5)	C(68)-C(69)	1.433(5)
C(27)-C(28)	1.405(6)	C(69)-C(74)	1.402(5)
C(28)-C(29)	1.361(5)	C(69)-C(70)	1.427(5)
C(30)-C(37)	1.421(5)	C(70)-C(71)	1.370(5)
C(30)-C(31)	1.427(5)	C(71)-C(72)	1.396(6)
C(31)-C(33)	1.400(5)	C(72)-C(73)	1.370(5)
C(31)-C(32)	1.529(5)	C(73)-C(74)	1.415(6)
C(33)-C(34)	1.382(5)	C(74)-C(75)	1.407(5)
C(34)-C(36)	1.373(5)	C(75)-C(76)	1.359(5)
C(34)-C(35)	1.514(5)	C(77)-C(78)	1.417(5)
C(36)-C(37)	1.400(5)	C(77)-C(84)	1.418(5)

C(78)-C(80)	1.397(5)
C(78)-C(79)	1.523(5)
C(80)-C(81)	1.350(5)
C(81)-C(83)	1.378(5)
C(81)-C(82)	1.531(5)
C(83)-C(84)	1.399(5)
C(84)-C(85)	1.501(5)
C(86)-C(93)	1.424(5)
C(86)-C(87)	1.424(5)
C(87)-C(89)	1.390(5)
C(87)-C(88)	1.523(5)
C(89)-C(90)	1.382(6)
C(90)-C(92)	1.374(5)
C(90)-C(91)	1.507(6)
C(92)-C(93)	1.364(5)
C(93)-C(94)	1.542(5)

C(21)-N(1)-C(29)	115.7(3)
C(21)-N(1)-B(1)	124.2(3)
C(29)-N(1)-B(1)	120.0(3)
C(19)-N(2)-C(8)	114.3(3)
C(19)-N(2)-C(12)	115.8(3)
C(8)-N(2)-C(12)	129.3(3)
C(68)-N(3)-C(76)	117.8(3)
C(68)-N(3)-B(2)	123.7(3)
C(76)-N(3)-B(2)	118.4(3)
C(66)-N(4)-C(55)	113.9(3)
C(66)-N(4)-C(59)	115.3(3)
C(55)-N(4)-C(59)	130.2(3)
C(39)-B(1)-C(1)	109.9(3)
C(39)-B(1)-C(30)	118.8(3)
C(1)-B(1)-C(30)	107.4(3)
C(39)-B(1)-N(1)	106.1(3)
C(1)-B(1)-N(1)	105.1(3)
C(30)-B(1)-N(1)	108.7(3)
C(86)-B(2)-C(48)	109.7(3)
C(86)-B(2)-C(77)	118.3(3)
C(48)-B(2)-C(77)	110.3(3)
C(86)-B(2)-N(3)	104.2(3)
C(48)-B(2)-N(3)	105.5(3)
C(77)-B(2)-N(3)	107.9(3)
C(6)-C(1)-C(2)	115.3(3)
C(6)-C(1)-B(1)	120.5(3)
C(2)-C(1)-B(1)	123.8(3)
C(3)-C(2)-C(1)	123.8(4)
C(4)-C(3)-C(2)	119.2(4)
C(3)-C(4)-C(5)	119.5(4)
C(6)-C(5)-C(4)	122.1(4)
C(5)-C(6)-C(1)	120.0(3)
C(5)-C(6)-C(7)	119.1(3)
C(1)-C(6)-C(7)	120.8(3)
C(20)-C(7)-C(8)	107.0(3)
C(20)-C(7)-C(6)	126.8(3)
C(8)-C(7)-C(6)	126.1(3)
N(2)-C(8)-C(9)	114.6(4)
N(2)-C(8)-C(7)	104.8(3)
C(9)-C(8)-C(7)	140.2(4)
C(8)-C(9)-C(10)	118.4(4)
C(11)-C(10)-C(9)	123.4(4)
C(12)-C(11)-C(10)	120.7(4)
C(11)-C(12)-N(2)	113.4(4)
C(11)-C(12)-C(13)	143.0(4)
N(2)-C(12)-C(13)	103.4(3)
C(14)-C(13)-C(12)	131.7(4)
C(14)-C(13)-C(18)	119.9(4)
C(12)-C(13)-C(18)	108.4(4)
C(15)-C(14)-C(13)	119.9(4)
C(14)-C(15)-C(16)	120.0(4)
C(17)-C(16)-C(15)	122.2(4)
C(16)-C(17)-C(18)	118.9(4)
C(17)-C(18)-C(13)	119.0(4)
C(17)-C(18)-C(19)	133.5(4)
C(13)-C(18)-C(19)	107.5(3)
N(2)-C(19)-C(20)	104.0(3)
N(2)-C(19)-C(18)	104.9(3)
C(20)-C(19)-C(18)	150.2(4)
C(7)-C(20)-C(19)	109.9(3)
C(7)-C(20)-C(21)	127.4(3)
C(19)-C(20)-C(21)	122.6(3)
N(1)-C(21)-C(22)	121.5(4)
N(1)-C(21)-C(20)	118.4(3)
C(22)-C(21)-C(20)	120.0(3)
C(27)-C(22)-C(23)	118.1(3)
C(27)-C(22)-C(21)	120.2(4)
C(23)-C(22)-C(21)	121.7(4)
C(24)-C(23)-C(22)	120.5(4)
C(23)-C(24)-C(25)	121.7(4)
C(24)-C(25)-C(26)	119.3(4)

C(25)-C(26)-C(27)	120.5(4)	C(55)-C(54)-C(67)	106.8(3)
C(22)-C(27)-C(28)	116.6(4)	C(55)-C(54)-C(53)	125.0(3)
C(22)-C(27)-C(26)	119.9(4)	C(67)-C(54)-C(53)	127.8(3)
C(28)-C(27)-C(26)	123.5(4)	N(4)-C(55)-C(56)	113.2(3)
C(29)-C(28)-C(27)	120.2(4)	N(4)-C(55)-C(54)	105.6(3)
C(28)-C(29)-N(1)	125.4(4)	C(56)-C(55)-C(54)	140.9(4)
C(37)-C(30)-C(31)	113.7(3)	C(57)-C(56)-C(55)	119.4(4)
C(37)-C(30)-B(1)	123.1(3)	C(56)-C(57)-C(58)	123.6(4)
C(31)-C(30)-B(1)	122.5(3)	C(59)-C(58)-C(57)	118.8(4)
C(33)-C(31)-C(30)	122.9(3)	C(58)-C(59)-N(4)	114.6(4)
C(33)-C(31)-C(32)	113.1(3)	C(58)-C(59)-C(60)	140.9(4)
C(30)-C(31)-C(32)	124.0(3)	N(4)-C(59)-C(60)	104.5(3)
C(34)-C(33)-C(31)	122.0(4)	C(61)-C(60)-C(65)	120.8(4)
C(36)-C(34)-C(33)	115.7(4)	C(61)-C(60)-C(59)	131.4(4)
C(36)-C(34)-C(35)	122.5(3)	C(65)-C(60)-C(59)	107.8(3)
C(33)-C(34)-C(35)	121.8(4)	C(62)-C(61)-C(60)	119.3(4)
C(34)-C(36)-C(37)	124.2(3)	C(61)-C(62)-C(63)	120.1(4)
C(36)-C(37)-C(30)	121.1(3)	C(64)-C(63)-C(62)	122.3(4)
C(36)-C(37)-C(38)	115.0(3)	C(63)-C(64)-C(65)	118.6(4)
C(30)-C(37)-C(38)	124.0(4)	C(64)-C(65)-C(60)	118.9(3)
C(46)-C(39)-C(40)	115.2(3)	C(64)-C(65)-C(66)	133.5(4)
C(46)-C(39)-B(1)	124.5(4)	C(60)-C(65)-C(66)	107.6(3)
C(40)-C(39)-B(1)	120.2(3)	N(4)-C(66)-C(67)	104.5(3)
C(42)-C(40)-C(39)	120.9(4)	N(4)-C(66)-C(65)	104.8(3)
C(42)-C(40)-C(41)	115.7(4)	C(67)-C(66)-C(65)	150.0(3)
C(39)-C(40)-C(41)	123.3(4)	C(54)-C(67)-C(66)	109.2(3)
C(43)-C(42)-C(40)	122.6(4)	C(54)-C(67)-C(68)	125.8(3)
C(45)-C(43)-C(42)	116.9(4)	C(66)-C(67)-C(68)	125.0(3)
C(45)-C(43)-C(44)	121.4(5)	N(3)-C(68)-C(69)	121.2(3)
C(42)-C(43)-C(44)	121.6(5)	N(3)-C(68)-C(67)	119.6(3)
C(43)-C(45)-C(46)	122.6(4)	C(69)-C(68)-C(67)	119.1(3)
C(45)-C(46)-C(39)	121.1(4)	C(74)-C(69)-C(70)	118.1(3)
C(45)-C(46)-C(47)	115.1(4)	C(74)-C(69)-C(68)	119.6(3)
C(39)-C(46)-C(47)	123.7(4)	C(70)-C(69)-C(68)	122.2(3)
C(53)-C(48)-C(49)	115.5(3)	C(71)-C(70)-C(69)	120.5(4)
C(53)-C(48)-B(2)	122.3(3)	C(70)-C(71)-C(72)	121.0(4)
C(49)-C(48)-B(2)	122.0(3)	C(73)-C(72)-C(71)	119.6(4)
C(50)-C(49)-C(48)	123.7(3)	C(72)-C(73)-C(74)	120.9(4)
C(49)-C(50)-C(51)	118.7(4)	C(69)-C(74)-C(75)	117.3(4)
C(50)-C(51)-C(52)	120.0(4)	C(69)-C(74)-C(73)	119.8(4)
C(53)-C(52)-C(51)	121.1(4)	C(75)-C(74)-C(73)	122.9(4)
C(52)-C(53)-C(48)	121.0(3)	C(76)-C(75)-C(74)	120.8(4)
C(52)-C(53)-C(54)	118.4(3)	C(75)-C(76)-N(3)	123.0(3)
C(48)-C(53)-C(54)	120.5(3)	C(78)-C(77)-C(84)	113.1(3)

C(78)-C(77)-B(2)	124.3(3)	C(93)-C(86)-B(2)	120.3(3)
C(84)-C(77)-B(2)	122.4(3)	C(87)-C(86)-B(2)	124.2(3)
C(80)-C(78)-C(77)	121.0(4)	C(89)-C(87)-C(86)	121.0(4)
C(80)-C(78)-C(79)	115.2(3)	C(89)-C(87)-C(88)	114.7(4)
C(77)-C(78)-C(79)	123.8(3)	C(86)-C(87)-C(88)	124.1(3)
C(81)-C(80)-C(78)	125.1(4)	C(90)-C(89)-C(87)	121.7(4)
C(80)-C(81)-C(83)	115.5(4)	C(92)-C(90)-C(89)	117.0(4)
C(80)-C(81)-C(82)	123.6(4)	C(92)-C(90)-C(91)	123.3(4)
C(83)-C(81)-C(82)	120.9(4)	C(89)-C(90)-C(91)	119.7(4)
C(81)-C(83)-C(84)	121.7(4)	C(93)-C(92)-C(90)	123.6(4)
C(83)-C(84)-C(77)	123.5(4)	C(92)-C(93)-C(86)	120.7(4)
C(83)-C(84)-C(85)	113.2(3)	C(92)-C(93)-C(94)	116.8(4)
C(77)-C(84)-C(85)	123.2(3)	C(86)-C(93)-C(94)	122.4(3)
C(93)-C(86)-C(87)	115.4(3)		

Table S71. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for b3a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... \ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	45(2)	34(2)	34(2)	13(2)	-12(2)	-18(2)
N(2)	37(2)	34(2)	33(2)	6(2)	-5(1)	-4(2)
N(3)	33(2)	43(2)	26(2)	5(2)	-2(1)	-15(1)
N(4)	37(2)	30(2)	27(2)	2(2)	-6(1)	-5(1)
B(1)	37(3)	37(3)	32(3)	7(2)	-9(2)	-11(2)
B(2)	34(2)	30(2)	30(3)	2(2)	-3(2)	-13(2)
C(1)	36(2)	32(2)	33(2)	4(2)	-5(2)	-11(2)
C(2)	45(3)	41(2)	48(3)	3(2)	-10(2)	-16(2)
C(3)	62(3)	54(3)	62(3)	3(2)	-19(2)	-32(2)
C(4)	53(3)	57(3)	72(3)	10(3)	-30(2)	-24(2)
C(5)	43(3)	46(3)	47(3)	0(2)	-14(2)	-10(2)
C(6)	30(2)	39(2)	36(2)	-1(2)	-6(2)	-9(2)
C(7)	32(2)	32(2)	26(2)	3(2)	-7(2)	-6(2)
C(8)	33(2)	31(2)	37(3)	-6(2)	-8(2)	4(2)
C(9)	56(3)	47(3)	37(3)	-4(2)	-11(2)	-10(2)
C(10)	69(3)	51(3)	32(3)	7(2)	-21(2)	-11(2)
C(11)	63(3)	43(3)	38(3)	11(2)	-5(2)	-7(2)
C(12)	37(2)	30(2)	39(3)	7(2)	7(2)	-1(2)
C(13)	40(2)	38(2)	40(3)	5(2)	-2(2)	-8(2)

C(14)	55(3)	53(3)	60(3)	21(2)	-2(2)	-27(2)
C(15)	68(3)	69(3)	84(4)	24(3)	-20(3)	-41(3)
C(16)	62(3)	64(3)	71(3)	17(3)	-25(2)	-33(2)
C(17)	44(3)	44(3)	62(3)	11(2)	-11(2)	-21(2)
C(18)	38(2)	31(2)	40(3)	7(2)	-4(2)	-8(2)
C(19)	29(2)	40(2)	29(2)	2(2)	-6(2)	-6(2)
C(20)	35(2)	34(2)	27(2)	14(2)	-7(2)	-8(2)
C(21)	29(2)	40(2)	39(2)	13(2)	-13(2)	-13(2)
C(22)	48(2)	41(3)	31(2)	3(2)	-12(2)	-23(2)
C(23)	40(2)	42(3)	32(2)	3(2)	-5(2)	-13(2)
C(24)	49(3)	54(3)	49(3)	-6(2)	-7(2)	-21(2)
C(25)	77(3)	62(3)	45(3)	-4(3)	-4(2)	-33(3)
C(26)	99(4)	76(4)	28(3)	10(3)	-20(2)	-47(3)
C(27)	62(3)	56(3)	37(3)	10(2)	-16(2)	-32(2)
C(28)	86(3)	54(3)	45(3)	15(2)	-31(2)	-30(3)
C(29)	64(3)	47(3)	49(3)	23(2)	-22(2)	-23(2)
C(30)	35(2)	32(2)	42(2)	11(2)	-2(2)	-8(2)
C(31)	37(2)	31(2)	45(3)	9(2)	-7(2)	-7(2)
C(32)	43(2)	42(3)	53(3)	7(2)	0(2)	-9(2)
C(33)	35(2)	44(3)	50(3)	13(2)	-7(2)	-17(2)
C(34)	36(2)	33(2)	54(3)	9(2)	-18(2)	-7(2)
C(35)	59(3)	36(3)	64(3)	13(2)	-13(2)	-9(2)
C(36)	39(2)	38(3)	53(3)	7(2)	-4(2)	-2(2)
C(37)	34(2)	43(3)	48(3)	16(2)	-9(2)	-10(2)
C(38)	36(3)	51(3)	83(4)	19(2)	7(2)	3(2)
C(39)	37(2)	30(2)	47(3)	10(2)	-14(2)	-6(2)
C(40)	31(2)	39(2)	55(3)	6(2)	-4(2)	-1(2)
C(41)	58(3)	71(3)	47(3)	-8(2)	-3(2)	-14(2)
C(42)	43(3)	62(3)	46(3)	14(2)	3(2)	-9(2)
C(43)	39(3)	58(3)	67(4)	21(3)	12(2)	-8(2)
C(44)	62(3)	91(4)	106(4)	44(3)	28(3)	-17(3)
C(45)	31(2)	51(3)	83(4)	12(3)	6(2)	-10(2)
C(46)	43(3)	41(3)	50(3)	8(2)	-7(2)	-9(2)
C(47)	50(3)	83(4)	81(4)	6(3)	-13(2)	-32(2)
C(48)	35(2)	30(2)	33(2)	6(2)	-9(2)	-15(2)
C(49)	40(2)	51(3)	37(2)	6(2)	-7(2)	-19(2)
C(50)	45(3)	61(3)	59(3)	-1(2)	-6(2)	-36(2)
C(51)	45(3)	67(3)	56(3)	6(3)	-4(2)	-26(2)

C(52)	33(2)	49(3)	48(3)	7(2)	0(2)	-19(2)
C(53)	36(2)	34(2)	33(2)	11(2)	-7(2)	-14(2)
C(54)	24(2)	33(2)	27(2)	3(2)	-1(2)	-5(2)
C(55)	21(2)	28(2)	37(2)	6(2)	-2(2)	-2(2)
C(56)	36(2)	42(2)	38(3)	12(2)	4(2)	-5(2)
C(57)	50(3)	61(3)	35(3)	17(2)	-3(2)	-15(2)
C(58)	45(3)	58(3)	36(3)	10(2)	-12(2)	-14(2)
C(59)	38(2)	36(2)	36(2)	3(2)	-9(2)	1(2)
C(60)	33(2)	42(2)	43(3)	-6(2)	-10(2)	-3(2)
C(61)	45(3)	61(3)	47(3)	-3(2)	-11(2)	-6(2)
C(62)	55(3)	93(4)	62(3)	-23(3)	-12(2)	-32(3)
C(63)	53(3)	68(3)	64(3)	-11(3)	-2(2)	-33(2)
C(64)	44(3)	50(3)	48(3)	-4(2)	-3(2)	-20(2)
C(65)	31(2)	33(2)	31(2)	-1(2)	-4(2)	-3(2)
C(66)	35(2)	31(2)	32(2)	7(2)	-2(2)	-5(2)
C(67)	24(2)	33(2)	28(2)	4(2)	-3(2)	-5(2)
C(68)	29(2)	33(2)	35(2)	2(2)	-6(2)	-12(2)
C(69)	32(2)	30(2)	35(2)	8(2)	-8(2)	-9(2)
C(70)	33(2)	37(2)	39(2)	8(2)	-4(2)	-5(2)
C(71)	51(3)	35(3)	57(3)	12(2)	-4(2)	-2(2)
C(72)	85(3)	49(3)	58(3)	19(3)	2(3)	-10(3)
C(73)	80(3)	58(3)	38(3)	20(2)	0(2)	-21(3)
C(74)	54(3)	46(3)	24(2)	11(2)	-6(2)	-17(2)
C(75)	65(3)	53(3)	25(2)	13(2)	-2(2)	-31(2)
C(76)	43(2)	51(3)	33(2)	-1(2)	2(2)	-20(2)
C(77)	32(2)	44(2)	36(2)	5(2)	-4(2)	-22(2)
C(78)	32(2)	46(2)	34(2)	0(2)	-1(2)	-8(2)
C(79)	31(2)	57(3)	54(3)	-11(2)	-3(2)	4(2)
C(80)	45(2)	51(3)	43(3)	-11(2)	-1(2)	-9(2)
C(81)	56(3)	54(3)	44(3)	-13(2)	4(2)	-20(2)
C(82)	98(4)	84(4)	58(3)	-34(3)	-4(3)	-11(3)
C(83)	50(3)	58(3)	38(3)	-4(2)	-7(2)	-21(2)
C(84)	44(2)	45(2)	30(2)	0(2)	0(2)	-21(2)
C(85)	52(3)	54(3)	35(2)	5(2)	-10(2)	-19(2)
C(86)	28(2)	28(2)	31(2)	-3(2)	-2(2)	-7(2)
C(87)	28(2)	38(2)	46(3)	-3(2)	-10(2)	-6(2)
C(88)	36(2)	50(3)	71(3)	8(2)	-12(2)	-21(2)
C(89)	36(2)	50(3)	54(3)	-12(2)	-9(2)	-14(2)

C(90)	43(3)	65(3)	36(3)	-5(2)	-12(2)	-12(2)
C(91)	79(3)	125(4)	52(3)	11(3)	-28(3)	-45(3)
C(92)	42(2)	59(3)	31(2)	7(2)	-12(2)	-13(2)
C(93)	28(2)	33(2)	35(2)	-3(2)	-1(2)	-7(2)
C(94)	56(3)	48(3)	45(3)	14(2)	-9(2)	-12(2)

Table S72. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for b3a.

	x	y	z	U(eq)
H(2)	5465	3721	7179	53
H(3)	3937	3907	6744	66
H(4)	3099	5229	6257	68
H(5)	3835	6345	6162	54
H(9)	5104	6609	4940	56
H(10)	5718	7545	4076	61
H(11)	6706	8353	4399	61
H(14)	7923	9089	5320	67
H(15)	8704	9415	6269	83
H(16)	8472	8831	7492	74
H(17)	7489	7891	7793	58
H(23)	5221	8113	7909	46
H(24)	4922	9035	8920	59
H(25)	5287	8518	10118	71
H(26)	6078	7050	10289	75
H(28)	6852	5552	9704	69
H(29)	7086	4667	8702	61
H(32A)	5314	4667	8445	72
H(32B)	5557	4086	9188	72
H(32C)	4886	3856	8629	72
H(33)	6180	2463	8792	51
H(35A)	7696	740	7739	82
H(35B)	7060	979	8580	82
H(35C)	8274	817	8427	82
H(36)	8752	1879	7266	55
H(38A)	8662	3463	6227	95

H(38B)	9472	2830	6704	95
H(38C)	9023	3834	6910	95
H(41A)	6174	4597	5490	91
H(41B)	6882	3830	5939	91
H(41C)	7234	3991	5049	91
H(42)	7909	5121	4623	65
H(44A)	9484	5716	4183	143
H(44B)	9517	6457	4724	143
H(44C)	8553	6591	4297	143
H(45)	9117	6203	6033	70
H(47A)	9234	5626	7263	103
H(47B)	8460	5131	7694	103
H(47C)	8079	6158	7599	103
H(49)	6580	8646	1165	50
H(50)	5028	8466	1741	61
H(51)	4016	9406	2724	66
H(52)	4652	10416	3193	52
H(56)	5600	10049	4338	50
H(57)	6018	10376	5470	60
H(58)	7061	11253	5514	56
H(61)	8476	12328	5001	63
H(62)	9500	13090	4296	80
H(63)	9572	13233	2976	71
H(64)	8646	12623	2325	56
H(70)	6369	12905	2370	46
H(71)	6194	14276	1872	62
H(72)	6737	14485	570	82
H(73)	7520	13305	-222	72
H(75)	8208	11696	-378	55
H(76)	8362	10345	119	50
H(79A)	10529	7626	1076	77
H(79B)	9561	7910	1744	77
H(79C)	10100	8606	1358	77
H(80)	10160	7332	4	57
H(82A)	9397	7515	-1701	125
H(82B)	8842	6874	-1224	125
H(82C)	10010	6781	-1171	125
H(83)	7707	8579	-917	57

H(85A)	6870	10084	-439	69
H(85B)	6575	10143	473	69
H(85C)	6219	9497	15	69
H(88A)	9659	10169	1104	76
H(88B)	10302	10453	1653	76
H(88C)	9160	11039	1588	76
H(89)	10087	10220	2933	55
H(91A)	10629	9275	4078	121
H(91B)	9778	8892	4565	121
H(91C)	9578	9913	4501	121
H(92)	8662	8515	3851	53
H(94A)	7799	8101	2256	76
H(94B)	7012	8534	2997	76
H(94C)	8022	7760	3092	76

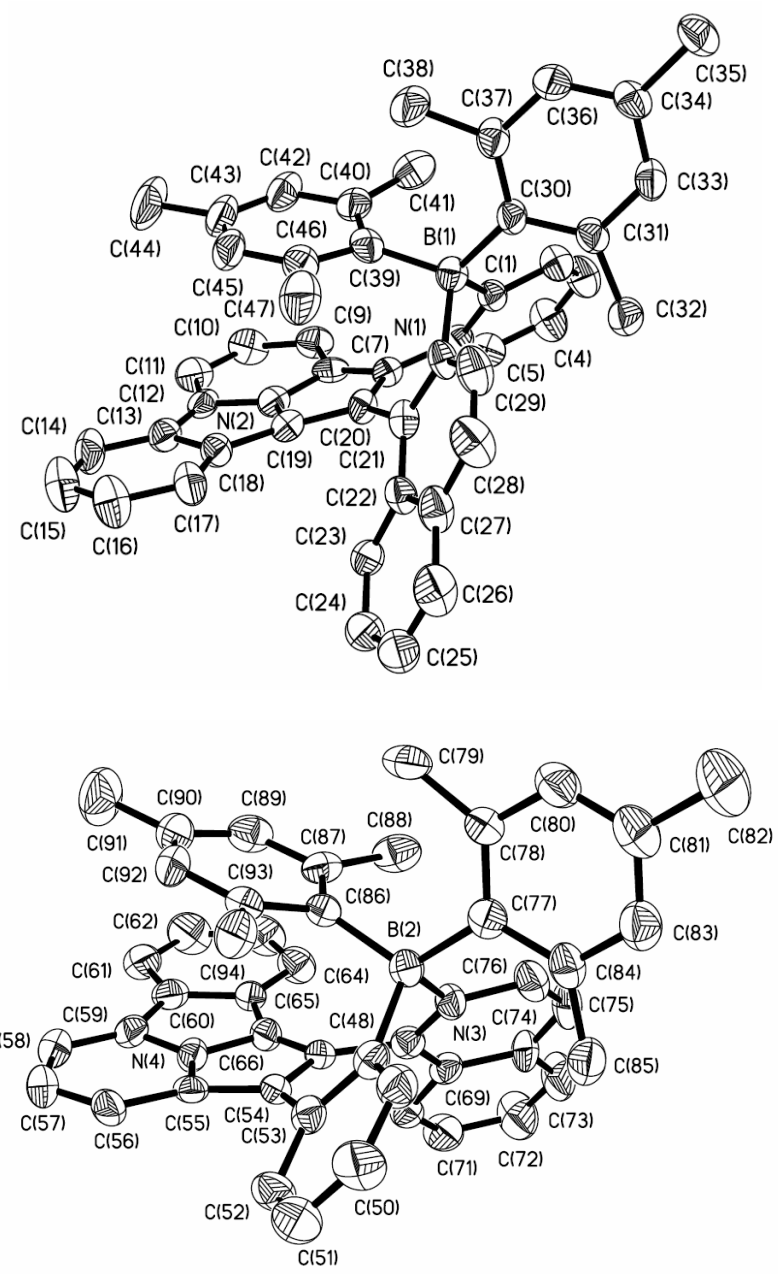


Figure S105. A diagram showing the two independent molecules in the crystal lattice of **B3a** with labeling schemes and 35% thermal ellipsoids. H atoms are omitted for clarity.

Table S73. Crystal data and structure refinement for B3b.

Identification code	B3b	
Empirical formula	C95 H81 B2 Cl2 N4	
Formula weight	1371.15	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 22.13(4) Å	α= 90°.
	b = 17.76(3) Å	β= 106.15(6)°.
	c = 19.24(3) Å	γ = 90°.
Volume	7262(23) $Å^3$	
Z	4	
Density (calculated)	1.254 Mg/m^3	
Absorption coefficient	0.143 mm^{-1}	
F(000)	2892	
Crystal size	0.160 x 0.145 x 0.120 mm^3	
Theta range for data collection	2.545 to 27.232°.	
Index ranges	-28<=h<=28, -22<=k<=22, -24<=l<=24	
Reflections collected	41480	
Independent reflections	15059 [R(int) = 0.1775]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.983 and 0.978	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15059 / 2 / 942	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.1236, wR2 = 0.3025	
R indices (all data)	R1 = 0.2104, wR2 = 0.3516	
Absolute structure parameter	0.1(3)	
Extinction coefficient	0.0070(11)	
Largest diff. peak and hole	0.694 and -0.539 $e.Å^{-3}$	

Table S74. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for B3b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	2898(6)	4419(7)	4174(7)	29(3)
B(2)	8328(5)	4366(7)	5952(7)	25(3)
N(1)	3450(4)	3910(5)	4786(5)	29(2)
N(2)	1790(4)	2927(5)	5442(5)	31(2)
N(3)	8599(4)	4852(5)	5324(4)	25(2)
N(4)	6636(5)	5813(6)	4542(5)	36(2)
C(1)	2505(5)	3803(7)	3558(6)	32(3)
C(2)	2438(6)	3891(7)	2821(6)	39(3)
C(3)	2066(6)	3418(8)	2290(7)	46(3)
C(4)	1758(6)	2821(8)	2493(7)	47(3)
C(5)	1811(5)	2694(6)	3208(6)	34(3)
C(6)	2175(5)	3175(7)	3739(6)	31(3)
C(7)	2137(5)	3062(6)	4487(6)	29(2)
C(8)	1601(5)	2917(6)	4703(6)	29(2)
C(9)	922(6)	2921(6)	4505(7)	36(3)
C(10)	463(6)	2931(8)	3856(7)	45(3)
C(11)	-162(7)	2933(9)	3887(10)	63(4)
C(12)	-321(6)	2896(8)	4515(9)	57(4)
C(13)	125(6)	2864(8)	5185(8)	49(4)
C(14)	748(6)	2880(6)	5177(7)	37(3)
C(15)	1314(6)	2936(7)	5764(7)	36(3)
C(16)	1505(6)	3023(7)	6509(7)	42(3)
C(17)	2143(6)	3123(7)	6850(7)	42(3)
C(18)	2600(6)	3176(7)	6483(6)	35(3)
C(19)	2412(5)	3056(6)	5748(6)	27(2)
C(20)	2658(5)	3158(6)	5115(5)	26(2)
C(21)	3304(5)	3303(6)	5169(5)	24(2)
C(22)	4063(6)	4119(8)	4930(6)	41(3)
C(23)	4535(6)	3782(8)	5416(7)	42(3)
C(24)	4419(6)	3132(7)	5779(6)	38(3)
C(25)	4915(6)	2699(8)	6272(6)	43(3)
C(26)	4768(6)	2074(8)	6593(7)	49(3)
C(27)	4146(6)	1820(7)	6438(6)	37(3)

C(28)	3666(6)	2218(7)	5966(6)	34(3)
C(29)	3797(6)	2880(7)	5643(6)	33(3)
C(30)	3281(6)	4999(7)	3774(6)	35(3)
C(31)	3216(5)	5811(7)	3748(6)	35(3)
C(32)	3520(6)	6243(7)	3358(6)	40(3)
C(33)	3896(6)	5961(7)	2956(6)	39(3)
C(34)	3988(6)	5177(8)	2983(6)	43(3)
C(35)	3696(6)	4711(7)	3367(6)	34(3)
C(36)	3857(6)	3878(7)	3336(7)	41(3)
C(37)	2812(8)	6251(9)	4129(8)	59(4)
C(38)	2433(5)	4749(6)	4638(6)	33(3)
C(39)	1770(6)	4813(7)	4320(6)	36(3)
C(40)	1363(6)	4875(7)	4769(8)	48(3)
C(41)	1573(6)	4965(8)	5513(8)	48(3)
C(42)	2215(7)	5004(7)	5811(7)	47(3)
C(43)	2626(5)	4911(7)	5373(6)	32(3)
C(44)	3313(6)	5049(8)	5768(7)	45(3)
C(45)	1457(7)	4816(8)	3518(8)	57(4)
C(46)	4245(7)	6463(9)	2554(8)	62(4)
C(47)	1126(8)	4988(9)	5971(10)	66(5)
C(48)	8236(5)	5036(6)	6518(6)	29(2)
C(49)	8526(6)	5022(8)	7251(6)	40(3)
C(50)	8415(6)	5553(7)	7742(6)	42(3)
C(51)	8005(7)	6130(8)	7499(7)	46(3)
C(52)	7673(6)	6161(7)	6778(5)	33(3)
C(53)	7789(5)	5635(6)	6290(5)	28(2)
C(54)	7426(5)	5705(6)	5544(5)	27(2)
C(55)	6772(5)	5836(7)	5289(6)	31(2)
C(56)	6165(5)	5860(6)	5432(7)	34(3)
C(57)	5994(6)	5860(7)	6081(7)	41(3)
C(58)	5364(7)	5866(9)	6035(8)	60(4)
C(59)	4906(7)	5874(9)	5381(9)	58(4)
C(60)	5061(6)	5876(9)	4736(9)	56(4)
C(61)	5708(5)	5861(6)	4779(6)	35(3)
C(62)	6007(6)	5793(7)	4175(8)	44(3)
C(63)	5868(6)	5689(7)	3459(7)	42(3)
C(64)	6352(6)	5573(9)	3148(7)	52(4)
C(65)	6987(6)	5561(8)	3536(6)	41(3)

C(66)	7144(5)	5675(6)	4296(6)	29(2)
C(67)	7645(5)	5603(6)	4916(6)	27(2)
C(68)	8296(5)	5418(6)	4918(5)	26(2)
C(69)	8575(5)	5848(7)	4451(5)	30(2)
C(70)	8282(6)	6519(7)	4089(6)	35(3)
C(71)	8562(7)	6877(8)	3633(6)	47(3)
C(72)	9126(6)	6636(8)	3521(7)	44(3)
C(73)	9420(7)	6005(8)	3883(7)	47(3)
C(74)	9148(5)	5605(6)	4346(6)	31(3)
C(75)	9418(5)	4962(8)	4717(6)	38(3)
C(76)	9148(5)	4605(7)	5198(6)	30(2)
C(77)	8879(6)	3744(7)	6367(6)	35(3)
C(78)	9483(6)	3991(7)	6736(5)	33(3)
C(79)	9941(7)	3467(8)	7094(7)	45(3)
C(80)	9829(8)	2698(8)	7091(7)	51(4)
C(81)	9239(7)	2455(8)	6713(7)	47(3)
C(82)	8756(6)	2957(7)	6363(7)	42(3)
C(83)	8142(7)	2553(8)	6005(8)	55(4)
C(84)	10334(9)	2156(11)	7478(8)	77(5)
C(85)	9723(6)	4789(7)	6794(6)	40(3)
C(86)	7619(5)	4053(6)	5524(5)	29(2)
C(87)	7126(5)	4004(6)	5869(6)	32(3)
C(88)	6512(6)	3929(7)	5481(7)	43(3)
C(89)	6325(6)	3850(7)	4737(7)	41(3)
C(90)	6797(6)	3786(7)	4406(7)	43(3)
C(91)	7426(5)	3842(7)	4766(6)	34(3)
C(92)	7894(6)	3704(7)	4349(7)	42(3)
C(93)	7262(7)	4029(8)	6701(7)	49(4)
C(94)	5636(7)	3810(10)	4314(9)	60(4)
C(95)	6507(7)	1872(10)	4941(8)	62(4)
Cl(1)	6162(3)	1799(3)	4008(3)	91(2)
Cl(2)	5929(3)	1951(3)	5406(3)	91(2)

Table S75. Bond lengths [Å] and angles [°] for B3b.

B(1)-C(38)	1.646(16)	B(1)-N(1)	1.700(15)
B(1)-C(30)	1.655(17)	B(2)-C(86)	1.652(16)
B(1)-C(1)	1.669(18)	B(2)-C(48)	1.662(16)

B(2)-C(77)	1.673(17)	C(24)-C(29)	1.401(17)
B(2)-N(3)	1.724(14)	C(24)-C(25)	1.454(18)
N(1)-C(22)	1.358(15)	C(25)-C(26)	1.35(2)
N(1)-C(21)	1.394(13)	C(26)-C(27)	1.398(19)
N(2)-C(19)	1.359(14)	C(27)-C(28)	1.385(16)
N(2)-C(15)	1.362(14)	C(28)-C(29)	1.396(16)
N(2)-C(8)	1.366(14)	C(30)-C(31)	1.448(17)
N(3)-C(68)	1.333(14)	C(30)-C(35)	1.455(16)
N(3)-C(76)	1.375(13)	C(31)-C(32)	1.374(16)
N(4)-C(66)	1.358(14)	C(31)-C(37)	1.521(18)
N(4)-C(62)	1.375(16)	C(32)-C(33)	1.378(18)
N(4)-C(55)	1.383(15)	C(33)-C(34)	1.406(19)
C(1)-C(2)	1.392(15)	C(33)-C(46)	1.524(17)
C(1)-C(6)	1.428(16)	C(34)-C(35)	1.383(17)
C(2)-C(3)	1.400(18)	C(35)-C(36)	1.526(18)
C(3)-C(4)	1.37(2)	C(38)-C(43)	1.389(16)
C(4)-C(5)	1.366(18)	C(38)-C(39)	1.429(16)
C(5)-C(6)	1.401(15)	C(39)-C(40)	1.415(17)
C(6)-C(7)	1.478(15)	C(39)-C(45)	1.505(18)
C(7)-C(8)	1.387(15)	C(40)-C(41)	1.39(2)
C(7)-C(20)	1.429(16)	C(41)-C(42)	1.378(19)
C(8)-C(9)	1.442(16)	C(41)-C(47)	1.498(19)
C(9)-C(10)	1.373(18)	C(42)-C(43)	1.409(16)
C(9)-C(14)	1.451(18)	C(43)-C(44)	1.519(17)
C(10)-C(11)	1.40(2)	C(48)-C(49)	1.378(16)
C(11)-C(12)	1.35(2)	C(48)-C(53)	1.435(16)
C(12)-C(13)	1.39(2)	C(49)-C(50)	1.405(17)
C(13)-C(14)	1.384(17)	C(50)-C(51)	1.362(18)
C(14)-C(15)	1.439(18)	C(51)-C(52)	1.379(17)
C(15)-C(16)	1.385(18)	C(52)-C(53)	1.398(15)
C(16)-C(17)	1.394(19)	C(53)-C(54)	1.443(15)
C(17)-C(18)	1.389(17)	C(54)-C(55)	1.412(16)
C(18)-C(19)	1.375(16)	C(54)-C(67)	1.433(14)
C(19)-C(20)	1.475(14)	C(55)-C(56)	1.444(16)
C(20)-C(21)	1.429(15)	C(56)-C(61)	1.376(17)
C(21)-C(29)	1.425(16)	C(56)-C(57)	1.403(16)
C(22)-C(23)	1.335(18)	C(57)-C(58)	1.37(2)
C(23)-C(24)	1.409(18)	C(58)-C(59)	1.38(2)

C(59)-C(60)	1.38(2)		
C(60)-C(61)	1.412(17)	C(38)-B(1)-C(30)	120.6(10)
C(61)-C(62)	1.493(18)	C(38)-B(1)-C(1)	109.7(9)
C(62)-C(63)	1.339(18)	C(30)-B(1)-C(1)	108.1(8)
C(63)-C(64)	1.380(19)	C(38)-B(1)-N(1)	104.6(8)
C(64)-C(65)	1.397(18)	C(30)-B(1)-N(1)	106.9(9)
C(65)-C(66)	1.420(16)	C(1)-B(1)-N(1)	106.0(9)
C(66)-C(67)	1.390(16)	C(86)-B(2)-C(48)	107.1(8)
C(67)-C(68)	1.476(15)	C(86)-B(2)-C(77)	118.7(9)
C(68)-C(69)	1.444(14)	C(48)-B(2)-C(77)	111.5(9)
C(69)-C(74)	1.406(16)	C(86)-B(2)-N(3)	106.6(8)
C(69)-C(70)	1.440(16)	C(48)-B(2)-N(3)	103.3(8)
C(70)-C(71)	1.365(16)	C(77)-B(2)-N(3)	108.4(8)
C(71)-C(72)	1.390(19)	C(22)-N(1)-C(21)	117.9(9)
C(72)-C(73)	1.385(19)	C(22)-N(1)-B(1)	118.7(9)
C(73)-C(74)	1.399(16)	C(21)-N(1)-B(1)	123.3(8)
C(74)-C(75)	1.391(17)	C(19)-N(2)-C(15)	128.2(10)
C(75)-C(76)	1.386(15)	C(19)-N(2)-C(8)	115.7(8)
C(77)-C(78)	1.398(18)	C(15)-N(2)-C(8)	115.0(9)
C(77)-C(82)	1.423(18)	C(68)-N(3)-C(76)	117.5(8)
C(78)-C(79)	1.407(17)	C(68)-N(3)-B(2)	124.9(8)
C(78)-C(85)	1.507(18)	C(76)-N(3)-B(2)	117.4(8)
C(79)-C(80)	1.39(2)	C(66)-N(4)-C(62)	129.3(10)
C(80)-C(81)	1.38(2)	C(66)-N(4)-C(55)	113.9(9)
C(80)-C(84)	1.507(19)	C(62)-N(4)-C(55)	115.5(10)
C(81)-C(82)	1.411(19)	C(2)-C(1)-C(6)	114.9(10)
C(82)-C(83)	1.52(2)	C(2)-C(1)-B(1)	122.4(10)
C(86)-C(87)	1.430(15)	C(6)-C(1)-B(1)	122.6(9)
C(86)-C(91)	1.450(15)	C(1)-C(2)-C(3)	123.3(12)
C(87)-C(88)	1.362(18)	C(4)-C(3)-C(2)	119.6(11)
C(87)-C(93)	1.546(16)	C(5)-C(4)-C(3)	120.1(11)
C(88)-C(89)	1.382(18)	C(4)-C(5)-C(6)	120.3(11)
C(89)-C(90)	1.372(17)	C(5)-C(6)-C(1)	121.8(10)
C(89)-C(94)	1.518(19)	C(5)-C(6)-C(7)	116.8(10)
C(90)-C(91)	1.376(17)	C(1)-C(6)-C(7)	121.0(10)
C(91)-C(92)	1.496(16)	C(8)-C(7)-C(20)	108.9(9)
C(95)-Cl(1)	1.748(17)	C(8)-C(7)-C(6)	127.0(11)
C(95)-Cl(2)	1.761(17)	C(20)-C(7)-C(6)	123.9(10)

N(2)-C(8)-C(7)	105.6(9)	C(28)-C(29)-C(21)	120.7(10)
N(2)-C(8)-C(9)	105.7(9)	C(24)-C(29)-C(21)	119.2(11)
C(7)-C(8)-C(9)	146.6(11)	C(31)-C(30)-C(35)	113.8(10)
C(10)-C(9)-C(8)	133.9(11)	C(31)-C(30)-B(1)	125.2(10)
C(10)-C(9)-C(14)	119.9(11)	C(35)-C(30)-B(1)	120.8(10)
C(8)-C(9)-C(14)	106.3(11)	C(32)-C(31)-C(30)	121.0(11)
C(9)-C(10)-C(11)	116.8(13)	C(32)-C(31)-C(37)	114.8(12)
C(12)-C(11)-C(10)	122.9(15)	C(30)-C(31)-C(37)	124.1(11)
C(11)-C(12)-C(13)	122.6(12)	C(31)-C(32)-C(33)	124.6(12)
C(14)-C(13)-C(12)	116.1(13)	C(32)-C(33)-C(34)	116.3(10)
C(13)-C(14)-C(15)	130.2(12)	C(32)-C(33)-C(46)	122.9(13)
C(13)-C(14)-C(9)	121.6(12)	C(34)-C(33)-C(46)	120.6(12)
C(15)-C(14)-C(9)	107.9(10)	C(35)-C(34)-C(33)	121.8(12)
N(2)-C(15)-C(16)	114.9(11)	C(34)-C(35)-C(30)	122.4(11)
N(2)-C(15)-C(14)	104.8(10)	C(34)-C(35)-C(36)	114.2(11)
C(16)-C(15)-C(14)	140.2(11)	C(30)-C(35)-C(36)	123.4(10)
C(15)-C(16)-C(17)	118.6(10)	C(43)-C(38)-C(39)	114.0(10)
C(18)-C(17)-C(16)	123.7(11)	C(43)-C(38)-B(1)	124.4(10)
C(19)-C(18)-C(17)	117.3(11)	C(39)-C(38)-B(1)	121.3(10)
N(2)-C(19)-C(18)	116.9(9)	C(40)-C(39)-C(38)	119.8(10)
N(2)-C(19)-C(20)	103.0(9)	C(40)-C(39)-C(45)	115.8(11)
C(18)-C(19)-C(20)	139.0(10)	C(38)-C(39)-C(45)	124.4(11)
C(21)-C(20)-C(7)	129.6(9)	C(41)-C(40)-C(39)	123.5(12)
C(21)-C(20)-C(19)	123.6(9)	C(42)-C(41)-C(40)	116.5(11)
C(7)-C(20)-C(19)	106.8(9)	C(42)-C(41)-C(47)	121.8(13)
N(1)-C(21)-C(29)	119.8(9)	C(40)-C(41)-C(47)	121.6(13)
N(1)-C(21)-C(20)	118.4(9)	C(41)-C(42)-C(43)	120.5(12)
C(29)-C(21)-C(20)	121.6(10)	C(38)-C(43)-C(42)	124.5(11)
C(23)-C(22)-N(1)	124.2(12)	C(38)-C(43)-C(44)	121.6(10)
C(22)-C(23)-C(24)	120.1(11)	C(42)-C(43)-C(44)	113.8(10)
C(29)-C(24)-C(23)	118.2(11)	C(49)-C(48)-C(53)	114.3(10)
C(29)-C(24)-C(25)	118.5(12)	C(49)-C(48)-B(2)	123.4(10)
C(23)-C(24)-C(25)	123.2(11)	C(53)-C(48)-B(2)	122.0(9)
C(26)-C(25)-C(24)	119.8(12)	C(48)-C(49)-C(50)	123.9(11)
C(25)-C(26)-C(27)	121.0(12)	C(51)-C(50)-C(49)	119.9(10)
C(28)-C(27)-C(26)	120.3(12)	C(50)-C(51)-C(52)	119.6(11)
C(27)-C(28)-C(29)	120.3(11)	C(51)-C(52)-C(53)	120.2(11)
C(28)-C(29)-C(24)	120.0(11)	C(52)-C(53)-C(48)	122.0(10)

C(52)-C(53)-C(54)	117.0(10)	C(73)-C(72)-C(71)	119.2(11)
C(48)-C(53)-C(54)	120.9(9)	C(72)-C(73)-C(74)	120.4(12)
C(55)-C(54)-C(67)	106.4(9)	C(75)-C(74)-C(73)	122.9(11)
C(55)-C(54)-C(53)	126.4(9)	C(75)-C(74)-C(69)	117.1(9)
C(67)-C(54)-C(53)	127.0(9)	C(73)-C(74)-C(69)	120.0(11)
N(4)-C(55)-C(54)	105.2(9)	C(76)-C(75)-C(74)	120.9(10)
N(4)-C(55)-C(56)	104.7(10)	N(3)-C(76)-C(75)	122.6(10)
C(54)-C(55)-C(56)	148.8(10)	C(78)-C(77)-C(82)	117.7(11)
C(61)-C(56)-C(57)	120.1(11)	C(78)-C(77)-B(2)	120.2(10)
C(61)-C(56)-C(55)	108.2(10)	C(82)-C(77)-B(2)	122.1(11)
C(57)-C(56)-C(55)	131.7(12)	C(77)-C(78)-C(79)	119.9(12)
C(58)-C(57)-C(56)	117.5(13)	C(77)-C(78)-C(85)	126.9(10)
C(57)-C(58)-C(59)	122.4(13)	C(79)-C(78)-C(85)	113.2(12)
C(60)-C(59)-C(58)	121.3(13)	C(80)-C(79)-C(78)	123.0(14)
C(59)-C(60)-C(61)	116.7(14)	C(81)-C(80)-C(79)	117.0(12)
C(56)-C(61)-C(60)	122.0(12)	C(81)-C(80)-C(84)	121.8(15)
C(56)-C(61)-C(62)	109.7(10)	C(79)-C(80)-C(84)	121.3(16)
C(60)-C(61)-C(62)	128.2(12)	C(80)-C(81)-C(82)	122.4(13)
C(63)-C(62)-N(4)	116.3(11)	C(81)-C(82)-C(77)	120.0(12)
C(63)-C(62)-C(61)	141.9(11)	C(81)-C(82)-C(83)	112.4(12)
N(4)-C(62)-C(61)	101.7(11)	C(77)-C(82)-C(83)	127.7(12)
C(62)-C(63)-C(64)	118.9(12)	C(87)-C(86)-C(91)	113.7(10)
C(63)-C(64)-C(65)	123.9(12)	C(87)-C(86)-B(2)	122.1(9)
C(64)-C(65)-C(66)	118.0(11)	C(91)-C(86)-B(2)	124.2(9)
N(4)-C(66)-C(67)	105.0(9)	C(88)-C(87)-C(86)	121.7(10)
N(4)-C(66)-C(65)	113.4(10)	C(88)-C(87)-C(93)	116.6(10)
C(67)-C(66)-C(65)	141.0(10)	C(86)-C(87)-C(93)	121.7(10)
C(66)-C(67)-C(54)	109.5(9)	C(87)-C(88)-C(89)	122.9(11)
C(66)-C(67)-C(68)	124.6(9)	C(90)-C(89)-C(88)	116.2(11)
C(54)-C(67)-C(68)	125.8(10)	C(90)-C(89)-C(94)	121.9(12)
N(3)-C(68)-C(69)	122.0(9)	C(88)-C(89)-C(94)	121.8(12)
N(3)-C(68)-C(67)	120.1(9)	C(89)-C(90)-C(91)	123.7(11)
C(69)-C(68)-C(67)	117.8(9)	C(90)-C(91)-C(86)	119.9(10)
C(74)-C(69)-C(70)	119.3(10)	C(90)-C(91)-C(92)	118.2(10)
C(74)-C(69)-C(68)	119.1(10)	C(86)-C(91)-C(92)	121.9(10)
C(70)-C(69)-C(68)	121.7(10)	Cl(1)-C(95)-Cl(2)	110.8(9)
C(71)-C(70)-C(69)	118.1(12)		
C(70)-C(71)-C(72)	123.0(13)		

Table S76. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for B3b. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	33(7)	23(7)	35(7)	9(5)	15(6)	2(5)
B(2)	21(6)	20(6)	40(7)	4(5)	18(5)	-4(5)
N(1)	24(5)	31(5)	33(5)	4(4)	10(4)	3(4)
N(2)	28(5)	28(5)	40(6)	-1(4)	14(4)	-4(4)
N(3)	33(5)	18(5)	26(4)	-1(3)	11(4)	-4(4)
N(4)	29(5)	40(6)	39(5)	4(4)	9(5)	1(4)
C(1)	28(6)	46(7)	27(5)	-6(5)	12(5)	-4(5)
C(2)	44(7)	48(8)	26(6)	6(5)	11(5)	3(6)
C(3)	49(8)	56(9)	32(6)	-10(6)	11(6)	-8(7)
C(4)	39(7)	48(9)	46(8)	-22(6)	0(6)	-2(6)
C(5)	36(6)	27(6)	36(6)	-11(5)	5(5)	-9(5)
C(6)	26(6)	39(7)	25(5)	2(5)	2(5)	2(5)
C(7)	26(6)	30(6)	31(6)	7(4)	9(5)	2(5)
C(8)	27(6)	23(6)	39(7)	-4(4)	8(5)	-7(5)
C(9)	30(6)	24(6)	57(8)	-5(5)	18(6)	-2(5)
C(10)	27(6)	52(9)	50(8)	-8(6)	1(6)	5(6)
C(11)	33(8)	66(10)	83(11)	-27(9)	4(8)	-7(7)
C(12)	16(6)	59(9)	96(12)	-35(8)	18(7)	3(6)
C(13)	28(7)	48(8)	75(10)	-13(7)	20(7)	1(6)
C(14)	34(6)	14(6)	64(8)	-11(5)	18(6)	-3(5)
C(15)	37(7)	27(7)	47(7)	-1(5)	17(6)	-4(5)
C(16)	43(8)	40(8)	58(8)	-5(6)	41(7)	2(6)
C(17)	54(8)	46(8)	34(6)	-3(5)	23(6)	4(6)
C(18)	39(7)	32(7)	33(6)	-1(5)	8(5)	1(5)
C(19)	20(5)	33(6)	30(6)	1(4)	8(5)	-5(4)
C(20)	22(5)	35(6)	20(5)	-6(4)	6(4)	-1(5)
C(21)	24(5)	23(6)	28(5)	-5(4)	10(5)	2(4)
C(22)	32(7)	62(9)	31(6)	7(6)	12(5)	-6(6)
C(23)	24(6)	55(9)	52(8)	3(6)	16(6)	0(6)
C(24)	37(7)	49(8)	33(6)	-7(5)	18(6)	4(6)
C(25)	27(6)	62(9)	38(7)	4(6)	3(5)	11(6)
C(26)	43(8)	52(9)	46(8)	-2(6)	3(6)	22(7)
C(27)	47(8)	30(7)	31(6)	3(5)	6(6)	11(5)

C(28)	32(6)	43(7)	29(6)	7(5)	13(5)	-3(5)
C(29)	32(6)	43(7)	28(5)	-7(5)	12(5)	-1(5)
C(30)	43(7)	38(7)	18(5)	-9(4)	0(5)	-6(5)
C(31)	33(6)	38(7)	30(6)	3(5)	4(5)	3(5)
C(32)	43(7)	34(7)	35(6)	13(5)	-1(6)	-2(5)
C(33)	39(7)	48(8)	24(6)	16(5)	-2(5)	-14(6)
C(34)	38(7)	63(10)	23(6)	1(5)	1(5)	-16(6)
C(35)	36(6)	35(7)	31(6)	-6(5)	6(5)	-6(5)
C(36)	43(7)	43(8)	42(7)	-10(5)	21(6)	-6(6)
C(37)	78(11)	46(9)	53(8)	0(6)	19(8)	11(8)
C(38)	31(6)	30(7)	38(6)	-5(5)	11(5)	-2(5)
C(39)	30(6)	38(7)	36(6)	-8(5)	2(5)	8(5)
C(40)	40(7)	39(8)	66(9)	-7(6)	15(7)	4(6)
C(41)	38(7)	47(8)	66(9)	-18(6)	25(7)	6(6)
C(42)	56(9)	44(8)	49(8)	-8(6)	30(7)	4(7)
C(43)	31(6)	39(7)	25(5)	-5(5)	6(5)	2(5)
C(44)	37(7)	54(9)	34(6)	-5(6)	-4(6)	6(6)
C(45)	52(9)	48(9)	57(9)	-11(7)	-7(7)	18(7)
C(46)	61(10)	64(10)	55(9)	23(7)	5(8)	-12(8)
C(47)	75(11)	48(9)	93(12)	-17(8)	52(10)	-14(8)
C(48)	33(6)	32(6)	30(6)	4(4)	20(5)	-2(5)
C(49)	39(7)	57(8)	29(6)	12(5)	17(5)	13(6)
C(50)	59(8)	51(8)	14(5)	-4(5)	7(5)	13(6)
C(51)	58(9)	47(8)	34(7)	-12(6)	18(6)	-2(7)
C(52)	38(7)	46(8)	18(5)	-3(5)	12(5)	5(5)
C(53)	20(5)	42(7)	24(5)	4(5)	9(4)	-7(5)
C(54)	24(6)	30(6)	30(6)	4(4)	12(5)	6(5)
C(55)	28(6)	36(7)	31(6)	3(5)	14(5)	2(5)
C(56)	33(6)	21(6)	51(7)	-4(5)	17(6)	2(5)
C(57)	41(7)	42(8)	52(8)	-11(6)	30(6)	-13(6)
C(58)	58(10)	75(11)	57(9)	-12(7)	36(8)	-6(8)
C(59)	39(8)	55(10)	85(11)	-28(8)	22(8)	-4(7)
C(60)	29(7)	63(10)	74(10)	-26(8)	11(7)	-3(6)
C(61)	28(6)	28(6)	48(7)	-9(5)	9(6)	5(5)
C(62)	29(7)	34(7)	67(9)	-3(6)	11(6)	-3(5)
C(63)	34(7)	49(8)	35(7)	-8(5)	-3(6)	7(6)
C(64)	35(7)	71(10)	42(7)	5(6)	0(6)	4(7)
C(65)	38(7)	53(8)	34(6)	-1(5)	12(6)	-3(6)

C(66)	31(6)	34(7)	26(5)	0(4)	13(5)	1(5)
C(67)	31(6)	24(6)	30(6)	-4(4)	14(5)	-2(5)
C(68)	26(5)	33(6)	22(5)	-1(4)	13(4)	3(5)
C(69)	30(6)	42(7)	19(5)	0(4)	7(5)	-2(5)
C(70)	42(7)	38(7)	21(5)	7(5)	4(5)	-4(5)
C(71)	67(9)	44(8)	35(7)	-7(5)	24(7)	-17(7)
C(72)	55(8)	46(8)	37(7)	2(6)	23(6)	-10(6)
C(73)	46(8)	53(9)	46(7)	-3(6)	22(6)	-9(6)
C(74)	31(6)	35(7)	31(6)	-13(5)	16(5)	-11(5)
C(75)	26(6)	60(9)	30(6)	1(6)	11(5)	-4(6)
C(76)	20(5)	41(7)	30(6)	10(5)	10(5)	8(5)
C(77)	47(7)	33(7)	28(6)	1(5)	15(6)	8(5)
C(78)	42(7)	37(7)	21(5)	4(4)	11(5)	16(5)
C(79)	52(8)	49(9)	39(7)	11(6)	21(6)	16(6)
C(80)	78(11)	50(9)	33(7)	9(6)	29(7)	35(8)
C(81)	69(10)	42(8)	36(7)	-5(5)	24(7)	2(7)
C(82)	51(8)	40(8)	34(6)	1(5)	10(6)	8(6)
C(83)	76(10)	29(8)	53(8)	4(6)	7(8)	-4(7)
C(84)	100(14)	72(12)	49(9)	11(8)	4(9)	48(10)
C(85)	40(7)	45(8)	33(6)	3(5)	6(6)	1(6)
C(86)	33(6)	39(7)	16(5)	-4(4)	8(5)	-5(5)
C(87)	37(7)	32(7)	29(6)	-6(5)	15(5)	-16(5)
C(88)	42(7)	41(8)	54(8)	-13(6)	25(6)	-12(6)
C(89)	38(7)	34(7)	51(8)	-8(5)	11(6)	-7(6)
C(90)	41(7)	44(8)	42(7)	-21(6)	8(6)	-8(6)
C(91)	33(7)	33(7)	36(6)	-2(5)	11(5)	-8(5)
C(92)	49(8)	41(8)	40(7)	-11(5)	20(6)	-12(6)
C(93)	61(9)	60(9)	37(7)	2(6)	30(7)	-21(7)
C(94)	43(8)	63(10)	73(10)	-17(8)	16(8)	-1(7)
C(95)	48(9)	61(10)	70(11)	4(7)	2(8)	-5(7)
Cl(1)	121(4)	80(3)	66(3)	2(2)	15(3)	30(3)
Cl(2)	119(4)	77(3)	86(3)	10(2)	40(3)	13(3)

Table S77. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for B3b.

	x	y	z	U(eq)

H(2)	2657	4292	2671	47
H(3)	2027	3509	1793	55
H(4)	1507	2496	2135	56
H(5)	1601	2277	3346	41
H(8)	1634	2358	4667	35
H(10)	565	2937	3407	54
H(11)	-488	2961	3446	76
H(12)	-754	2891	4498	68
H(13)	8	2834	5624	59
H(16)	1206	3015	6781	50
H(17)	2273	3158	7363	51
H(18)	3025	3289	6730	42
H(22)	4162	4532	4667	50
H(23)	4949	3981	5518	51
H(25)	5341	2854	6367	52
H(26)	5091	1804	6929	58
H(27)	4053	1372	6658	44
H(28)	3245	2040	5861	41
H(32)	3468	6774	3367	48
H(34)	4258	4961	2730	52
H(36A)	3685	3691	2842	61
H(36B)	3676	3593	3666	61
H(36C)	4316	3816	3483	61
H(37A)	2929	6784	4152	88
H(37B)	2878	6055	4621	88
H(37C)	2367	6196	3861	88
H(40)	923	4853	4549	58
H(42)	2383	5095	6315	56
H(44A)	3463	4651	6128	67
H(44B)	3356	5539	6012	67
H(44C)	3563	5045	5420	67
H(45A)	1363	4297	3348	85
H(45B)	1738	5047	3266	85
H(45C)	1065	5105	3419	85
H(46A)	3968	6872	2314	93
H(46B)	4373	6164	2190	93
H(46C)	4619	6675	2898	93
H(47A)	1099	4488	6174	99

H(47B)	709	5142	5674	99
H(47C)	1278	5351	6365	99
H(49)	8818	4629	7435	48
H(50)	8626	5511	8243	50
H(51)	7947	6508	7824	55
H(52)	7365	6542	6612	40
H(57)	6304	5857	6537	50
H(58)	5239	5865	6469	71
H(59)	4475	5877	5376	70
H(60)	4747	5887	4283	67
H(63)	5443	5696	3170	50
H(64)	6247	5496	2639	62
H(65)	7305	5478	3299	50
H(70)	7904	6708	4167	41
H(71)	8363	7310	3380	56
H(72)	9306	6903	3200	53
H(73)	9809	5841	3817	56
H(75)	9794	4764	4641	46
H(76)	9349	4173	5449	36
H(79)	10346	3648	7348	54
H(81)	9153	1930	6686	56
H(83A)	8177	2023	6153	83
H(83B)	8056	2584	5478	83
H(83C)	7798	2791	6152	83
H(84A)	10419	2224	8002	116
H(84B)	10719	2252	7335	116
H(84C)	10193	1638	7349	116
H(85A)	9799	4964	7294	61
H(85B)	9410	5113	6471	61
H(85C)	10117	4807	6656	61
H(88)	6199	3930	5733	52
H(90)	6683	3697	3899	51
H(92A)	7708	3372	3938	63
H(92B)	8271	3466	4665	63
H(92C)	8010	4185	4170	63
H(93A)	7271	4554	6861	74
H(93B)	7669	3792	6925	74
H(93C)	6930	3757	6846	74

H(94A)	5496	3284	4279	90
H(94B)	5582	4013	3826	90
H(94C)	5385	4107	4562	90
H(95A)	6785	2319	5043	75
H(95B)	6769	1421	5114	75

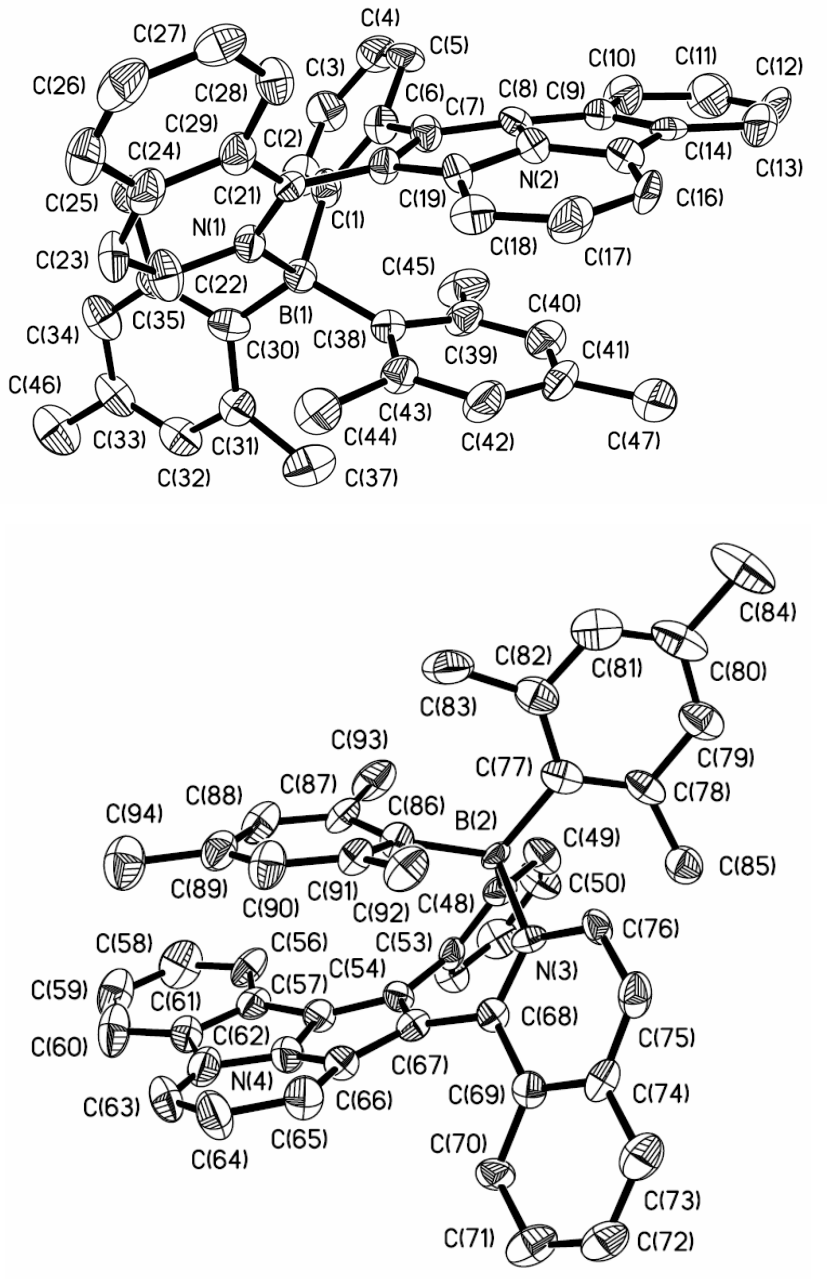


Figure S106. A diagram showing the two independent molecules in the crystal lattice of **B3b** with labeling schemes and 35% thermal ellipsoids. H atoms are omitted for clarity.

Table S78. Crystal data and structure refinement for B4a.

Identification code	B4a	
Empirical formula	C45 H37 B N2 S	
Formula weight	648.63	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.145(10) Å	α= 64.16(3)°.
	b = 12.992(13) Å	β= 75.45(3)°.
	c = 14.196(13) Å	γ = 73.97(3)°.
Volume	1758(3) $Å^3$	
Z	2	
Density (calculated)	1.225 Mg/m^3	
Absorption coefficient	0.127 mm^{-1}	
F(000)	684	
Crystal size	0.160 x 0.140 x 0.120 mm^3	
Theta range for data collection	2.691 to 27.276°.	
Index ranges	-14<=h<=14, -16<=k<=16, -18<=l<=18	
Reflections collected	25091	
Independent reflections	7700 [R(int) = 0.1272]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.985 and 0.980	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7700 / 0 / 449	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0651, wR2 = 0.1416	
R indices (all data)	R1 = 0.1388, wR2 = 0.1681	
Extinction coefficient	0.011(2)	
Largest diff. peak and hole	0.292 and -0.306 $e.Å^{-3}$	

Table S79. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for B4a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	2156(1)	6165(1)	2505(1)	35(1)
N(1)	4284(2)	3457(2)	754(2)	30(1)
N(2)	4470(2)	5067(2)	2813(2)	35(1)
C(1)	919(2)	3424(2)	3260(2)	28(1)
C(2)	-352(2)	3532(3)	3750(2)	37(1)
C(3)	-1329(3)	4332(3)	3218(2)	41(1)
C(4)	-1051(3)	5075(3)	2185(3)	43(1)
C(5)	196(3)	5016(2)	1670(2)	39(1)
C(6)	1184(2)	4195(2)	2198(2)	28(1)
C(7)	2508(2)	4132(2)	1620(2)	28(1)
C(8)	2985(2)	3585(2)	887(2)	29(1)
C(9)	2580(3)	3144(2)	298(2)	39(1)
C(10)	3475(3)	2603(3)	-313(2)	46(1)
C(11)	4800(3)	2450(3)	-360(2)	41(1)
C(12)	5222(3)	2869(2)	210(2)	33(1)
C(13)	6375(3)	2911(2)	479(2)	32(1)
C(14)	7642(3)	2397(3)	247(2)	41(1)
C(15)	8556(3)	2521(3)	673(2)	44(1)
C(16)	8241(3)	3161(3)	1315(2)	43(1)
C(17)	7004(3)	3676(2)	1562(2)	37(1)
C(18)	6053(2)	3553(2)	1150(2)	30(1)
C(19)	4682(2)	3886(2)	1318(2)	28(1)
C(20)	3563(2)	4365(2)	1845(2)	28(1)
C(21)	3514(2)	5091(2)	2412(2)	28(1)
C(22)	4148(3)	5914(2)	3245(2)	35(1)
C(23)	4940(3)	6118(3)	3740(3)	55(1)
C(24)	4503(4)	6979(3)	4145(3)	66(1)
C(25)	3269(3)	7629(3)	4081(3)	56(1)
C(26)	2460(3)	7461(3)	3581(2)	44(1)
C(27)	2918(3)	6589(2)	3161(2)	33(1)
C(28)	1638(2)	1936(2)	5175(2)	29(1)
C(29)	1450(2)	2754(2)	5645(2)	33(1)
C(30)	1699(3)	3995(3)	4998(2)	46(1)

C(31)	1089(2)	2435(3)	6733(2)	38(1)
C(32)	891(2)	1298(3)	7400(2)	37(1)
C(33)	451(3)	982(3)	8567(2)	59(1)
C(34)	1125(2)	479(3)	6950(2)	36(1)
C(35)	1503(2)	765(2)	5869(2)	30(1)
C(36)	1743(3)	-216(2)	5486(2)	40(1)
C(37)	2960(2)	1586(2)	3370(2)	26(1)
C(38)	2662(2)	1075(2)	2768(2)	29(1)
C(39)	1319(3)	1162(3)	2662(2)	43(1)
C(40)	3629(3)	412(2)	2303(2)	35(1)
C(41)	4894(3)	236(3)	2389(2)	38(1)
C(42)	5905(3)	-474(3)	1844(3)	62(1)
C(43)	5177(2)	732(2)	2978(2)	35(1)
C(44)	4249(2)	1383(2)	3477(2)	29(1)
C(45)	4650(2)	1877(3)	4117(2)	38(1)
B(1)	1885(3)	2328(3)	3934(2)	28(1)

Table S80. Bond lengths [Å] and angles [°] for B4a.

S(1)-C(27)	1.731(3)	C(10)-C(11)	1.423(4)
S(1)-C(21)	1.774(3)	C(11)-C(12)	1.375(4)
N(1)-C(19)	1.360(3)	C(12)-C(13)	1.451(4)
N(1)-C(8)	1.384(4)	C(13)-C(14)	1.409(4)
N(1)-C(12)	1.392(3)	C(13)-C(18)	1.443(4)
N(2)-C(21)	1.316(3)	C(14)-C(15)	1.385(4)
N(2)-C(22)	1.406(3)	C(15)-C(16)	1.408(4)
C(1)-C(6)	1.409(4)	C(16)-C(17)	1.386(4)
C(1)-C(2)	1.411(4)	C(17)-C(18)	1.407(4)
C(1)-B(1)	1.608(4)	C(18)-C(19)	1.457(4)
C(2)-C(3)	1.394(4)	C(19)-C(20)	1.418(4)
C(3)-C(4)	1.372(4)	C(20)-C(21)	1.467(4)
C(4)-C(5)	1.396(4)	C(22)-C(23)	1.395(4)
C(5)-C(6)	1.407(4)	C(22)-C(27)	1.410(4)
C(6)-C(7)	1.497(4)	C(23)-C(24)	1.392(4)
C(7)-C(8)	1.424(4)	C(24)-C(25)	1.404(5)
C(7)-C(20)	1.432(4)	C(25)-C(26)	1.390(4)
C(8)-C(9)	1.407(4)	C(26)-C(27)	1.419(4)
C(9)-C(10)	1.397(4)	C(28)-C(29)	1.430(4)

C(28)-C(35)	1.433(4)	N(1)-C(8)-C(9)	113.7(2)
C(28)-B(1)	1.579(4)	N(1)-C(8)-C(7)	104.9(2)
C(29)-C(31)	1.393(4)	C(9)-C(8)-C(7)	141.4(3)
C(29)-C(30)	1.532(4)	C(10)-C(9)-C(8)	119.5(3)
C(31)-C(32)	1.407(4)	C(9)-C(10)-C(11)	123.2(3)
C(32)-C(34)	1.402(4)	C(12)-C(11)-C(10)	118.5(3)
C(32)-C(33)	1.505(4)	C(11)-C(12)-N(1)	115.5(3)
C(34)-C(35)	1.392(4)	C(11)-C(12)-C(13)	141.4(3)
C(35)-C(36)	1.527(4)	N(1)-C(12)-C(13)	103.1(2)
C(37)-C(44)	1.422(4)	C(14)-C(13)-C(18)	120.0(3)
C(37)-C(38)	1.428(4)	C(14)-C(13)-C(12)	131.2(3)
C(37)-B(1)	1.599(4)	C(18)-C(13)-C(12)	108.7(2)
C(38)-C(40)	1.402(4)	C(15)-C(14)-C(13)	118.7(3)
C(38)-C(39)	1.512(4)	C(14)-C(15)-C(16)	121.2(3)
C(40)-C(41)	1.392(4)	C(17)-C(16)-C(15)	121.7(3)
C(41)-C(43)	1.390(4)	C(16)-C(17)-C(18)	118.4(3)
C(41)-C(42)	1.526(4)	C(17)-C(18)-C(13)	120.1(2)
C(43)-C(44)	1.399(4)	C(17)-C(18)-C(19)	132.6(2)
C(44)-C(45)	1.519(4)	C(13)-C(18)-C(19)	107.2(2)
		N(1)-C(19)-C(20)	105.3(2)
C(27)-S(1)-C(21)	89.53(14)	N(1)-C(19)-C(18)	104.6(2)
C(19)-N(1)-C(8)	114.0(2)	C(20)-C(19)-C(18)	149.8(2)
C(19)-N(1)-C(12)	116.4(2)	C(19)-C(20)-C(7)	108.2(2)
C(8)-N(1)-C(12)	129.3(2)	C(19)-C(20)-C(21)	124.9(2)
C(21)-N(2)-C(22)	110.1(2)	C(7)-C(20)-C(21)	126.6(2)
C(6)-C(1)-C(2)	117.1(2)	N(2)-C(21)-C(20)	123.9(2)
C(6)-C(1)-B(1)	126.7(2)	N(2)-C(21)-S(1)	115.2(2)
C(2)-C(1)-B(1)	115.7(2)	C(20)-C(21)-S(1)	120.63(19)
C(3)-C(2)-C(1)	122.7(3)	C(23)-C(22)-N(2)	125.1(3)
C(4)-C(3)-C(2)	119.2(3)	C(23)-C(22)-C(27)	119.2(3)
C(3)-C(4)-C(5)	120.3(3)	N(2)-C(22)-C(27)	115.6(2)
C(4)-C(5)-C(6)	120.8(3)	C(24)-C(23)-C(22)	119.6(3)
C(5)-C(6)-C(1)	119.9(2)	C(23)-C(24)-C(25)	120.9(3)
C(5)-C(6)-C(7)	119.7(3)	C(26)-C(25)-C(24)	121.1(3)
C(1)-C(6)-C(7)	120.4(2)	C(25)-C(26)-C(27)	117.5(3)
C(8)-C(7)-C(20)	107.4(2)	C(22)-C(27)-C(26)	121.6(3)
C(8)-C(7)-C(6)	124.0(2)	C(22)-C(27)-S(1)	109.5(2)
C(20)-C(7)-C(6)	127.4(2)	C(26)-C(27)-S(1)	128.9(2)

C(29)-C(28)-C(35)	117.6(2)
C(29)-C(28)-B(1)	121.3(2)
C(35)-C(28)-B(1)	121.0(2)
C(31)-C(29)-C(28)	121.0(3)
C(31)-C(29)-C(30)	116.7(3)
C(28)-C(29)-C(30)	122.2(3)
C(29)-C(31)-C(32)	120.9(3)
C(34)-C(32)-C(31)	118.4(3)
C(34)-C(32)-C(33)	121.5(3)
C(31)-C(32)-C(33)	120.2(3)
C(35)-C(34)-C(32)	122.2(3)
C(34)-C(35)-C(28)	119.9(3)
C(34)-C(35)-C(36)	116.7(3)
C(28)-C(35)-C(36)	123.4(2)
C(44)-C(37)-C(38)	117.5(2)
C(44)-C(37)-B(1)	121.0(2)
C(38)-C(37)-B(1)	121.5(2)
C(40)-C(38)-C(37)	119.8(2)
C(40)-C(38)-C(39)	117.8(2)
C(37)-C(38)-C(39)	122.3(2)
C(41)-C(40)-C(38)	122.6(3)
C(43)-C(41)-C(40)	117.3(2)
C(43)-C(41)-C(42)	122.7(3)
C(40)-C(41)-C(42)	120.1(3)
C(41)-C(43)-C(44)	122.6(2)
C(43)-C(44)-C(37)	120.2(2)
C(43)-C(44)-C(45)	118.7(2)
C(37)-C(44)-C(45)	121.1(2)
C(28)-B(1)-C(37)	121.5(2)
C(28)-B(1)-C(1)	117.6(2)
C(37)-B(1)-C(1)	120.5(2)

Table S81 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for B4a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	37(1)	30(1)	38(1)	-17(1)	-8(1)	3(1)
N(1)	32(1)	32(1)	27(1)	-15(1)	-2(1)	-3(1)
N(2)	37(1)	33(1)	41(2)	-22(1)	-5(1)	-5(1)
C(1)	25(1)	33(2)	28(2)	-18(1)	-4(1)	0(1)
C(2)	29(2)	44(2)	34(2)	-17(2)	-4(1)	2(1)
C(3)	27(2)	50(2)	49(2)	-26(2)	-8(1)	3(1)
C(4)	29(2)	46(2)	56(2)	-23(2)	-20(1)	8(1)
C(5)	42(2)	35(2)	38(2)	-12(1)	-14(1)	-1(1)
C(6)	27(1)	28(2)	33(2)	-17(1)	-9(1)	0(1)
C(7)	30(1)	24(1)	27(2)	-10(1)	-6(1)	1(1)
C(8)	36(2)	26(2)	26(2)	-10(1)	-8(1)	-3(1)
C(9)	44(2)	37(2)	36(2)	-14(2)	-15(1)	-2(1)
C(10)	59(2)	48(2)	41(2)	-28(2)	-18(2)	-1(2)
C(11)	48(2)	43(2)	35(2)	-23(2)	-9(1)	1(2)
C(12)	36(2)	31(2)	27(2)	-13(1)	-1(1)	0(1)
C(13)	38(2)	28(2)	25(2)	-9(1)	1(1)	-4(1)
C(14)	40(2)	38(2)	30(2)	-12(1)	4(1)	2(1)
C(15)	31(2)	40(2)	47(2)	-13(2)	1(1)	0(1)
C(16)	32(2)	42(2)	55(2)	-20(2)	-2(1)	-8(1)
C(17)	34(2)	37(2)	42(2)	-18(2)	-1(1)	-9(1)
C(18)	31(2)	22(1)	30(2)	-7(1)	0(1)	-6(1)
C(19)	34(2)	24(1)	28(2)	-12(1)	-4(1)	-4(1)
C(20)	32(1)	25(1)	26(2)	-10(1)	-5(1)	-3(1)
C(21)	31(2)	23(1)	26(2)	-9(1)	-2(1)	-3(1)
C(22)	40(2)	31(2)	38(2)	-18(1)	-5(1)	-7(1)
C(23)	50(2)	59(2)	74(3)	-43(2)	-20(2)	-2(2)
C(24)	76(3)	70(3)	81(3)	-52(2)	-27(2)	-6(2)
C(25)	82(3)	43(2)	55(2)	-32(2)	-6(2)	-11(2)
C(26)	58(2)	30(2)	38(2)	-16(2)	0(2)	-5(2)
C(27)	40(2)	26(2)	29(2)	-11(1)	-1(1)	-5(1)

C(28)	21(1)	29(2)	33(2)	-13(1)	-6(1)	4(1)
C(29)	31(2)	34(2)	32(2)	-16(1)	-4(1)	3(1)
C(30)	62(2)	35(2)	40(2)	-18(2)	-3(2)	-5(2)
C(31)	38(2)	41(2)	35(2)	-22(2)	-5(1)	2(1)
C(32)	32(2)	41(2)	27(2)	-10(1)	-3(1)	3(1)
C(33)	64(2)	61(2)	33(2)	-16(2)	1(2)	3(2)
C(34)	30(2)	33(2)	34(2)	-7(1)	-4(1)	-3(1)
C(35)	23(1)	33(2)	33(2)	-13(1)	-6(1)	1(1)
C(36)	44(2)	30(2)	37(2)	-10(1)	-3(1)	-3(1)
C(37)	26(1)	23(1)	26(1)	-8(1)	-5(1)	-3(1)
C(38)	26(1)	31(2)	30(2)	-13(1)	-5(1)	-3(1)
C(39)	37(2)	54(2)	45(2)	-27(2)	-7(1)	-8(2)
C(40)	41(2)	34(2)	39(2)	-22(1)	-7(1)	-4(1)
C(41)	34(2)	36(2)	46(2)	-22(2)	-5(1)	2(1)
C(42)	49(2)	67(2)	78(3)	-51(2)	-3(2)	9(2)
C(43)	23(1)	36(2)	42(2)	-17(2)	-6(1)	2(1)
C(44)	28(1)	25(1)	30(2)	-8(1)	-6(1)	-2(1)
C(45)	30(2)	46(2)	40(2)	-21(2)	-11(1)	-2(1)
B(1)	23(2)	28(2)	34(2)	-13(2)	-5(1)	-6(1)

Table S82. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for B4a.

	x	y	z	U(eq)
H(2)	-549	3038	4473	44
H(3)	-2178	4362	3566	50
H(4)	-1708	5633	1819	52
H(5)	379	5535	955	47
H(9)	1704	3213	316	47
H(10)	3185	2323	-716	55
H(11)	5381	2066	-777	49
H(14)	7864	1974	-194	49
H(15)	9412	2169	530	52
H(16)	8892	3242	1585	52
H(17)	6804	4102	1999	45
H(23)	5772	5673	3800	66
H(24)	5049	7128	4470	80
H(25)	2981	8193	4384	67
H(26)	1630	7912	3522	52
H(30A)	1177	4395	4431	69
H(30B)	2593	3963	4688	69
H(30C)	1487	4421	5461	69
H(31)	974	2991	7029	45
H(33A)	546	1590	8761	88
H(33B)	960	237	8967	88
H(33C)	-439	914	8734	88
H(34)	1021	-297	7398	43
H(36A)	1149	-26	5003	59
H(36B)	1624	-945	6095	59
H(36C)	2610	-306	5115	59
H(39A)	1319	754	2221	64
H(39B)	925	1983	2330	64
H(39C)	841	804	3364	64
H(40)	3413	70	1914	42
H(42A)	6634	-88	1509	93

H(42B)	5560	-534	1303	93
H(42C)	6171	-1256	2369	93
H(43)	6034	625	3046	42
H(45A)	5565	1843	3943	57
H(45B)	4430	1418	4874	57
H(45C)	4214	2689	3946	57

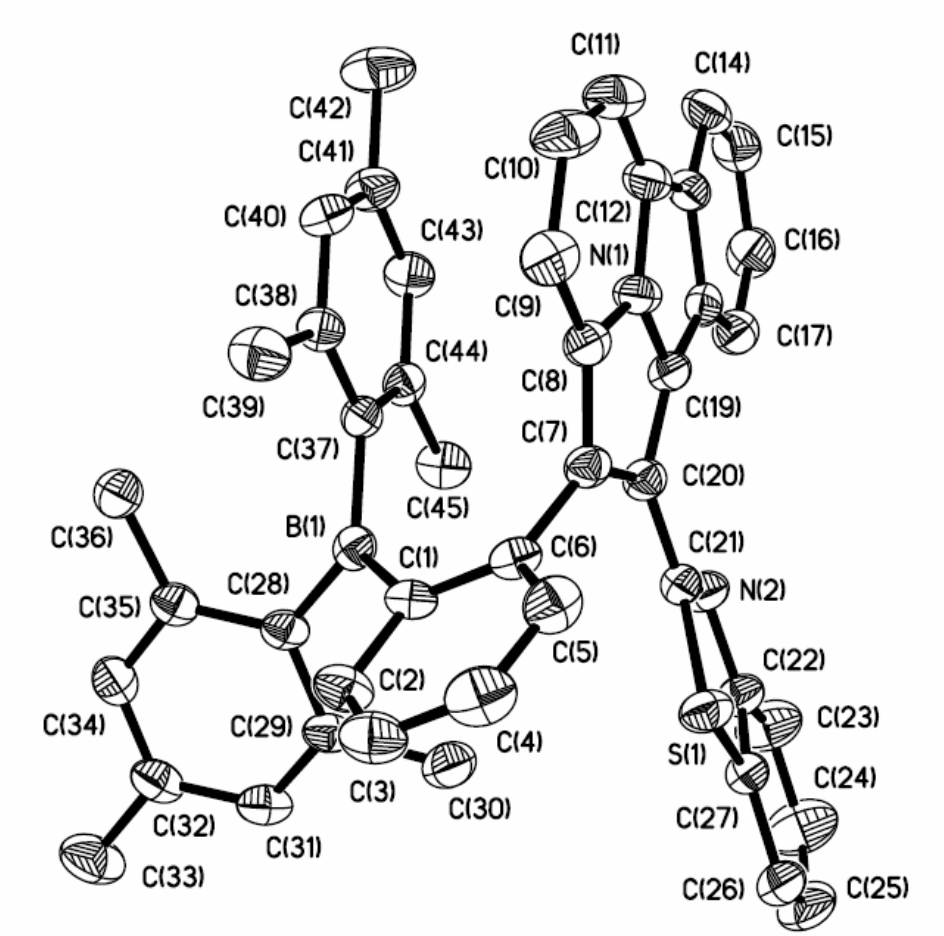


Figure S107. A diagram showing the structure of **4a** with labeling schemes and 35% thermal ellipsoids. H atoms are omitted for clarity.

Table S83. Crystal data and structure refinement for b4b.

Identification code	b4b	
Empirical formula	C4.09 H3.36 B0.09 N0.18 S0.09	
Formula weight	58.97	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.741(4) Å	α= 63.989(11)°.
	b = 13.927(5) Å	β= 89.736(13)°.
	c = 15.334(6) Å	γ = 69.795(12)°.
Volume	1727.6(11) $Å^3$	
Z	22	
Density (calculated)	1.247 Mg/m^3	
Absorption coefficient	0.128 mm^{-1}	
F(000)	684	
Crystal size	0.200 x 0.147 x 0.145 mm^3	
Theta range for data collection	2.681 to 27.248°.	
Index ranges	-12<=h<=12, -17<=k<=17, -19<=l<=19	
Reflections collected	27025	
Independent reflections	7646 [R(int) = 0.1469]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.982 and 0.975	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7646 / 0 / 448	
Goodness-of-fit on F^2	1.022	
Final R indices [I>2sigma(I)]	R1 = 0.0650, wR2 = 0.1326	
R indices (all data)	R1 = 0.1403, wR2 = 0.1594	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.290 and -0.287 $e.Å^{-3}$	

Table S84. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for b4b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	3226(3)	3556(3)	3917(2)	27(1)
S(1)	5440(1)	1425(1)	2476(1)	29(1)
N(1)	3729(2)	5623(2)	673(2)	27(1)
N(2)	2760(2)	2594(2)	1459(2)	30(1)
C(1)	4932(3)	2994(2)	3925(2)	27(1)
C(2)	5822(3)	2214(3)	4858(2)	41(1)
C(3)	7349(3)	1828(3)	5006(2)	53(1)
C(4)	8055(3)	2186(3)	4215(2)	54(1)
C(5)	7237(3)	2913(3)	3280(2)	40(1)
C(6)	5693(3)	3311(2)	3114(2)	28(1)
C(7)	4876(3)	4070(2)	2088(2)	25(1)
C(8)	3940(3)	3824(2)	1574(2)	26(1)
C(9)	3172(3)	4846(2)	685(2)	26(1)
C(10)	2053(3)	5282(2)	-114(2)	32(1)
C(11)	1602(3)	6436(3)	-803(2)	38(1)
C(12)	2243(3)	7184(3)	-763(2)	37(1)
C(13)	3356(3)	6761(2)	9(2)	31(1)
C(14)	4311(3)	7125(2)	414(2)	32(1)
C(15)	4501(3)	8175(3)	65(2)	40(1)
C(16)	5537(3)	8265(3)	596(2)	47(1)
C(17)	6380(3)	7326(3)	1485(2)	43(1)
C(18)	6229(3)	6277(3)	1853(2)	35(1)
C(19)	5189(3)	6157(2)	1321(2)	30(1)
C(20)	4770(3)	5205(2)	1478(2)	26(1)
C(21)	3886(3)	2717(2)	1798(2)	25(1)
C(22)	3070(3)	1443(2)	1731(2)	28(1)
C(23)	4474(3)	666(2)	2299(2)	26(1)
C(24)	4923(3)	-515(2)	2621(2)	31(1)
C(25)	3953(3)	-909(2)	2357(2)	38(1)
C(26)	2555(3)	-140(3)	1788(2)	40(1)
C(27)	2105(3)	1025(2)	1474(2)	35(1)

C(28)	2316(3)	4866(2)	3140(2)	25(1)
C(29)	2779(3)	5758(2)	3042(2)	28(1)
C(30)	4060(3)	5553(3)	3751(2)	38(1)
C(31)	2036(3)	6882(2)	2301(2)	31(1)
C(32)	834(3)	7176(2)	1625(2)	33(1)
C(33)	81(4)	8395(3)	807(2)	49(1)
C(34)	363(3)	6307(2)	1731(2)	33(1)
C(35)	1048(3)	5171(2)	2477(2)	28(1)
C(36)	436(3)	4288(3)	2529(2)	39(1)
C(37)	2489(3)	2840(2)	4757(2)	29(1)
C(38)	2465(3)	1778(2)	4870(2)	31(1)
C(39)	3075(3)	1304(3)	4178(2)	43(1)
C(40)	1825(3)	1162(2)	5617(2)	32(1)
C(41)	1201(3)	1533(3)	6272(2)	34(1)
C(42)	560(3)	821(3)	7092(2)	50(1)
C(43)	1229(3)	2564(3)	6175(2)	35(1)
C(44)	1861(3)	3219(2)	5442(2)	32(1)
C(45)	1923(3)	4285(3)	5444(2)	41(1)

Table S85. Bond lengths [Å] and angles [°] for b4b.

B(1)-C(1)	1.571(4)	C(11)-C(12)	1.408(4)
B(1)-C(28)	1.587(4)	C(12)-C(13)	1.373(4)
B(1)-C(37)	1.589(4)	C(13)-C(14)	1.455(4)
S(1)-C(23)	1.738(3)	C(14)-C(15)	1.399(4)
S(1)-C(21)	1.761(3)	C(14)-C(19)	1.433(4)
N(1)-C(9)	1.363(3)	C(15)-C(16)	1.372(4)
N(1)-C(20)	1.365(3)	C(16)-C(17)	1.396(4)
N(1)-C(13)	1.367(3)	C(17)-C(18)	1.379(4)
N(2)-C(21)	1.310(3)	C(18)-C(19)	1.401(4)
N(2)-C(22)	1.383(3)	C(19)-C(20)	1.441(4)
C(1)-C(2)	1.405(4)	C(22)-C(27)	1.400(4)
C(1)-C(6)	1.424(3)	C(22)-C(23)	1.400(4)
C(2)-C(3)	1.377(4)	C(23)-C(24)	1.390(4)
C(3)-C(4)	1.376(4)	C(24)-C(25)	1.384(4)
C(4)-C(5)	1.377(4)	C(25)-C(26)	1.395(4)
C(5)-C(6)	1.392(3)	C(26)-C(27)	1.372(4)
C(6)-C(7)	1.482(3)	C(28)-C(29)	1.412(4)
C(7)-C(20)	1.406(4)	C(28)-C(35)	1.417(3)
C(7)-C(8)	1.423(3)	C(29)-C(31)	1.389(4)
C(8)-C(9)	1.420(3)	C(29)-C(30)	1.522(4)
C(8)-C(21)	1.446(4)	C(31)-C(32)	1.385(4)
C(9)-C(10)	1.399(3)	C(32)-C(34)	1.383(4)
C(10)-C(11)	1.385(4)	C(32)-C(33)	1.508(4)

C(34)-C(35)	1.396(4)
C(35)-C(36)	1.514(4)
C(37)-C(44)	1.418(4)
C(37)-C(38)	1.420(4)
C(38)-C(40)	1.392(3)
C(38)-C(39)	1.501(4)
C(40)-C(41)	1.370(4)
C(41)-C(43)	1.387(4)
C(41)-C(42)	1.511(4)
C(43)-C(44)	1.398(4)
C(44)-C(45)	1.509(4)

C(1)-B(1)-C(28)	119.3(2)
C(1)-B(1)-C(37)	119.0(2)
C(28)-B(1)-C(37)	121.4(2)
C(23)-S(1)-C(21)	89.12(13)
C(9)-N(1)-C(20)	114.2(2)
C(9)-N(1)-C(13)	130.1(2)
C(20)-N(1)-C(13)	115.7(2)
C(21)-N(2)-C(22)	110.9(2)
C(2)-C(1)-C(6)	116.5(2)
C(2)-C(1)-B(1)	115.9(2)
C(6)-C(1)-B(1)	126.9(2)
C(3)-C(2)-C(1)	122.7(3)
C(4)-C(3)-C(2)	119.6(3)
C(3)-C(4)-C(5)	120.0(3)
C(4)-C(5)-C(6)	121.3(3)
C(5)-C(6)-C(1)	119.8(2)
C(5)-C(6)-C(7)	118.8(2)
C(1)-C(6)-C(7)	121.4(2)
C(20)-C(7)-C(8)	107.4(2)
C(20)-C(7)-C(6)	126.2(2)
C(8)-C(7)-C(6)	126.1(2)
C(9)-C(8)-C(7)	108.2(2)
C(9)-C(8)-C(21)	122.9(2)
C(7)-C(8)-C(21)	128.3(2)
N(1)-C(9)-C(10)	114.6(2)
N(1)-C(9)-C(8)	104.4(2)
C(10)-C(9)-C(8)	140.9(3)
C(11)-C(10)-C(9)	118.1(3)
C(10)-C(11)-C(12)	123.7(3)
C(13)-C(12)-C(11)	118.7(3)
N(1)-C(13)-C(12)	114.8(3)
N(1)-C(13)-C(14)	104.0(2)
C(12)-C(13)-C(14)	141.2(3)
C(15)-C(14)-C(19)	120.1(3)
C(15)-C(14)-C(13)	132.0(3)
C(19)-C(14)-C(13)	107.9(2)
C(16)-C(15)-C(14)	119.4(3)
C(15)-C(16)-C(17)	120.5(3)
C(18)-C(17)-C(16)	121.8(3)
C(17)-C(18)-C(19)	118.8(3)
C(18)-C(19)-C(14)	119.3(3)
C(18)-C(19)-C(20)	133.2(3)
C(14)-C(19)-C(20)	107.5(2)
N(1)-C(20)-C(7)	105.6(2)
N(1)-C(20)-C(19)	104.9(2)
C(7)-C(20)-C(19)	149.4(2)
N(2)-C(21)-C(8)	123.8(2)
N(2)-C(21)-S(1)	115.1(2)
C(8)-C(21)-S(1)	120.89(18)
N(2)-C(22)-C(27)	125.0(2)
N(2)-C(22)-C(23)	115.6(2)
C(27)-C(22)-C(23)	119.4(3)
C(24)-C(23)-C(22)	121.3(2)
C(24)-C(23)-S(1)	129.3(2)
C(22)-C(23)-S(1)	109.3(2)
C(25)-C(24)-C(23)	118.3(3)
C(24)-C(25)-C(26)	120.8(3)
C(27)-C(26)-C(25)	121.0(3)
C(26)-C(27)-C(22)	119.2(3)
C(29)-C(28)-C(35)	117.5(2)
C(29)-C(28)-B(1)	121.8(2)
C(35)-C(28)-B(1)	120.7(2)
C(31)-C(29)-C(28)	120.6(2)
C(31)-C(29)-C(30)	117.0(2)
C(28)-C(29)-C(30)	122.3(2)
C(32)-C(31)-C(29)	122.2(3)
C(34)-C(32)-C(31)	117.3(3)
C(34)-C(32)-C(33)	121.7(3)
C(31)-C(32)-C(33)	121.0(3)
C(32)-C(34)-C(35)	122.8(3)
C(34)-C(35)-C(28)	119.6(3)
C(34)-C(35)-C(36)	118.4(2)
C(28)-C(35)-C(36)	121.9(2)
C(44)-C(37)-C(38)	117.0(2)
C(44)-C(37)-B(1)	121.5(2)
C(38)-C(37)-B(1)	121.4(2)
C(40)-C(38)-C(37)	120.4(3)
C(40)-C(38)-C(39)	117.9(3)
C(37)-C(38)-C(39)	121.6(2)
C(41)-C(40)-C(38)	122.7(3)
C(40)-C(41)-C(43)	117.5(2)
C(40)-C(41)-C(42)	121.1(3)
C(43)-C(41)-C(42)	121.3(3)
C(41)-C(43)-C(44)	122.4(3)
C(43)-C(44)-C(37)	120.0(3)
C(43)-C(44)-C(45)	118.0(3)
C(37)-C(44)-C(45)	121.9(2)

Table S86. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for b4b. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	33(2)	29(2)	25(2)	-16(2)	2(1)	-16(1)
S(1)	26(1)	26(1)	32(1)	-12(1)	2(1)	-9(1)
N(1)	28(1)	22(1)	25(1)	-7(1)	3(1)	-8(1)
N(2)	28(1)	27(1)	33(1)	-14(1)	2(1)	-9(1)
C(1)	29(1)	20(1)	28(2)	-8(1)	-1(1)	-9(1)
C(2)	35(2)	41(2)	30(2)	-6(2)	-1(1)	-11(1)
C(3)	37(2)	56(2)	37(2)	-3(2)	-13(2)	-8(2)
C(4)	24(2)	70(3)	49(2)	-17(2)	-7(2)	-11(2)
C(5)	27(2)	46(2)	39(2)	-15(2)	5(1)	-13(1)
C(6)	25(1)	24(2)	32(2)	-11(1)	-1(1)	-10(1)
C(7)	24(1)	24(2)	29(2)	-12(1)	7(1)	-9(1)
C(8)	23(1)	26(2)	28(2)	-12(1)	7(1)	-9(1)
C(9)	24(1)	27(2)	26(2)	-11(1)	4(1)	-10(1)
C(10)	35(2)	32(2)	28(2)	-14(1)	4(1)	-11(1)
C(11)	39(2)	39(2)	26(2)	-12(1)	-1(1)	-9(1)
C(12)	44(2)	29(2)	25(2)	-5(1)	5(1)	-8(1)
C(13)	35(2)	26(2)	24(2)	-6(1)	9(1)	-10(1)
C(14)	37(2)	27(2)	32(2)	-13(1)	14(1)	-14(1)
C(15)	49(2)	31(2)	41(2)	-15(2)	18(2)	-19(1)
C(16)	57(2)	41(2)	61(2)	-30(2)	26(2)	-31(2)
C(17)	40(2)	45(2)	59(2)	-31(2)	16(2)	-25(2)
C(18)	29(2)	38(2)	42(2)	-20(2)	7(1)	-13(1)
C(19)	28(1)	27(2)	36(2)	-16(1)	12(1)	-11(1)
C(20)	23(1)	29(2)	25(2)	-12(1)	2(1)	-8(1)
C(21)	22(1)	27(2)	25(1)	-11(1)	4(1)	-10(1)
C(22)	28(1)	30(2)	26(2)	-13(1)	6(1)	-10(1)
C(23)	27(1)	29(2)	25(1)	-14(1)	8(1)	-13(1)
C(24)	35(2)	26(2)	29(2)	-8(1)	6(1)	-12(1)
C(25)	50(2)	26(2)	42(2)	-15(2)	15(2)	-18(1)
C(26)	38(2)	43(2)	51(2)	-25(2)	9(2)	-23(2)
C(27)	30(2)	36(2)	43(2)	-21(2)	4(1)	-14(1)

C(28)	26(1)	26(2)	25(1)	-11(1)	4(1)	-12(1)
C(29)	27(1)	25(2)	28(2)	-11(1)	2(1)	-8(1)
C(30)	38(2)	37(2)	38(2)	-16(2)	-2(1)	-17(1)
C(31)	37(2)	25(2)	31(2)	-13(1)	5(1)	-13(1)
C(32)	37(2)	27(2)	30(2)	-13(1)	3(1)	-5(1)
C(33)	65(2)	33(2)	36(2)	-13(2)	-3(2)	-8(2)
C(34)	24(1)	35(2)	34(2)	-19(1)	-2(1)	-2(1)
C(35)	25(1)	30(2)	32(2)	-18(1)	4(1)	-8(1)
C(36)	28(2)	43(2)	47(2)	-22(2)	1(1)	-14(1)
C(37)	25(1)	27(2)	26(2)	-7(1)	1(1)	-7(1)
C(38)	27(1)	31(2)	30(2)	-11(1)	3(1)	-9(1)
C(39)	55(2)	38(2)	45(2)	-22(2)	19(2)	-23(2)
C(40)	30(2)	30(2)	32(2)	-8(1)	3(1)	-15(1)
C(41)	25(1)	39(2)	30(2)	-11(1)	6(1)	-11(1)
C(42)	53(2)	55(2)	41(2)	-15(2)	22(2)	-28(2)
C(43)	29(2)	41(2)	34(2)	-19(2)	7(1)	-10(1)
C(44)	26(1)	31(2)	30(2)	-12(1)	-1(1)	-7(1)
C(45)	44(2)	43(2)	42(2)	-24(2)	11(1)	-17(2)

Table S87. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for b4b.

	x	y	z	U(eq)
H(2)	5351	1942	5408	49
H(3)	7911	1318	5651	64
H(4)	9107	1933	4313	65
H(5)	7736	3147	2737	47
H(10)	1616	4800	-183	38
H(11)	816	6740	-1331	45
H(12)	1913	7965	-1262	45
H(15)	3918	8820	-535	47
H(16)	5682	8972	357	56
H(17)	7078	7413	1847	51
H(18)	6819	5646	2457	42
H(24)	5872	-1038	3013	38

H(25)	4242	-1712	2565	46
H(26)	1905	-428	1615	48
H(27)	1150	1542	1087	42
H(30A)	4713	5921	3376	57
H(30B)	4625	4720	4144	57
H(30C)	3668	5886	4188	57
H(31)	2363	7468	2256	37
H(33A)	553	8479	226	73
H(33B)	175	8939	1023	73
H(33C)	-972	8559	640	73
H(34)	-461	6491	1276	40
H(36A)	-503	4682	2066	58
H(36B)	264	3879	3199	58
H(36C)	1152	3733	2355	58
H(39A)	2434	1792	3529	65
H(39B)	3108	515	4436	65
H(39C)	4080	1297	4117	65
H(40)	1820	456	5675	38
H(42A)	-404	1325	7133	76
H(42B)	1240	447	7718	76
H(42C)	429	229	6957	76
H(43)	804	2836	6622	42
H(45A)	2952	4145	5655	62
H(45B)	1305	4467	5899	62
H(45C)	1553	4937	4778	62

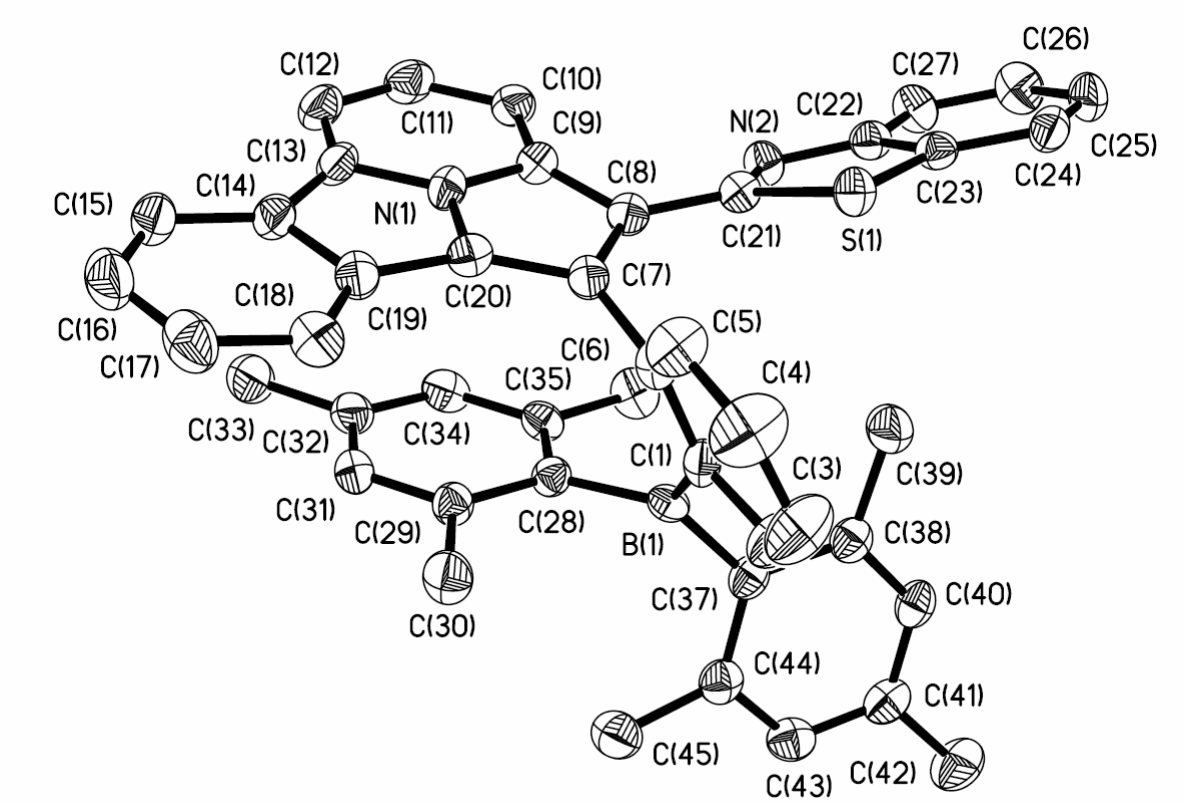


Figure S108. A diagram showing the crystal structure of **B4b** with labeling schemes and 35% thermal ellipsoids. H atoms are omitted for clarity.

Table S88. Crystal data and structure refinement for 5a.

Identification code	zc5a	
Empirical formula	C41 H35 B N2 S	
Formula weight	598.58	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.384(3) Å	α= 90°.
	b = 12.918(3) Å	β= 125.50(2)°.
	c = 22.321(7) Å	γ = 90°.
Volume	3141.8(16) $Å^3$	
Z	4	
Density (calculated)	1.265 Mg/m^3	
Absorption coefficient	0.136 mm^{-1}	
F(000)	1264	
Crystal size	0.170 x 0.130 x 0.100 mm^3	
Theta range for data collection	2.191 to 27.699°.	
Index ranges	-17<=h<=17, -16<=k<=16, -29<=l<=28	
Reflections collected	51049	
Independent reflections	7337 [R(int) = 0.1109]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7337 / 0 / 412	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0507, wR2 = 0.1088	
R indices (all data)	R1 = 0.0922, wR2 = 0.1251	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.267 and -0.361 $e.Å^{-3}$	

Table S89. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	7885(2)	1665(2)	5222(1)	22(1)
C(1)	7917(2)	2413(1)	5831(1)	24(1)
N(1)	9160(1)	1975(1)	5276(1)	22(1)
S(1)	10661(1)	2949(1)	5132(1)	31(1)
C(2)	7785(2)	1993(2)	6361(1)	29(1)
N(2)	7393(1)	5115(1)	4318(1)	24(1)
C(3)	7695(2)	2590(2)	6843(1)	35(1)
C(4)	7755(2)	3652(2)	6822(1)	34(1)
C(5)	7896(2)	4106(2)	6317(1)	29(1)
C(6)	7958(2)	3499(1)	5816(1)	24(1)
C(7)	7944(2)	4047(1)	5236(1)	23(1)
C(8)	8595(2)	3803(1)	4933(1)	23(1)
C(9)	9382(2)	2912(1)	5128(1)	23(1)
C(10)	10035(2)	1271(1)	5388(1)	27(1)
C(11)	10902(2)	1659(2)	5331(1)	32(1)
C(12)	8254(2)	4503(1)	4357(1)	23(1)
C(13)	8243(2)	4794(1)	3729(1)	27(1)
C(14)	8936(2)	4496(2)	3475(1)	38(1)
C(15)	8687(2)	4936(2)	2841(1)	49(1)
C(16)	7754(2)	5666(2)	2446(1)	55(1)
C(17)	7068(2)	5986(2)	2686(1)	46(1)
C(18)	7312(2)	5561(2)	3331(1)	31(1)
C(19)	6756(2)	5751(1)	3714(1)	28(1)
C(20)	5819(2)	6299(2)	3647(1)	38(1)
C(21)	5568(2)	6155(2)	4169(1)	38(1)
C(22)	6206(2)	5466(2)	4747(1)	31(1)
C(23)	7168(2)	4890(1)	4830(1)	24(1)
C(24)	6759(2)	2032(1)	4373(1)	23(1)
C(25)	5690(2)	2534(2)	4216(1)	31(1)
C(26)	4939(2)	3099(2)	3569(1)	46(1)
C(27)	5168(2)	3185(2)	3047(1)	53(1)

C(28)	6112(2)	2598(2)	3155(1)	46(1)
C(29)	6869(2)	2005(2)	3782(1)	33(1)
C(30)	7767(2)	1297(2)	3772(1)	53(1)
C(31)	4365(3)	3852(2)	2373(2)	94(1)
C(32)	5265(2)	2460(2)	4709(1)	53(1)
C(33)	8043(2)	446(1)	5476(1)	24(1)
C(34)	9086(2)	124(1)	6174(1)	27(1)
C(35)	9208(2)	-891(2)	6419(1)	32(1)
C(36)	8327(2)	-1635(2)	6006(1)	33(1)
C(37)	7302(2)	-1336(2)	5332(1)	32(1)
C(38)	7137(2)	-327(1)	5061(1)	27(1)
C(39)	5937(2)	-138(2)	4323(1)	42(1)
C(40)	8463(2)	-2727(2)	6292(2)	48(1)
C(41)	10142(2)	828(2)	6727(1)	33(1)

Table S90. Bond lengths [Å] and angles [°] for 5a.

B(1)-C(33)	1.644(3)	C(7)-C(8)	1.414(2)
B(1)-C(1)	1.648(3)	C(8)-C(12)	1.414(3)
B(1)-C(24)	1.664(3)	C(8)-C(9)	1.446(2)
B(1)-N(1)	1.688(2)	C(10)-C(11)	1.337(3)
C(1)-C(2)	1.403(2)	C(12)-C(13)	1.443(3)
C(1)-C(6)	1.406(3)	C(13)-C(14)	1.393(3)
N(1)-C(9)	1.332(2)	C(13)-C(18)	1.427(3)
N(1)-C(10)	1.386(2)	C(14)-C(15)	1.374(3)
S(1)-C(11)	1.707(2)	C(15)-C(16)	1.396(3)
S(1)-C(9)	1.7079(18)	C(16)-C(17)	1.368(3)
C(2)-C(3)	1.384(3)	C(17)-C(18)	1.392(3)
N(2)-C(12)	1.358(2)	C(18)-C(19)	1.443(3)
N(2)-C(23)	1.370(2)	C(19)-C(20)	1.371(3)
N(2)-C(19)	1.373(2)	C(20)-C(21)	1.400(3)
C(3)-C(4)	1.376(3)	C(21)-C(22)	1.381(3)
C(4)-C(5)	1.377(3)	C(22)-C(23)	1.403(2)
C(5)-C(6)	1.406(2)	C(24)-C(29)	1.411(3)
C(6)-C(7)	1.466(3)	C(24)-C(25)	1.418(3)
C(7)-C(23)	1.412(2)	C(25)-C(26)	1.395(3)

C(25)-C(32)	1.506(3)	C(5)-C(6)-C(1)	121.12(17)
C(26)-C(27)	1.370(4)	C(5)-C(6)-C(7)	117.20(16)
C(27)-C(28)	1.370(4)	C(1)-C(6)-C(7)	121.42(15)
C(27)-C(31)	1.512(3)	C(23)-C(7)-C(8)	107.04(16)
C(28)-C(29)	1.387(3)	C(23)-C(7)-C(6)	124.50(15)
C(29)-C(30)	1.520(3)	C(8)-C(7)-C(6)	128.26(16)
C(33)-C(38)	1.422(3)	C(12)-C(8)-C(7)	109.18(15)
C(33)-C(34)	1.423(3)	C(12)-C(8)-C(9)	125.27(16)
C(34)-C(35)	1.393(3)	C(7)-C(8)-C(9)	125.24(16)
C(34)-C(41)	1.525(3)	N(1)-C(9)-C(8)	124.73(15)
C(35)-C(36)	1.379(3)	N(1)-C(9)-S(1)	113.02(13)
C(36)-C(37)	1.378(3)	C(8)-C(9)-S(1)	122.12(13)
C(36)-C(40)	1.516(3)	C(11)-C(10)-N(1)	115.18(17)
C(37)-C(38)	1.399(3)	C(10)-C(11)-S(1)	110.34(14)
C(38)-C(39)	1.511(3)	N(2)-C(12)-C(8)	104.15(15)
		N(2)-C(12)-C(13)	104.89(15)
C(33)-B(1)-C(1)	109.91(15)	C(8)-C(12)-C(13)	149.97(16)
C(33)-B(1)-C(24)	121.02(15)	C(14)-C(13)-C(18)	119.04(18)
C(1)-B(1)-C(24)	110.16(14)	C(14)-C(13)-C(12)	133.63(18)
C(33)-B(1)-N(1)	106.29(13)	C(18)-C(13)-C(12)	107.32(16)
C(1)-B(1)-N(1)	105.14(14)	C(15)-C(14)-C(13)	119.0(2)
C(24)-B(1)-N(1)	102.88(13)	C(14)-C(15)-C(16)	121.6(2)
C(2)-C(1)-C(6)	115.55(16)	C(17)-C(16)-C(15)	120.9(2)
C(2)-C(1)-B(1)	120.88(16)	C(16)-C(17)-C(18)	118.6(2)
C(6)-C(1)-B(1)	123.30(15)	C(17)-C(18)-C(13)	120.90(18)
C(9)-N(1)-C(10)	110.80(14)	C(17)-C(18)-C(19)	130.81(19)
C(9)-N(1)-B(1)	124.01(14)	C(13)-C(18)-C(19)	108.29(17)
C(10)-N(1)-B(1)	124.75(14)	C(20)-C(19)-N(2)	115.04(17)
C(11)-S(1)-C(9)	90.65(9)	C(20)-C(19)-C(18)	140.98(19)
C(3)-C(2)-C(1)	123.35(18)	N(2)-C(19)-C(18)	103.90(15)
C(12)-N(2)-C(23)	114.36(15)	C(19)-C(20)-C(21)	119.13(19)
C(12)-N(2)-C(19)	115.51(15)	C(22)-C(21)-C(20)	123.12(18)
C(23)-N(2)-C(19)	129.33(15)	C(21)-C(22)-C(23)	119.14(18)
C(4)-C(3)-C(2)	119.76(18)	N(2)-C(23)-C(22)	114.00(17)
C(3)-C(4)-C(5)	119.35(18)	N(2)-C(23)-C(7)	105.24(15)
C(4)-C(5)-C(6)	120.85(18)	C(22)-C(23)-C(7)	140.36(18)

C(29)-C(24)-C(25)	114.80(17)	C(38)-C(33)-C(34)	115.49(16)
C(29)-C(24)-B(1)	122.74(16)	C(38)-C(33)-B(1)	123.93(16)
C(25)-C(24)-B(1)	121.86(15)	C(34)-C(33)-B(1)	120.38(16)
C(26)-C(25)-C(24)	120.75(19)	C(35)-C(34)-C(33)	121.49(18)
C(26)-C(25)-C(32)	116.06(19)	C(35)-C(34)-C(41)	113.71(17)
C(24)-C(25)-C(32)	123.14(18)	C(33)-C(34)-C(41)	124.79(16)
C(27)-C(26)-C(25)	122.8(2)	C(36)-C(35)-C(34)	122.27(19)
C(26)-C(27)-C(28)	116.4(2)	C(37)-C(36)-C(35)	117.20(18)
C(26)-C(27)-C(31)	120.8(3)	C(37)-C(36)-C(40)	121.43(19)
C(28)-C(27)-C(31)	122.7(3)	C(35)-C(36)-C(40)	121.3(2)
C(27)-C(28)-C(29)	122.8(2)	C(36)-C(37)-C(38)	122.69(18)
C(28)-C(29)-C(24)	121.2(2)	C(37)-C(38)-C(33)	120.86(18)
C(28)-C(29)-C(30)	116.04(19)	C(37)-C(38)-C(39)	115.03(17)
C(24)-C(29)-C(30)	122.74(19)	C(33)-C(38)-C(39)	124.10(17)

Table S91. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 5a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	21(1)	25(1)	23(1)	1(1)	15(1)	-1(1)
C(1)	22(1)	28(1)	20(1)	0(1)	12(1)	2(1)
N(1)	22(1)	22(1)	24(1)	0(1)	15(1)	0(1)
S(1)	28(1)	27(1)	48(1)	2(1)	27(1)	0(1)
C(2)	36(1)	31(1)	26(1)	4(1)	20(1)	4(1)
N(2)	24(1)	21(1)	27(1)	0(1)	15(1)	1(1)
C(3)	42(1)	47(1)	26(1)	4(1)	25(1)	6(1)
C(4)	36(1)	46(1)	26(1)	-7(1)	21(1)	3(1)
C(5)	30(1)	32(1)	27(1)	-6(1)	16(1)	2(1)
C(6)	21(1)	29(1)	22(1)	-1(1)	13(1)	2(1)
C(7)	23(1)	21(1)	25(1)	-4(1)	14(1)	-2(1)
C(8)	23(1)	22(1)	24(1)	-3(1)	14(1)	-2(1)
C(9)	24(1)	22(1)	24(1)	-3(1)	15(1)	-2(1)
C(10)	28(1)	23(1)	36(1)	3(1)	21(1)	6(1)
C(11)	30(1)	29(1)	44(1)	2(1)	25(1)	6(1)
C(12)	24(1)	19(1)	29(1)	-3(1)	18(1)	-1(1)

C(13)	32(1)	23(1)	30(1)	-3(1)	20(1)	-4(1)
C(14)	47(1)	37(1)	41(1)	2(1)	32(1)	5(1)
C(15)	69(2)	53(1)	51(2)	5(1)	50(1)	9(1)
C(16)	81(2)	58(2)	44(2)	15(1)	46(2)	13(1)
C(17)	58(2)	46(1)	39(1)	12(1)	31(1)	13(1)
C(18)	35(1)	31(1)	30(1)	2(1)	20(1)	3(1)
C(19)	31(1)	25(1)	28(1)	2(1)	16(1)	1(1)
C(20)	35(1)	39(1)	33(1)	7(1)	16(1)	12(1)
C(21)	32(1)	39(1)	44(1)	3(1)	22(1)	12(1)
C(22)	28(1)	33(1)	37(1)	-3(1)	22(1)	2(1)
C(23)	26(1)	23(1)	26(1)	-4(1)	17(1)	-2(1)
C(24)	25(1)	25(1)	22(1)	-3(1)	14(1)	-6(1)
C(25)	25(1)	33(1)	27(1)	-5(1)	11(1)	-1(1)
C(26)	35(1)	36(1)	36(1)	-6(1)	2(1)	5(1)
C(27)	58(2)	38(1)	24(1)	2(1)	2(1)	-16(1)
C(28)	50(1)	58(2)	20(1)	-4(1)	15(1)	-28(1)
C(29)	32(1)	45(1)	23(1)	-10(1)	17(1)	-18(1)
C(30)	42(1)	88(2)	38(1)	-31(1)	29(1)	-18(1)
C(31)	111(3)	56(2)	38(2)	18(1)	-1(2)	-7(2)
C(32)	27(1)	90(2)	46(2)	-13(1)	23(1)	2(1)
C(33)	26(1)	26(1)	25(1)	-1(1)	18(1)	0(1)
C(34)	27(1)	28(1)	29(1)	2(1)	19(1)	2(1)
C(35)	32(1)	31(1)	33(1)	7(1)	20(1)	5(1)
C(36)	42(1)	25(1)	46(1)	6(1)	34(1)	3(1)
C(37)	38(1)	27(1)	42(1)	-5(1)	30(1)	-8(1)
C(38)	31(1)	28(1)	30(1)	-3(1)	22(1)	-3(1)
C(39)	40(1)	35(1)	34(1)	-3(1)	12(1)	-14(1)
C(40)	55(2)	30(1)	70(2)	12(1)	43(1)	4(1)
C(41)	32(1)	35(1)	27(1)	4(1)	14(1)	0(1)

Table S92. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 5a.

	x	y	z	U(eq)
H(2)	7756	1261	6391	35

H(3)	7592	2269	7186	42
H(4)	7701	4068	7153	41
H(5)	7952	4838	6306	35
H(10)	10020	563	5499	33
H(11)	11559	1272	5392	39
H(14)	9570	3996	3736	45
H(15)	9162	4739	2669	59
H(16)	7592	5945	2004	67
H(17)	6438	6487	2418	56
H(20)	5346	6771	3252	45
H(21)	4928	6550	4123	46
H(22)	5996	5383	5084	38
H(26)	4240	3439	3486	56
H(28)	6254	2598	2785	55
H(30A)	7374	1007	3278	79
H(30B)	8013	734	4126	79
H(30C)	8494	1695	3906	79
H(31A)	4048	4437	2496	141
H(31B)	3677	3439	1982	141
H(31C)	4848	4113	2204	141
H(32A)	5559	3064	5035	79
H(32B)	5594	1828	5005	79
H(32C)	4366	2441	4407	79
H(35)	9923	-1077	6886	38
H(37)	6682	-1835	5038	38
H(39A)	5479	-789	4134	63
H(39B)	6102	130	3977	63
H(39C)	5450	369	4378	63
H(40A)	9318	-2846	6708	72
H(40B)	8230	-3224	5900	72
H(40C)	7928	-2817	6456	72
H(41A)	10260	787	7202	50
H(41B)	9952	1544	6548	50
H(41C)	10895	608	6785	50

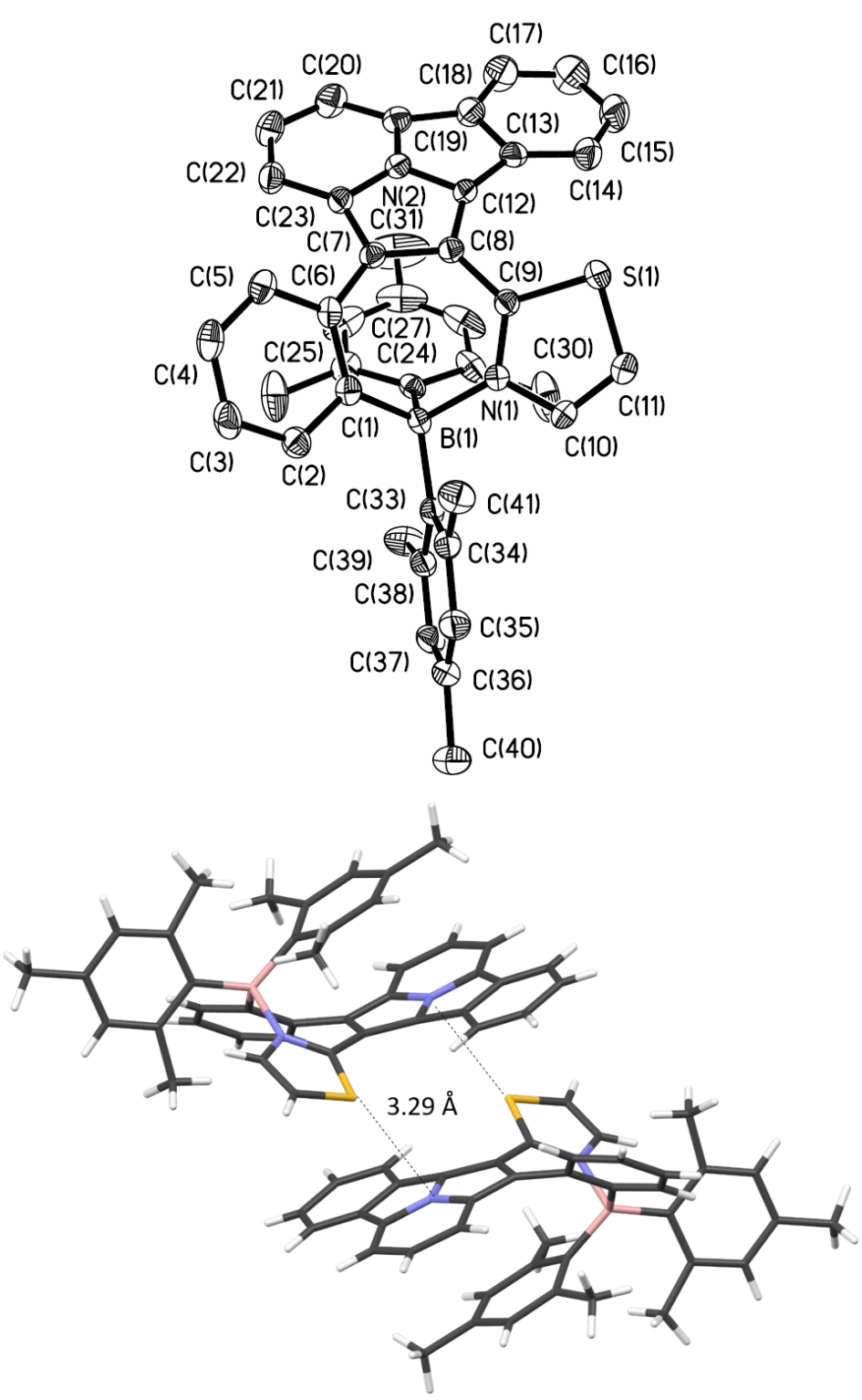


Figure S109. Top: A diagram showing the structure of **5a** with labeling schemes. H atoms are omitted for clarity. Bottom: a packing diagram showing key short contacts in the crystal lattice of **5a**.

Table S93. Crystal data and structure refinement for 5b.

Identification code	zc5b	
Empirical formula	C42 H37 B1 Cl2 N2 S1	
Formula weight	683.56	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.681(9) Å	α= 67.96(3)°.
	b = 11.761(11) Å	β= 84.76(4)°.
	c = 15.247(16) Å	γ = 83.27(3)°.
Volume	1761(3) $Å^3$	
Z	2	
Density (calculated)	1.289 Mg/m^3	
Absorption coefficient	0.277 mm^{-1}	
F(000)	716	
Crystal size	0.130 x 0.120 x 0.070 mm^3	
Theta range for data collection	2.344 to 25.245°.	
Index ranges	-12<=h<=12, -13<=k<=13, -17<=l<=17	
Reflections collected	17171	
Independent reflections	6055 [R(int) = 0.1381]	
Completeness to theta = 25.242°	94.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.756 and 0.546	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6055 / 0 / 439	
Goodness-of-fit on F^2	0.961	
Final R indices [I>2sigma(I)]	R1 = 0.0680, wR2 = 0.1613	
R indices (all data)	R1 = 0.1505, wR2 = 0.2048	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.367 and -0.460 $e.Å^{-3}$	

Table S94. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	3321(4)	8112(4)	8180(3)	22(1)
C(1)	4874(4)	8175(4)	7916(3)	23(1)
Cl(1)	2090(1)	7383(1)	2155(1)	56(1)
N(1)	3215(3)	6698(3)	9045(2)	24(1)
S(1)	3317(1)	4337(1)	9957(1)	34(1)
C(2)	5481(4)	9181(4)	7935(3)	27(1)
Cl(2)	222(2)	5648(2)	2412(1)	75(1)
N(2)	5007(3)	4614(3)	7036(3)	28(1)
C(3)	6737(4)	9373(4)	7629(3)	36(1)
C(4)	7460(4)	8526(4)	7300(3)	32(1)
C(5)	6924(4)	7501(4)	7284(3)	32(1)
C(6)	5649(4)	7324(4)	7558(3)	25(1)
C(7)	5174(4)	6221(4)	7471(3)	23(1)
C(8)	4295(4)	5456(4)	8111(3)	24(1)
C(9)	3636(4)	5608(4)	8947(3)	25(1)
C(10)	2544(4)	5301(4)	10505(3)	36(1)
C(11)	2577(4)	6507(4)	9929(3)	29(1)
C(12)	2712(4)	9127(4)	8684(3)	20(1)
C(13)	3250(4)	9157(4)	9518(3)	23(1)
C(14)	2739(4)	9978(4)	9978(3)	27(1)
C(15)	1679(4)	10812(4)	9666(3)	27(1)
C(16)	1149(4)	10795(4)	8865(3)	28(1)
C(17)	1626(4)	10009(4)	8369(3)	22(1)
C(18)	889(5)	10167(4)	7507(3)	39(1)
C(19)	1104(4)	11666(4)	10183(4)	40(1)
C(20)	4375(4)	8294(4)	10005(3)	30(1)
C(21)	2617(4)	8122(4)	7237(3)	25(1)
C(22)	2988(4)	8932(4)	6294(3)	30(1)
C(23)	2412(5)	8960(4)	5481(3)	39(1)
C(24)	1410(5)	8260(4)	5545(4)	40(1)
C(25)	1010(4)	7522(4)	6454(4)	36(1)

C(26)	1576(4)	7438(4)	7290(3)	27(1)
C(27)	879(4)	6706(4)	8218(3)	38(1)
C(28)	3916(5)	9902(4)	6101(3)	46(1)
C(29)	765(6)	8364(5)	4660(4)	62(2)
C(30)	4190(4)	4411(4)	7831(3)	25(1)
C(31)	3566(4)	3322(4)	8087(3)	33(1)
C(32)	3853(4)	2550(4)	7553(4)	38(1)
C(33)	4711(4)	2799(4)	6761(3)	35(1)
C(34)	5309(4)	3892(4)	6478(3)	28(1)
C(35)	6223(4)	4568(4)	5768(3)	31(1)
C(36)	6889(4)	4287(4)	5012(3)	39(1)
C(37)	7745(5)	5112(5)	4436(4)	45(1)
C(38)	7907(5)	6197(5)	4599(4)	47(1)
C(39)	7273(4)	6490(4)	5337(3)	38(1)
C(40)	6414(4)	5666(4)	5949(3)	28(1)
C(41)	5625(4)	5664(4)	6795(3)	27(1)
C(42)	961(5)	6479(5)	2939(4)	50(2)

Table S95. Bond lengths [Å] and angles [°] for 5b.

B(1)-C(1)	1.675(6)	C(3)-C(4)	1.402(6)
B(1)-C(21)	1.678(7)	C(4)-C(5)	1.401(6)
B(1)-C(12)	1.688(6)	C(5)-C(6)	1.404(6)
B(1)-N(1)	1.700(6)	C(6)-C(7)	1.502(6)
C(1)-C(2)	1.426(6)	C(7)-C(8)	1.419(5)
C(1)-C(6)	1.454(6)	C(7)-C(41)	1.438(6)
Cl(1)-C(42)	1.760(5)	C(8)-C(9)	1.460(6)
N(1)-C(9)	1.366(5)	C(8)-C(30)	1.463(6)
N(1)-C(11)	1.404(5)	C(10)-C(11)	1.362(6)
S(1)-C(9)	1.737(4)	C(12)-C(17)	1.449(6)
S(1)-C(10)	1.740(5)	C(12)-C(13)	1.456(6)
C(2)-C(3)	1.395(6)	C(13)-C(14)	1.427(6)
Cl(2)-C(42)	1.764(6)	C(13)-C(20)	1.529(6)
N(2)-C(41)	1.379(5)	C(14)-C(15)	1.400(6)
N(2)-C(30)	1.388(5)	C(15)-C(16)	1.400(6)
N(2)-C(34)	1.407(5)	C(15)-C(19)	1.539(6)

C(16)-C(17)	1.426(6)	C(9)-S(1)-C(10)	90.3(2)
C(17)-C(18)	1.534(6)	C(3)-C(2)-C(1)	123.5(4)
C(21)-C(26)	1.426(6)	C(41)-N(2)-C(30)	113.6(4)
C(21)-C(22)	1.445(6)	C(41)-N(2)-C(34)	117.0(4)
C(22)-C(23)	1.422(7)	C(30)-N(2)-C(34)	129.4(4)
C(22)-C(28)	1.527(6)	C(2)-C(3)-C(4)	118.9(4)
C(23)-C(24)	1.400(7)	C(5)-C(4)-C(3)	120.2(4)
C(24)-C(25)	1.390(7)	C(4)-C(5)-C(6)	121.2(4)
C(24)-C(29)	1.530(7)	C(5)-C(6)-C(1)	120.0(4)
C(25)-C(26)	1.425(7)	C(5)-C(6)-C(7)	116.2(4)
C(26)-C(27)	1.531(6)	C(1)-C(6)-C(7)	123.8(4)
C(30)-C(31)	1.419(6)	C(8)-C(7)-C(41)	107.3(4)
C(31)-C(32)	1.424(6)	C(8)-C(7)-C(6)	125.8(4)
C(32)-C(33)	1.408(6)	C(41)-C(7)-C(6)	126.5(4)
C(33)-C(34)	1.404(6)	C(7)-C(8)-C(9)	127.5(4)
C(34)-C(35)	1.449(6)	C(7)-C(8)-C(30)	108.6(4)
C(35)-C(36)	1.424(6)	C(9)-C(8)-C(30)	123.8(3)
C(35)-C(40)	1.457(6)	N(1)-C(9)-C(8)	126.4(4)
C(36)-C(37)	1.403(6)	N(1)-C(9)-S(1)	112.7(3)
C(37)-C(38)	1.421(7)	C(8)-C(9)-S(1)	120.9(3)
C(38)-C(39)	1.393(7)	C(11)-C(10)-S(1)	111.1(3)
C(39)-C(40)	1.424(6)	C(10)-C(11)-N(1)	114.4(4)
C(40)-C(41)	1.473(6)	C(17)-C(12)-C(13)	113.7(4)
		C(17)-C(12)-B(1)	125.3(4)
C(1)-B(1)-C(21)	108.7(3)	C(13)-C(12)-B(1)	121.0(4)
C(1)-B(1)-C(12)	112.7(3)	C(14)-C(13)-C(12)	122.6(4)
C(21)-B(1)-C(12)	117.7(3)	C(14)-C(13)-C(20)	113.6(4)
C(1)-B(1)-N(1)	103.7(3)	C(12)-C(13)-C(20)	123.8(4)
C(21)-B(1)-N(1)	107.5(3)	C(15)-C(14)-C(13)	122.7(4)
C(12)-B(1)-N(1)	105.4(3)	C(14)-C(15)-C(16)	115.5(4)
C(2)-C(1)-C(6)	116.0(4)	C(14)-C(15)-C(19)	122.6(4)
C(2)-C(1)-B(1)	119.9(4)	C(16)-C(15)-C(19)	121.9(4)
C(6)-C(1)-B(1)	123.8(4)	C(15)-C(16)-C(17)	124.3(4)
C(9)-N(1)-C(11)	111.4(3)	C(16)-C(17)-C(12)	121.2(4)
C(9)-N(1)-B(1)	124.9(3)	C(16)-C(17)-C(18)	114.7(4)
C(11)-N(1)-B(1)	123.5(3)	C(12)-C(17)-C(18)	124.1(4)

C(26)-C(21)-C(22)	115.0(4)	Cl(1)-C(42)-Cl(2)	111.8(3)
C(26)-C(21)-B(1)	124.5(4)		
C(22)-C(21)-B(1)	120.3(4)		
C(23)-C(22)-C(21)	121.7(4)		
C(23)-C(22)-C(28)	115.0(4)		
C(21)-C(22)-C(28)	123.1(4)		
C(24)-C(23)-C(22)	122.3(4)		
C(25)-C(24)-C(23)	116.2(5)		
C(25)-C(24)-C(29)	122.8(5)		
C(23)-C(24)-C(29)	121.0(5)		
C(24)-C(25)-C(26)	123.6(4)		
C(25)-C(26)-C(21)	121.0(4)		
C(25)-C(26)-C(27)	114.8(4)		
C(21)-C(26)-C(27)	123.8(4)		
N(2)-C(30)-C(31)	113.6(4)		
N(2)-C(30)-C(8)	104.1(3)		
C(31)-C(30)-C(8)	142.2(4)		
C(30)-C(31)-C(32)	119.2(4)		
C(33)-C(32)-C(31)	124.4(4)		
C(34)-C(33)-C(32)	117.3(4)		
C(33)-C(34)-N(2)	116.1(4)		
C(33)-C(34)-C(35)	140.4(4)		
N(2)-C(34)-C(35)	103.5(4)		
C(36)-C(35)-C(34)	130.0(4)		
C(36)-C(35)-C(40)	121.9(4)		
C(34)-C(35)-C(40)	108.1(4)		
C(37)-C(36)-C(35)	117.5(5)		
C(36)-C(37)-C(38)	120.5(5)		
C(39)-C(38)-C(37)	123.1(5)		
C(38)-C(39)-C(40)	118.2(5)		
C(39)-C(40)-C(35)	118.7(4)		
C(39)-C(40)-C(41)	132.8(4)		
C(35)-C(40)-C(41)	108.5(3)		
N(2)-C(41)-C(7)	106.3(4)		
N(2)-C(41)-C(40)	102.8(4)		
C(7)-C(41)-C(40)	150.8(4)		

Table S96. Anisotropic displacement parameters ($Å^2$x 10^3) for 5b. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	26(3)	18(3)	18(3)	-2(2)	-1(2)	1(2)
C(1)	31(2)	19(2)	17(2)	-5(2)	1(2)	-1(2)
Cl(1)	45(1)	60(1)	55(1)	-11(1)	2(1)	-10(1)
N(1)	29(2)	19(2)	22(2)	-6(2)	0(2)	0(2)
S(1)	45(1)	21(1)	29(1)	-3(1)	6(1)	0(1)
C(2)	33(3)	26(2)	21(3)	-11(2)	-2(2)	2(2)
Cl(2)	84(1)	76(1)	81(1)	-43(1)	25(1)	-37(1)
N(2)	34(2)	20(2)	28(2)	-7(2)	4(2)	-1(2)
C(3)	36(3)	30(3)	43(3)	-13(2)	3(2)	-14(2)
C(4)	26(2)	36(3)	33(3)	-11(2)	6(2)	-10(2)
C(5)	30(3)	29(3)	32(3)	-9(2)	4(2)	3(2)
C(6)	31(2)	23(2)	19(2)	-5(2)	-2(2)	-4(2)
C(7)	24(2)	17(2)	27(3)	-10(2)	-1(2)	4(2)
C(8)	22(2)	20(2)	29(3)	-7(2)	2(2)	2(2)
C(9)	29(2)	17(2)	27(3)	-5(2)	-6(2)	0(2)
C(10)	47(3)	28(3)	27(3)	-9(2)	11(2)	-1(2)
C(11)	36(3)	24(3)	25(3)	-8(2)	2(2)	1(2)
C(12)	23(2)	17(2)	18(2)	-4(2)	-3(2)	2(2)
C(13)	25(2)	24(2)	20(2)	-8(2)	-1(2)	-3(2)
C(14)	32(3)	28(2)	24(3)	-12(2)	-2(2)	-9(2)
C(15)	34(3)	19(2)	27(3)	-8(2)	3(2)	-6(2)
C(16)	25(2)	17(2)	38(3)	-7(2)	-2(2)	4(2)
C(17)	30(2)	17(2)	19(2)	-6(2)	0(2)	-1(2)
C(18)	47(3)	32(3)	38(3)	-15(2)	-15(2)	16(2)
C(19)	45(3)	34(3)	46(3)	-25(3)	10(3)	-2(2)
C(20)	34(3)	33(3)	22(3)	-10(2)	-8(2)	3(2)
C(21)	34(3)	15(2)	23(3)	-8(2)	4(2)	3(2)
C(22)	33(3)	29(3)	27(3)	-12(2)	2(2)	5(2)
C(23)	47(3)	41(3)	20(3)	-5(2)	-2(2)	8(3)
C(24)	48(3)	35(3)	40(3)	-19(3)	-14(3)	13(2)
C(25)	38(3)	29(3)	45(3)	-16(3)	-12(2)	1(2)
C(26)	30(2)	21(2)	29(3)	-11(2)	-4(2)	8(2)

C(27)	31(3)	36(3)	44(3)	-8(3)	-5(2)	-6(2)
C(28)	57(3)	42(3)	27(3)	4(2)	-5(3)	-13(3)
C(29)	79(4)	66(4)	48(4)	-28(3)	-31(3)	6(3)
C(30)	25(2)	22(2)	24(3)	-5(2)	3(2)	4(2)
C(31)	35(3)	24(2)	36(3)	-6(2)	-1(2)	-4(2)
C(32)	36(3)	27(3)	47(3)	-9(2)	-1(2)	-6(2)
C(33)	42(3)	22(2)	41(3)	-13(2)	0(2)	0(2)
C(34)	29(2)	25(2)	36(3)	-19(2)	-8(2)	5(2)
C(35)	26(2)	32(3)	32(3)	-13(2)	2(2)	5(2)
C(36)	40(3)	40(3)	41(3)	-23(3)	-1(3)	4(2)
C(37)	45(3)	55(3)	40(3)	-26(3)	10(3)	0(3)
C(38)	45(3)	49(3)	42(3)	-15(3)	13(3)	-6(3)
C(39)	42(3)	35(3)	35(3)	-14(2)	12(2)	-4(2)
C(40)	29(2)	24(2)	28(3)	-8(2)	2(2)	4(2)
C(41)	27(2)	17(2)	32(3)	-5(2)	-2(2)	0(2)
C(42)	57(3)	51(3)	40(3)	-14(3)	0(3)	-6(3)

Table S97. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 5b.

	x	y	z	U(eq)
H(2)	5005	9752	8169	32
H(3)	7097	10067	7644	43
H(4)	8315	8646	7086	38
H(5)	7434	6916	7085	38
H(10)	2151	5023	11124	43
H(11)	2200	7164	10110	35
H(14)	3135	9957	10518	32
H(16)	423	11345	8637	33
H(18A)	108	10697	7502	59
H(18B)	684	9360	7543	59
H(18C)	1405	10546	6926	59
H(19A)	353	11327	10568	60
H(19B)	868	12485	9717	60
H(19C)	1726	11728	10594	60
H(20A)	5043	8781	10032	44
H(20B)	4694	7773	9645	44

H(20C)	4107	7773	10649	44
H(23)	2719	9471	4872	47
H(25)	321	7048	6522	43
H(27A)	17	6628	8091	58
H(27B)	851	7137	8660	58
H(27C)	1323	5885	8498	58
H(28A)	4782	9520	6099	69
H(28B)	3794	10252	6597	69
H(28C)	3768	10557	5483	69
H(29A)	328	7625	4792	92
H(29B)	1401	8443	4139	92
H(29C)	153	9092	4480	92
H(31)	2965	3111	8609	40
H(32)	3437	1817	7744	45
H(33)	4879	2250	6431	42
H(36)	6759	3568	4900	46
H(37)	8219	4943	3934	54
H(38)	8475	6749	4185	56
H(39)	7409	7220	5429	46
H(42A)	314	7020	3140	60
H(42B)	1378	5895	3512	60

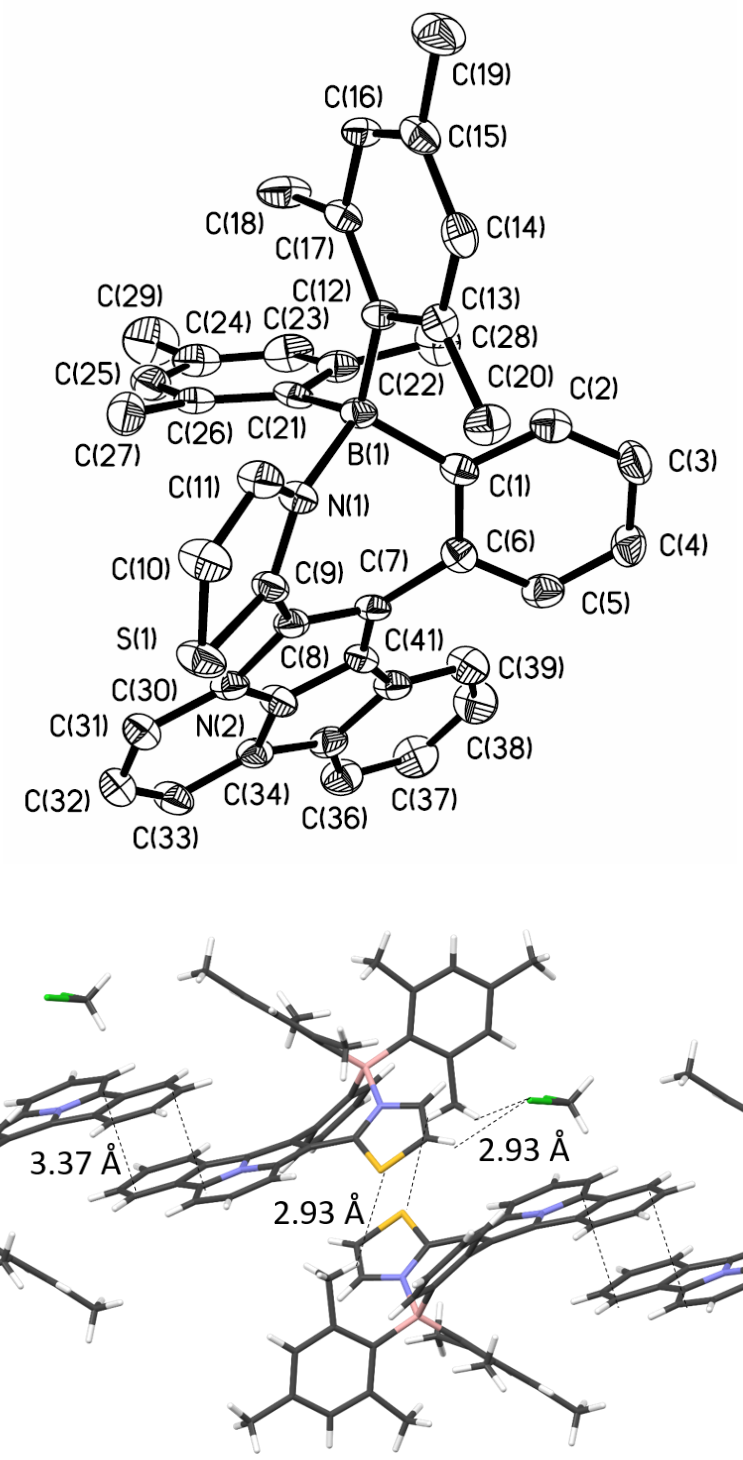


Figure S110. Top: A diagram showing the structure of **5b** with labeling schemes. H atoms are omitted for clarity. Bottom: a packing diagram showing key short contacts in the crystal lattice of **5b**.

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