

Supplementary Information For:

Late-Stage Direct Double Borylation of B/N-based Multi-Resonance Framework Enables High-Performance Ultra-Narrowband Deep-Blue Organic Light-Emitting Diodes

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Supplementary Tables

Supplementary Table 1: Summary of TD-DFT calculation. ν -DABNA-core, ν -DABNA-B-Mes, ν -DABNA-M and ν -DABNA-M-B-Mes were calculated at the B3LYP/6-31G(d) level of theory.

compound	HOMO-1 [eV]	HOMO [eV]	LUMO [eV]	LUMO+1 [eV]	$\lambda_{(S_0-S_1)}$ [nm]	E_S^a [eV]	f^b	$\lambda_{(S_0-T_1)}$ [nm]	E_T^c [eV]	ΔE_{ST}^d [eV]
ν -DABNA-core	-4.79	-4.56	-1.16	-0.67	425	2.92	0.4461	486	2.55	0.37
ν -DABNA-B-Mes	-5.35	-5.14	-1.80	-1.41	433	2.86	0.7267	486	2.55	0.31
ν -DABNA-M	-4.74	-4.49	-1.09	-0.58	425	2.92	0.4582	485	2.56	0.36
ν -DABNA-M-B-Mes	-5.28	-5.07	-1.72	-1.32	433	2.86	0.7370	485	2.56	0.30

^aSinglet-singlet excitation energy. ^bOscillator strength. ^cSinglet-triplet excitation energy. ^dEnergy gap between S_1 and T_1 states.

compound	transition	energy	coefficient of orbital		
ν -DABNA-core	S_0-S_1	2.92 eV (425 nm)	HOMO $\rightarrow$ LUMO (0.69256)	HOMO-1 $\rightarrow$ LUMO+1 (0.11430)	
	S_0-T_1	2.55 eV (486 nm)	HOMO $\rightarrow$ LUMO (0.67530)	HOMO-1 $\rightarrow$ LUMO+1 (0.16379)	
	S_0-T_2	2.72 eV (455 nm)	HOMO-1 $\rightarrow$ LUMO (0.62701)	HOMO $\rightarrow$ LUMO+1 (0.25778)	
ν -DABNA-B-Mes	S_0-S_1	2.86 eV (433 nm)	HOMO $\rightarrow$ LUMO (0.68526)	HOMO-2 $\rightarrow$ LUMO+1 (-0.10451)	
	S_0-T_1	2.55 eV (486 nm)	HOMO $\rightarrow$ LUMO (0.64425)	HOMO-1 $\rightarrow$ LUMO+1 (-0.23957)	
	S_0-T_2	2.61 eV (476 nm)	HOMO-2 $\rightarrow$ LUMO (-0.33290) HOMO $\rightarrow$ LUMO+1 (-0.33877)	HOMO-1 $\rightarrow$ LUMO (0.46593)	HOMO-1 $\rightarrow$ LUMO+3 (0.11076)
ν -DABNA-M	S_0-S_1	2.92 eV (425 nm)	HOMO $\rightarrow$ LUMO (0.69371)	HOMO-1 $\rightarrow$ LUMO+1 (0.10900)	
	S_0-T_1	2.56 eV (485 nm)	HOMO $\rightarrow$ LUMO (0.67787)	HOMO-1 $\rightarrow$ LUMO+1 (0.15545)	
	S_0-T_2	2.75 eV (451 nm)	HOMO-1 $\rightarrow$ LUMO (0.62751)	HOMO $\rightarrow$ LUMO+1 (0.25561)	HOMO $\rightarrow$ LUMO+9 (0.10045)
ν -DABNA-M-B-Mes	S_0-S_1	2.86 eV (433 nm)	HOMO $\rightarrow$ LUMO (0.68610)	HOMO-2 $\rightarrow$ LUMO+1 (-0.10429)	
	S_0-T_1	2.56 eV (485 nm)	HOMO $\rightarrow$ LUMO (0.64863)	HOMO-1 $\rightarrow$ LUMO+1 (-0.22530)	
	S_0-T_2	2.62 eV (473 nm)	HOMO-2 $\rightarrow$ LUMO (-0.32175)	HOMO-1 $\rightarrow$ LUMO (0.48838)	HOMO $\rightarrow$ LUMO+1 (-0.31581)

Supplementary Table 2: Summary of TD-DFT calculation. ν -DABNA-core, ν -DABNA-B-Mes, ν -DABNA-M and ν -DABNA-M-B-Mes were calculated at the M06-2X/6-31G(d) level of theory.

compound	HOMO-1 [eV]	HOMO [eV]	LUMO [eV]	LUMO+1 [eV]	$\lambda_{(S_0-S_1)}$ [nm]	E_S^a [eV]	f^b	$\lambda_{(S_0-T_1)}$ [nm]	E_T^c [eV]	ΔE_{ST}^d [eV]
ν -DABNA-core	-6.01	-5.74	-0.47	0.09	366	3.38	0.5678	422	2.93	0.45
ν -DABNA-B-Mes	-6.54	-6.30	-1.10	-0.64	366	3.38	1.1537	428	2.89	0.49
ν -DABNA-M	-5.98	-5.69	-0.43	0.15	367	3.38	0.5793	422	2.93	0.45
ν -DABNA-M-B-Mes	-6.48	-6.24	-1.06	-0.56	368	3.37	1.1494	428	2.90	0.47

^aSinglet-singlet excitation energy. ^bOscillator strength. ^cSinglet-triplet excitation energy. ^dEnergy gap between S_1 and T_1 states.

compound	transition	energy	coefficient of orbital		
ν -DABNA-core	S_0-S_1	3.38 eV (366 nm)	HOMO $\rightarrow$ LUMO (0.65170)	HOMO-1 $\rightarrow$ LUMO+1 (0.21552)	
	S_0-T_1	2.93 eV (422 nm)	HOMO $\rightarrow$ LUMO (0.62793)	HOMO-1 $\rightarrow$ LUMO+1 (0.23429)	
	S_0-T_2	3.12 eV (397 nm)	HOMO-2 $\rightarrow$ LUMO (0.11815)	HOMO-1 $\rightarrow$ LUMO (0.51135)	
			HOMO $\rightarrow$ LUMO+1 (0.39962)		
ν -DABNA-B-Mes	S_0-S_1	3.38 eV (366 nm)	HOMO $\rightarrow$ LUMO (0.62826)	HOMO-1 $\rightarrow$ LUMO+1 (0.19688)	HOMO-1 $\rightarrow$ LUMO+2 (-0.15081)
	S_0-T_1	2.89 eV (428 nm)	HOMO $\rightarrow$ LUMO (0.53547)	HOMO-3 $\rightarrow$ LUMO (0.12190)	HOMO-1 $\rightarrow$ LUMO+1 (0.35606)
			HOMO $\rightarrow$ LUMO+3 (0.12773)		
	S_0-T_2	2.92 eV (423 nm)	HOMO-2 $\rightarrow$ LUMO (-0.16093)	HOMO-2 $\rightarrow$ LUMO+3 (0.10477)	HOMO-1 $\rightarrow$ LUMO (0.43927)
			HOMO-1 $\rightarrow$ LUMO+3 (-0.19117)	HOMO $\rightarrow$ LUMO+1 (0.41361)	
ν -DABNA-M	S_0-S_1	3.38 eV (367 nm)	HOMO $\rightarrow$ LUMO (0.65366)	HOMO-1 $\rightarrow$ LUMO+1 (0.21051)	
	S_0-T_1	2.93 eV (422 nm)	HOMO $\rightarrow$ LUMO (0.63020)	HOMO-1 $\rightarrow$ LUMO+1 (0.23046)	
	S_0-T_2	3.13 eV (396 nm)	HOMO-2 $\rightarrow$ LUMO (0.10923)	HOMO-1 $\rightarrow$ LUMO (0.51491)	HOMO $\rightarrow$ LUMO+1 (0.39839)
			HOMO $\rightarrow$ LUMO+2 (0.11043)		
ν -DABNA-M-B-Mes	S_0-S_1	3.37 eV (368 nm)	HOMO $\rightarrow$ LUMO (0.63214)	HOMO-1 $\rightarrow$ LUMO+2 (0.14306)	HOMO-1 $\rightarrow$ LUMO+1 (-0.18575)
	S_0-T_1	2.90 eV (428 nm)	HOMO $\rightarrow$ LUMO (0.55052)	HOMO $\rightarrow$ LUMO+3 (0.10687)	
	S_0-T_2	2.94 eV (421 nm)	HOMO-1 $\rightarrow$ LUMO (0.45709)	HOMO-1 $\rightarrow$ LUMO+3 (0.17143)	
			HOMO-2 $\rightarrow$ LUMO (-0.15206)		

Supplementary Table 3: Transition-dipole moment. The values were calculated at the M06-2X/6-31G(d) level of theory.

compound	state	X	Y	Z	Dip. (μ) [D]	Osc. (f)
v-DABNA-core	S ₁	0.0791	−2.6163	0.0000	6.6529	0.5678
	S ₂	0.0000	0.0000	1.7977	4.5692	0.2952
	S ₃	0.0000	0.0000	0.4682	1.1900	0.0214
v-DABNA-B-Mes	S ₁	1.2247	−3.5241	0.0000	9.4825	1.1537
	S ₂	0.0000	0.0000	0.8900	2.2621	0.0705
	S ₃	0.0000	0.0000	−0.3938	1.0010	0.0143

Supplementary Table 4: S₁, T₁ and T₂ vertical excitation energies and vertical excitation energy gaps of v-DABNA-core and v-DABNA-B-Mes. The calculation was performed at the SCS-CC2/def2TZVP//M062X/6-31G(d) level of theory (TURBOMOL).

compound	$E_{S_0-S_1}$ [eV]	%t1/%t2 [%]	$E_{S_0-T_1}$ [eV]	%t1/%t2 [%]	$E_{S_0-T_2}$ [eV]	%t1/%t2 [%]	$\Delta E_{S_1-T_1}$ [meV]	$\Delta E_{S_1-T_2}$ [meV]
v-DABNA-core	3.073	87.06/12.94	3.030	88.32/11.68	3.160	88.18/11.82	43	87
v-DABNA-B-Mes	3.087	86.84/13.16	3.053	88.17/11.83	3.093	88.60/11.40	34	6

Supplementary Table 5: Summary of photophysical data. v-DABNA-M and v-DABNA-M-B-Mes were doped at 1 wt% in PMMA films.

compound	λ_{ab}^a [nm]	λ_{em}^b [nm]	FWHM ^c [nm]	Φ^d [%]	τ_F^e [ns]	k_r/k_{nr}^f [10 ⁷ s ^{−1}]	λ_{em}^g [nm]	ΔE_{ST}^h [meV]
v-DABNA-M	465	473	17	92	4.6	16.4/1.4	497	117
v-DABNA-M-B-Mes	456	463	16	93	2.6	25.7/1.9	484	109

^aMaximum wavelength of absorption. ^bMaximum wavelength of fluorescence at 77 K. ^cFull width at half maximum. ^dAbsolute photoluminescence quantum yield. ^eLifetime of fluorescent (prompt) component. ^fRadiative and non-radiative rate constants. ^gMaximum wavelength of phosphorescence. ^hEnergy gap between S₁ and T₁ states.

Supplementary Table 6: Summary of electrochemical data. Cyclic voltammetry (CV) measurements were performed on a CHI6048E electrochemical workstation using *n*-Bu₄NPF₆ (0.1 M) in DMF as electrolyte solution and ferrocene as an internal reference.

compound	E_{ox}^a [V]	E_{red}^a [V]	ΔE_g^b [V]	HOMO ^c [eV]	LUMO ^c [eV]
PtON-TBBI	0.48	−2.68	3.16	−5.28	−2.12
ν-DABNA-M	0.40	−2.34	2.74	−5.20	−2.34
ν-DABNA-M-B-Mes	0.56	−2.54	3.10	−5.36	−2.26

^a E_{ox} and E_{red} are the peak of anodic and cathodic potentials from DPV versus Ag/Ag⁺. In degassed DMF with 0.1 M [*n*-Bu₄N]PF₆ as the supporting electrolyte and Fc/Fc⁺ as the internal reference.

^b $\Delta E_g = E_{\text{ox}} - E_{\text{red}}$. ^c $E_{\text{HOMO/LUMO}} = -(E_{\text{ox}} / E_{\text{red}} + 4.8)$ eV.

Supplementary Table 7: Summary of the EL performance. The representative deep-blue TADF-OLEDs using MR-TADF emitters (CIE_y ≤ 0.1). The MR-TADF emitters highlighted in red show a smaller FWHM compared to this work.

Emitter	λ_{EL}^a [nm]	FWHM ^b [nm]	V_{on}^c [V]	EQE [%] ^d Max/100/1000	CIE ^e (x, y)	CE _{max} ^f [cd A ^{−1}]	PE _{max} ^g [lm W ^{−1}]	ref
ν-DABNA-M-B-Mes	467	16	3.3	32.0/25.4/18.2	(0.10, 0.09)	26.2	24.2	this work
V-DABNA-F	468	15	3.3	26.6/25.8/23.4	(0.12, 0.10)	22.3	21.5	16
DPA-B3	450	15	3.6	37.7/33.7/21.0	(0.15, 0.04)	17.3	15.1	17
DPA-B4	457	13	3.6	39.2/36.4/28.7	(0.14, 0.05)	21.8	18.2	
ν-DABNA-Az1	459	19	3.0	30.8/29.0/19.9	(0.13, 0.08)	24.0	25.8	18
ν-DABNA-Az2	458	17	3.0	29.9/28.0/16.0	(0.14, 0.06)	18.1	19.4	
ν-DABNA-Az3	459	20	3.0	33.0/29.2/22.4	(0.13, 0.10)	29.9	32.0	
BOBO-Z	445	18	4.5	13.6/9.8/3.3	(0.15, 0.04)	7.2	5.0	19
BOBS-Z	456	23	4.0	26.9/24.0/15.0	(0.14, 0.06)	16.7	12.9	
BSBS-Z	463	22	4.0	26.8/24.0/15.9	(0.13, 0.08)	23.2	15.0	
4F-ν-DABNA	464	18	3.7	35.8/-/-	(0.13, 0.08)	26.8	-	20
4F-m-ν-DABNA	461	18	3.7	33.7/-/-	(0.13, 0.06)	24.9	-	
ν-DABNA-OMe	465	23	3.4	29.5/28.8/26.9	(0.13, 0.10)	24.6	22.7	21
DABNA-1	459	28	-	13.6/6.0/-	(0.13, 0.09)	10.6	8.3	22
CzBO	448	30	4.1	13.4/8.4/3.5	(0.15, 0.05)	7.4	5.7	23
BN1	457	28	4.3	31.2/18.3/9.3	(0.14, 0.08)	20.9	14.9	24
BN3	458	23	4.1	37.6/34.0/26.2	(0.14, 0.08)	27.5	19.0	
t-DABNA	464	26	8.2	28.4/14.8/4.4	(0.13, 0.10)	-	-	25
t-DABNA-DPA	459	26	7.5	27.6/21.8/9.2	(0.13, 0.08)	-	-	
DPACzBN2	469	28	3.7	24.0/23.5/14.3	(0.13, 0.10)	31.6	-	26
B-O-dpa	443	32	4.0	12.6/1.7/-	(0.15, 0.04)	5.8	-	27
BisICz	437	24	-	6.5/-/-	(0.16, 0.04)	2.9	2.7	28
tBisICz	445	22	-	15.1/-/-	(0.16, 0.05)	8.4	8.3	
tPBisICz	452	21	-	23.1/-/-	(0.15, 0.05)	13.5	13.3	
NOBNacene	409	37	4.2	8.5/-/-	(0.17, 0.05)	-	-	29
BIC-mCz	431	38	4.1	7.0/-/-	(0.16, 0.04)	-	4.7	30

CZCO	432	35	3.4	15.6/6.0/5.9	(0.15, 0.04)	8.6	7.1	31
CZ2CO	445	23	3.4	13/9.9/3.9	(0.15, 0.06)	9.4	5.9	
1B-DTACrs	440	30	10	1.31/-/-	(0.15, 0.05)	-	-	32
2B-DTACrs	447	26	4	14.8/10.1/-	(0.15, 0.04)	-	-	
tDIDcz	401	16	4.25	2.46/-/-	(0.16, 0.05)	0.39	-	33
ym-lcz	412	36	3.75	3.04/-/-	(0.16, 0.03)	0.68	-	
o-lcz	433	40	3.5	3.01/-/-	(0.16, 0.04)	-	-	
MesB-DIDOBNA-N	402	21	4.1	16.1/3.5/-	(0.17, 0.05)	-	2.7	34
DIDOBNA-N	429	70	4.2	15.2/3.8/-	(0.15, 0.07)	-	6.5	
PAB	452	30	3.6	13.1/-/-	(0.15, 0.05)	9.43	6.43	35
Me-PABO	460	26	3.6	20.4/5.90/-	(0.13, 0.09)	16.55	12.99	
C-BN	453	25	3.5	26.6/20.1/8.9	(0.14, 0.07)	20.1	-	36
DBCz-Mes	452	17	3.1	33.9/-/-	(0.14, 0.06)	-	-	37
QPO	444	-	-	2.5/-/-	(0.16, 0.07)	1.5	0.6	38
CzAO	444	43	4.0	8.62/-/-	(0.15, 0.06)	5.46	4.28	39
SFQ	460	30	-	21.7/12.5/3.6	(0.13, 0.10)	20	17.3	40
SOQ	456	33	-	24.3/14.9/4.2	(0.14, 0.10)	20	17.6	40
SSQ	456	31	-	25.5/13.4/3.5	(0.14, 0.10)	20	17.2	40
SNA	457	32	3.8	4.5/-/-	(0.14, 0.08)	-	-	41
SNB	462	32	3.8	7.0/-/-	(0.13, 0.09)	-	-	41
BSS-TBCz	460	34	-	19.9/-/-	(0.13, 0.07)	12.7	-	42
Tp-DABNA	462	25	3.8	24.3/9.8/-	(0.14, 0.10)	19.6	11.4	43
<i>ν</i> -DABNA	445	24	5.0	19.5/15.6/7.5	(0.15, 0.04)	7.6	4.7	44
DOB2-DABNA-A	452	24	3.4	24.1/23.3/21.6	(0.14, 0.05)	12.1	11.3	45

^{a)}Maximum wavelength of EL spectrum. ^{b)}Full width at half maximum. ^{c)}Turn-on voltage at the luminescence of 1 cd m⁻². ^{d)}External quantum efficiency of maximum/at 100/1000 cd m⁻². ^{e)}CIE (x, y) coordinates. ^{f)}Maximum current efficiency. ^{g)}Maximum power efficiency.

Supplementary Table 8: Summary of the EL performance. The representative hyperfluorescent (HF) and phosphorescent sensitized fluorescence (PSF) OLEDs using *ν*-DABNA and its derivatives as emitters.

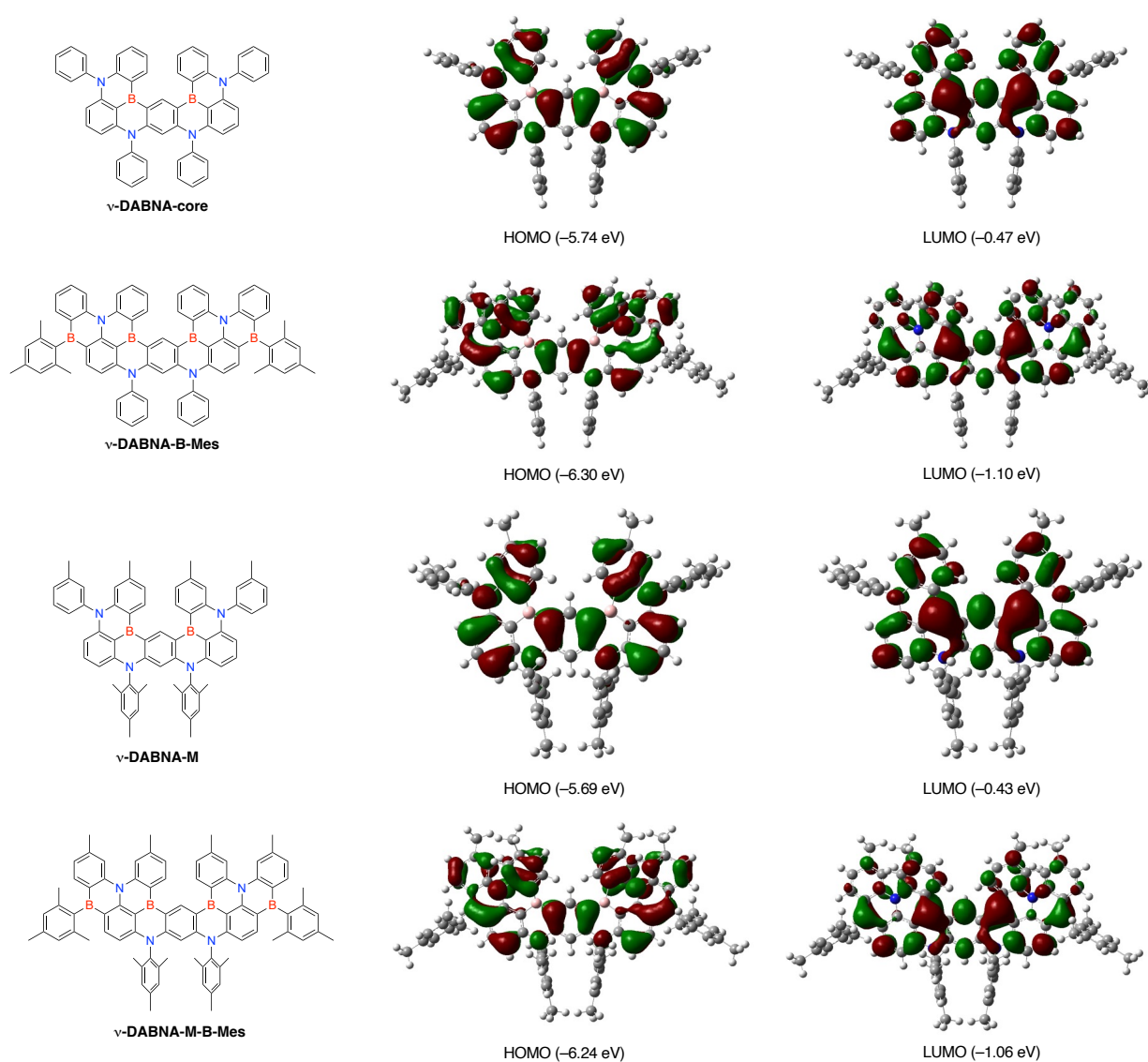
Final dopant	Sensitizer	λ_{EL}^a [nm]	FWHM ^b [nm]	EQE [%] ^c Max/100/1000	CIE ^d (x, y)	roll-off ^e [%]	CE _{max} ^f [cd A ⁻¹]	PE _{max} ^g [lm W ⁻¹]	LT ^h [h]	ref
<i>ν</i> -DABNA-M-B-Mes	PtON-TBBI	467	17	25.6/25.0/23.7	(0.12, 0.12)	7	25.6	31.2	LT80 = 1010 @ 100 nits	this work
<i>ν</i> -DABNA	5Cz-BO	468	18	33.1/-/-	(0.12, 0.11)	-	29.5	24.3	LT80 ≅ 3 @ 100 nits	46
<i>ν</i> -DABNA	HDT-1	470	18	27.0/24.0/20.0	(0.15, 0.20)	26	39.0	41.0	LT95 = 11 @ 1000 nits	47
<i>t</i> -BuCz-DABNA	4CzBN-PhCN	470	18	30.8/-/20.0	(0.14, 0.17)	35	-	-	LT95 = 221 @ 1000 nits	48
	4tCzBN-PhCN	470	21	27.8/-/24.2	(0.16, 0.27)	13	-	-	LT95 = 454 @ 1000 nits	

v-DABNA	PPCzTrz	473	19	33.0/-/25.2	(0.13, 0.20)	24	39.7	-	LT50 = 151 @ 1000 nits	49
	PCzTrz	473	19	33.5/-/23.8	(0.12, 0.18)	29	35.5	-	LT50 = 113 @ 1000 nits	
v-DABNA	DBA-DmICz	473	21	36.5/-/31.7	(0.13, 0.22)	13	42.5	-	-	50
	DBA-DTMCz	473	21	42.2/-/35.9	(0.12, 0.16)	15	40.1	-	-	
v-DABNA	4PhCz2BN	470	18	22.4/21.2/17.8	(0.13, 0.15)	20	25.4	25.0	LT90 = 7.5 @ 1000 nits	51
v-DABNA	ACRSA	473	19	28.5/24.6/18.6	(0.13, 0.17)	35	37	36	LT50 = 70 @ 2500 nits	52
v-DABNA	B-4-TMS	470	17	33.4/27.2/23.0	(0.12, 0.12)	31	33.4	34.4	LT50 = 4465 @ 100 nits	53
	B-5-TMS	470	17	33.4/28.7/24.1	(0.12, 0.12)	28	30.8	33.2	LT50 = 4552 @ 100 nits	
v-DABNA	PtON7-dtb	473	20	32.2/-/25.4	(0.11, 0.14)	21	32.0	-	LT50 = 156 @ 1000 nits	54
v-DABNA	m-2-tBu	472	21	22.0/18.9/14.9	(0.12, 0.15)	32	23.5	-	-	55
v-DABNA	CN-Ir	470	20	27.3/-/23.3	(0.13, 0.16)	15	31.2	-	LT50 = 121 @ 1000 nits	56
v-DABNA	3	471	-	15.3/-/10.4	(0.15, 0.27)	32	27.2	21.6	-	57
	6	472	-	15.7/-/10.5	(0.13, 0.19)	33	21.8	17.2	-	
v-DABNA	Ge-2/TCTA	471	20	30.0/-/25.6	(0.13, 0.14)	15	30.8	27.5	LT50 = 9.1 @ 500 nits	58
v-DABNA	f-ct3a	468	22	25.6/21.9/17.7	(0.13, 0.13)	31	25.7	23.0	-	59
	f-ct3b	468	22	29.0/23.1/18.5	(0.12, 0.13)	36	27.8	24.8	LT50 = 82 @ 1000 nits	

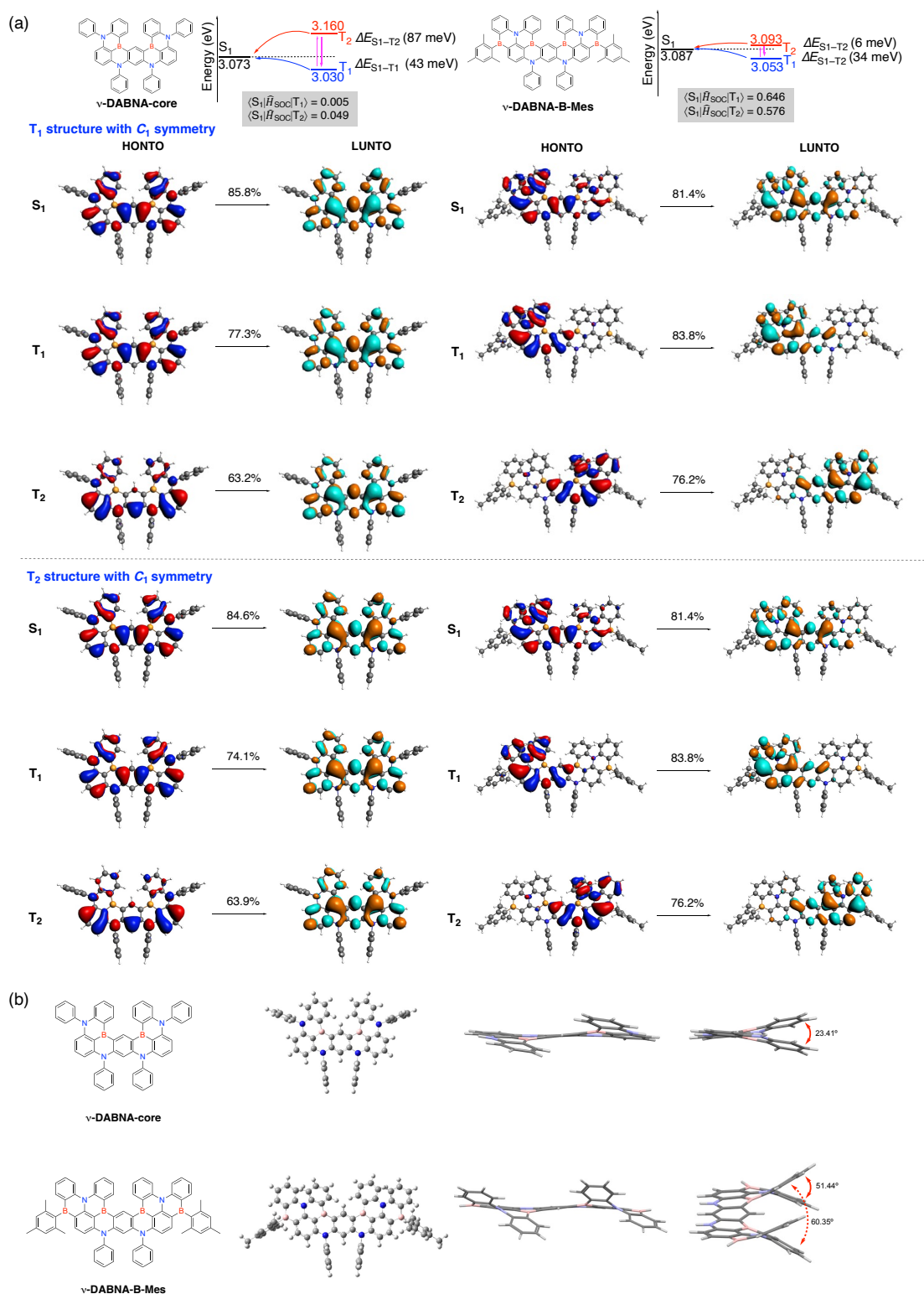
^{a)}Maximum wavelength of EL spectrum. ^{b)}Full width at half maximum. ^{c)}External quantum efficiency of maximum/at 100/1000 cd m⁻². ^{d)}CIE (x, y) coordinates. ^{e)}Efficiency roll-off at 1000 cd m⁻² from EQE_{max}.

^{f)}Maximum current efficiency. ^{g)}Maximum power efficiency. ^{h)}Lifetime of the devices of the specific initial luminance.

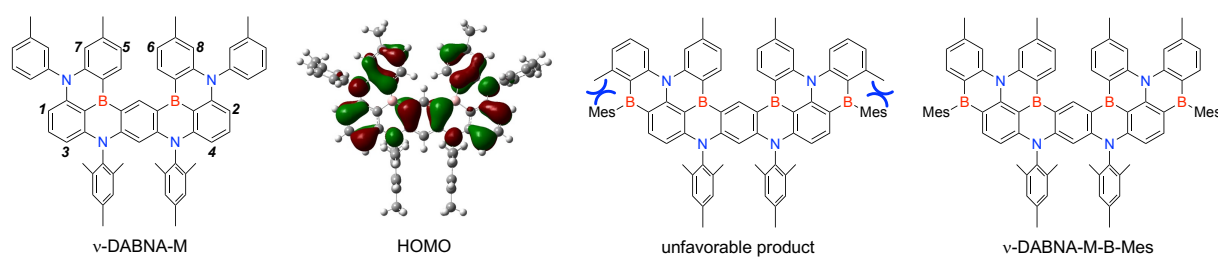
Supplementary Figures



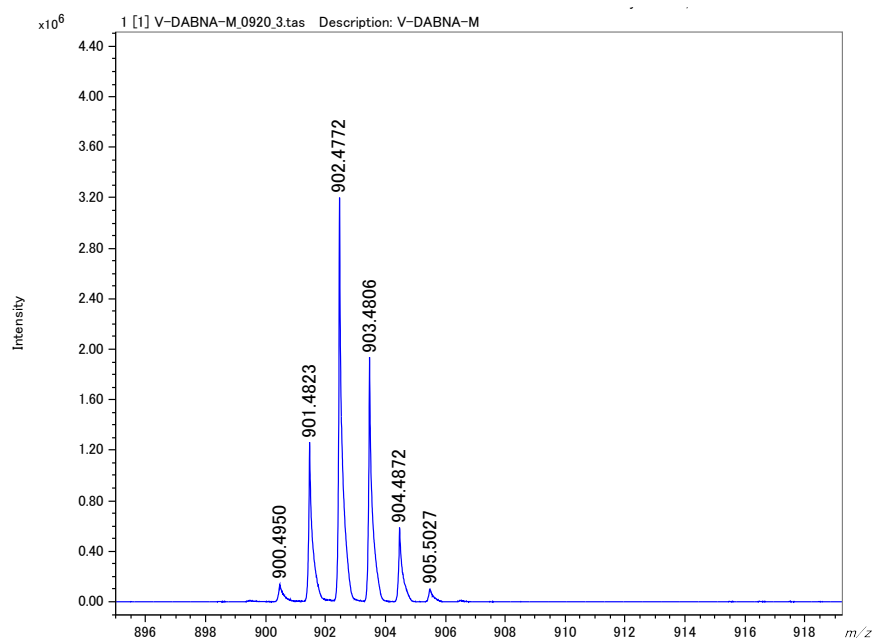
Supplementary Figure 1: Kohn–Sham frontier orbitals of v-DABNA-core, v-DABNA-B-Mes, v-DABNA-M and v-DABNA-M-B-Mes. They were calculated at the M06-2X/6-31G(d) level of theory (isovalue = 0.02).



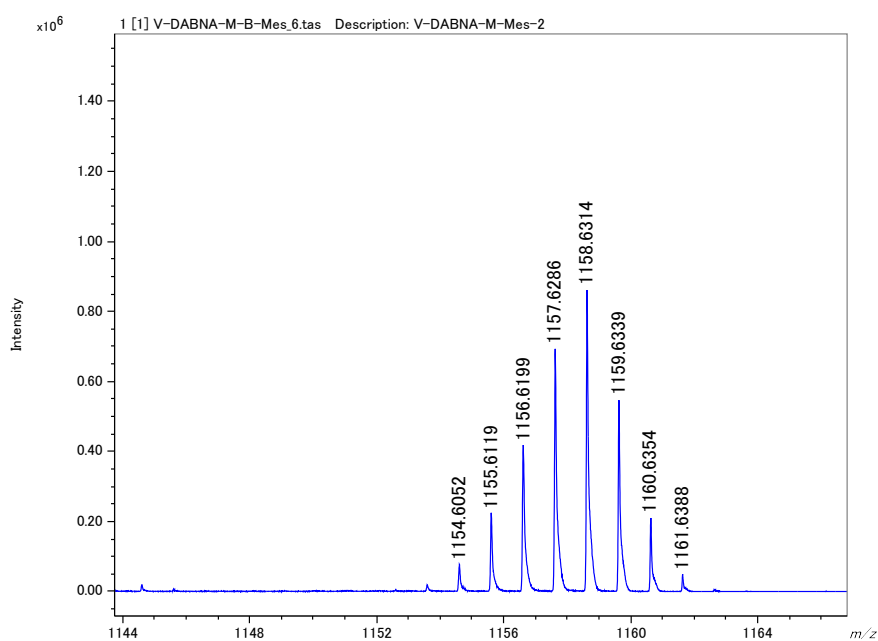
Supplementary Figure 2: Transition energies, spin orbital coupling (SOC) matrix elements, and natural transition orbitals (NTOs), along with optimized geometries and distortion angles of v-DABNA-core and v-DABNA-B-Mes. (a) Transition energies for S_1 , T_1 , and T_2 were calculated at the SCS-CC2/def2TZVP//M06-2X/6-31G(d) level of theory using the geometry of S_0 . SOC matrix elements, SOC (S_1-T_1) and SOC (S_1-T_2), were calculated at the M06-2X/TZP//M06-2X/6-31G(d) level of theory using the geometry of T_1 and T_2 , respectively. (b) Optimized geometries and distortion angles of v-DABNA-core and v-DABNA-B-Mes at the M06-2X/6-31G(d) level of theory. The peripheral phenyl rings are omitted for clarity in displaying the distortion angles.



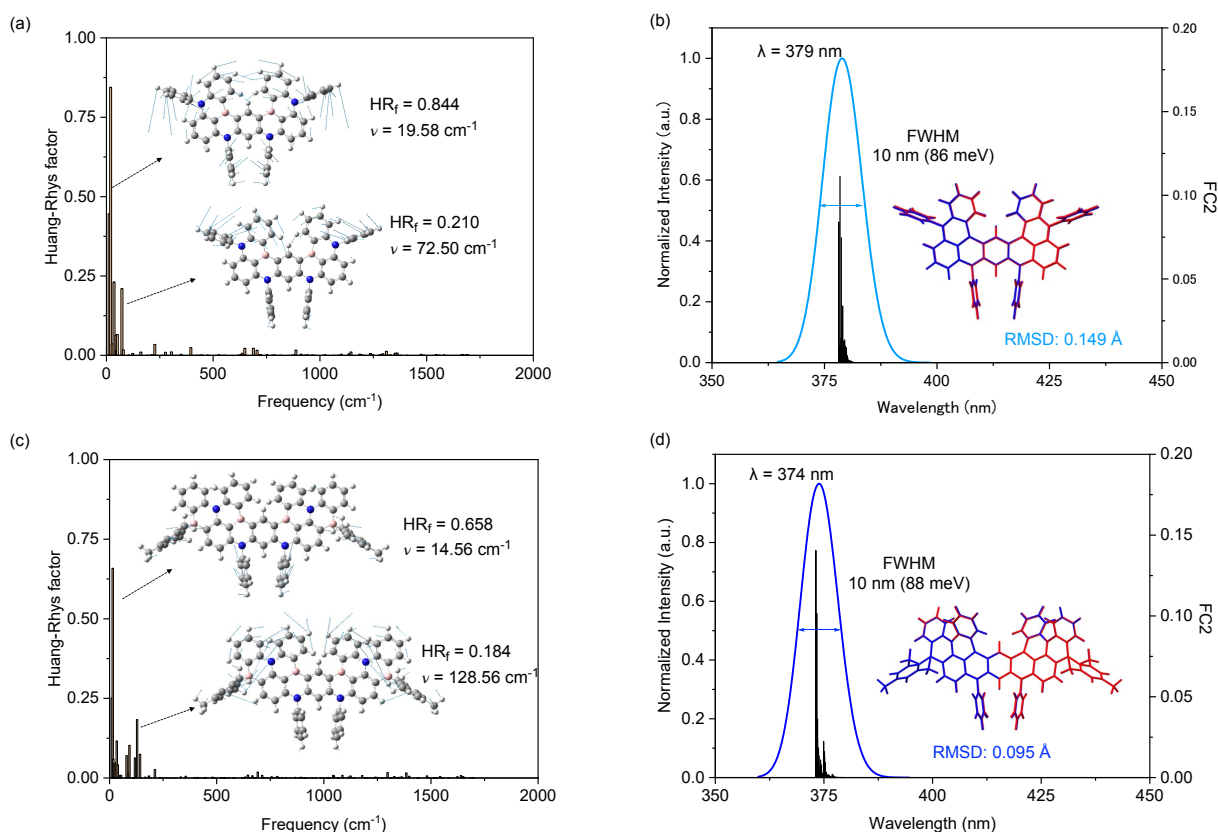
Supplementary Figure 3: HOMO distributions of v-DABNA-M. Two proposed structures of potential target products are shown.



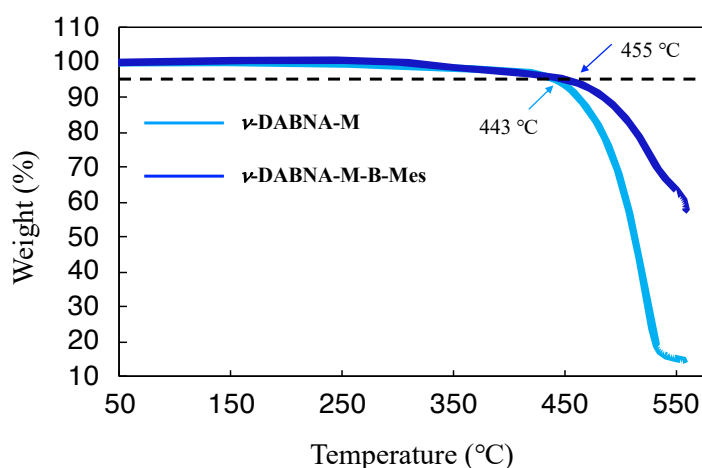
Supplementary Figure 4: HRMS data. High-resolution mass spectrometry of v-DABNA-M.



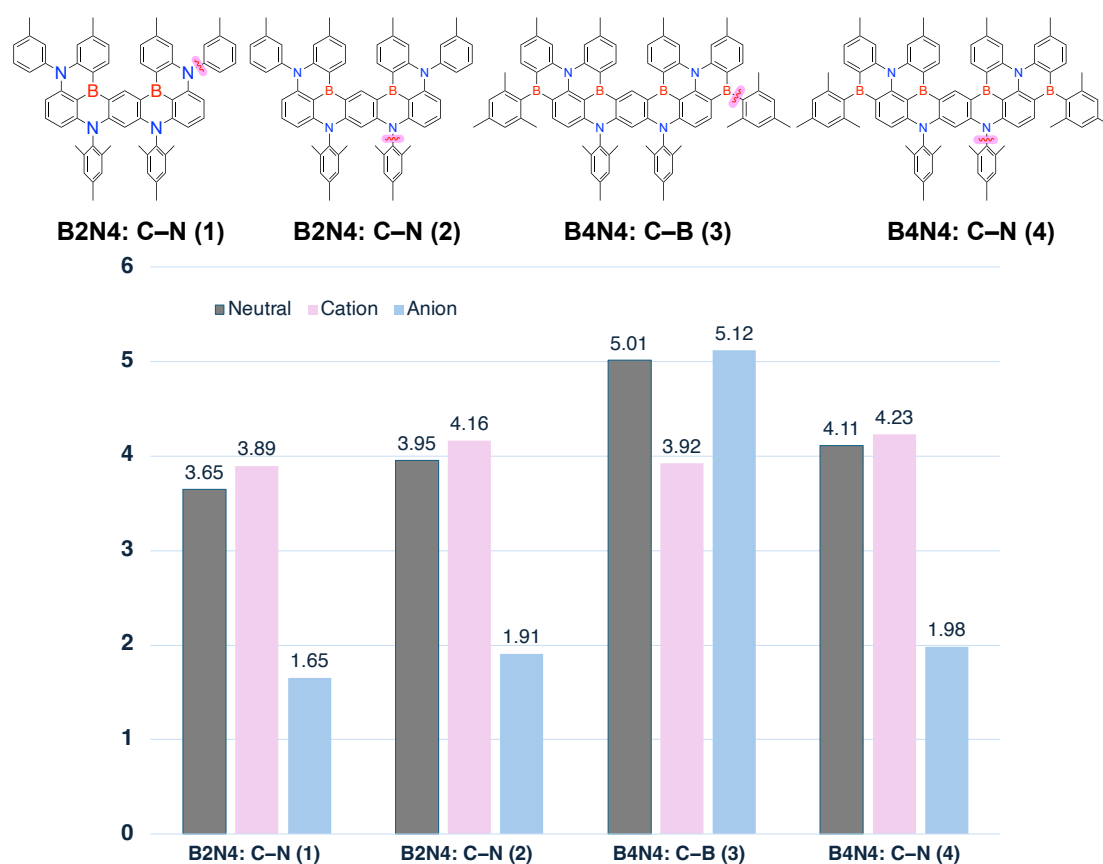
Supplementary Figure 5: HRMS data. High-resolution mass spectrometry of v-DABNA-M-B-Mes.



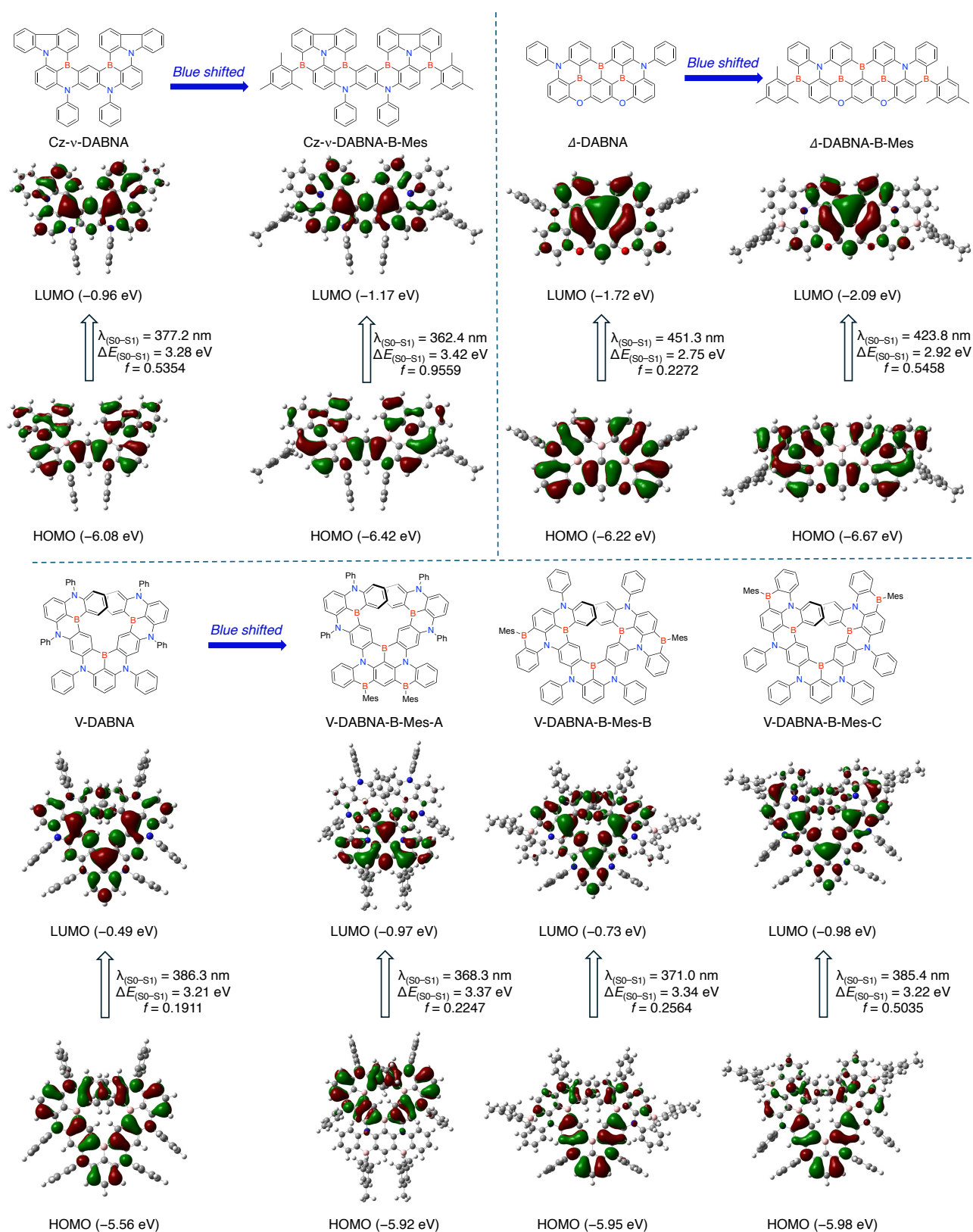
Supplementary Figure 6: Computational studies of two model compounds. Calculated Huang-Rhys factors for the $S_1 \rightarrow S_0$ transition of two model compounds are shown, with insets highlighting key vibrational modes: (a) for ν -DABNA-core and (c) for ν -DABNA-B-Mes. Panels (b) and (d) present the corresponding simulated emission spectra based on Franck-Condon analysis, where vertical lines indicate the squared Franck-Condon factors. Insets also compare the optimized structures in the S_0 (blue) and S_1 (red) state, along with RMSD values.



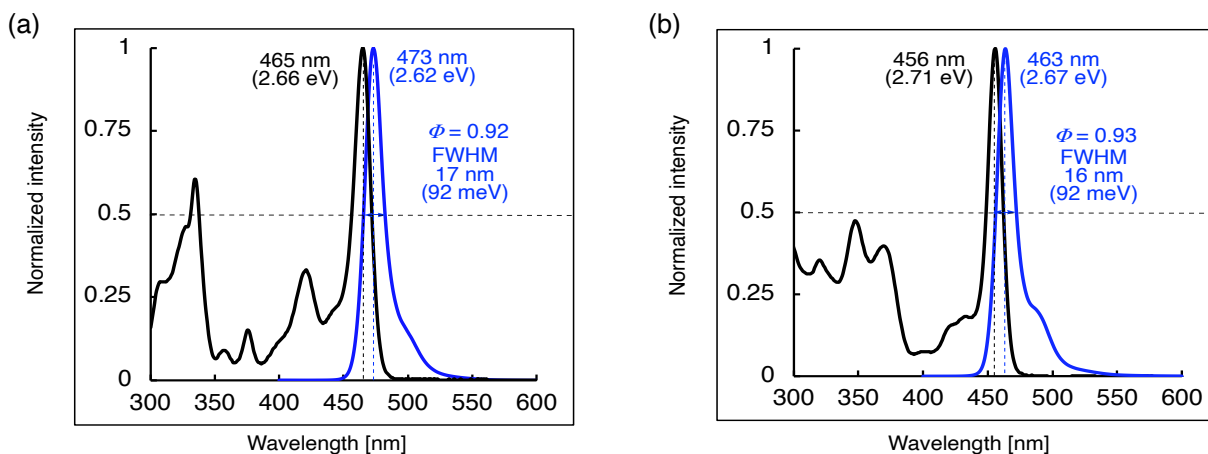
Supplementary Figure 7: TGA measurement. The decomposition temperatures (T_d) at 5% weight loss of ν -DABNA-M and ν -DABNA-M-B-Mes are presented in the inset.



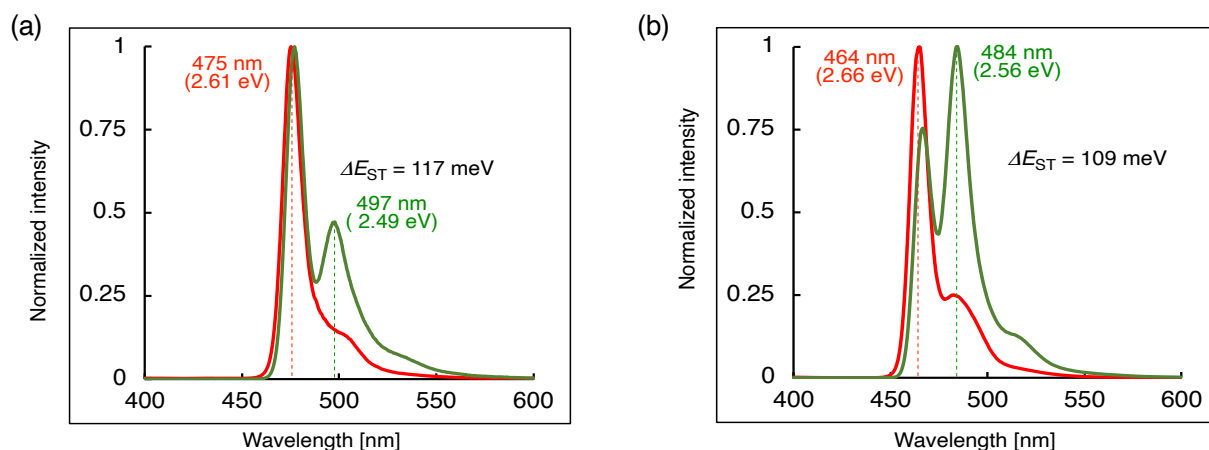
Supplementary Figure 8: Bond dissociation energy (BDE) values of v-DABNA-M and v-DABNA-M-B-Mes. The neutral (black bars), cationic (pink bars), and anionic (blue bars) states represent the BDEs of the fragile C–X bonds in each respective electronic state. All calculations were performed at the M06-2X/6-31+G(d,p) level. The calculation was performed at M06-2X/6-31+G(d,p) level of theory.



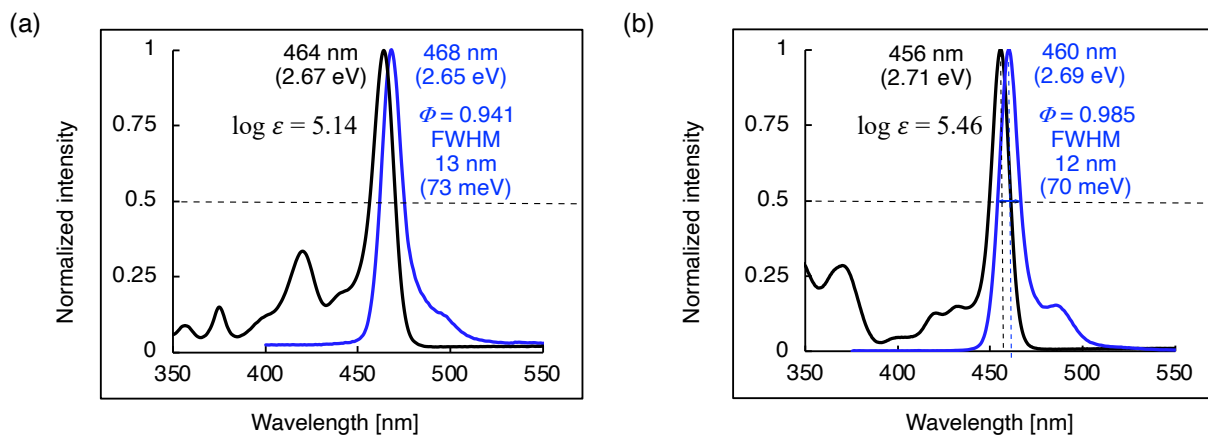
Supplementary Figure 9: Chemical structures of representative MR-TADF scaffolds and their B-Mes-substituted derivatives, along with Kohn–Sham frontier orbitals, oscillator strengths (f), and transition energies (ΔE , λ). They were calculated at the M06-2X/6-31G(d) level of theory (isovalue = 0.02).



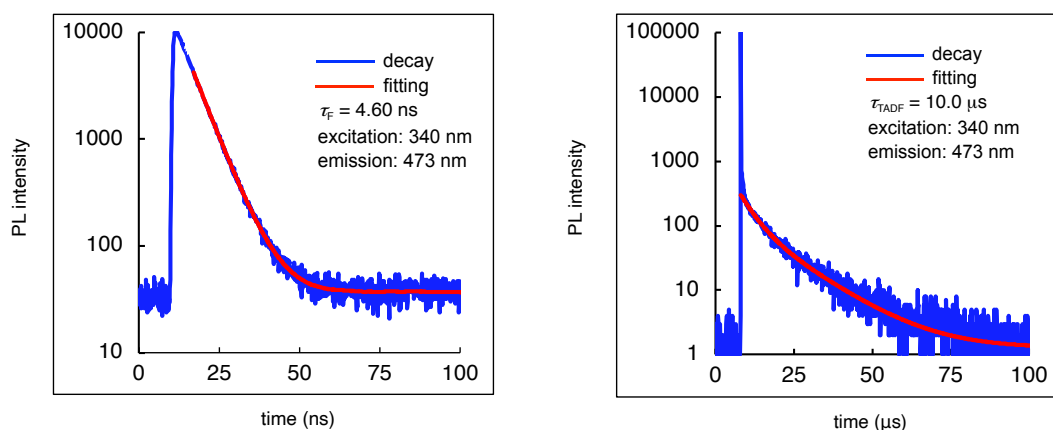
Supplementary Figure 10: Normalized absorption (black) and fluorescence (blue) spectra at 298 K. The spectra of (a) v-DABNA-M, (b) v-DABNA-M-B-Mes in 1 wt% doped PMMA film with absorption/emission maxima (nm, eV), absolute quantum yield (Φ), and full width at half maximum (nm, meV).



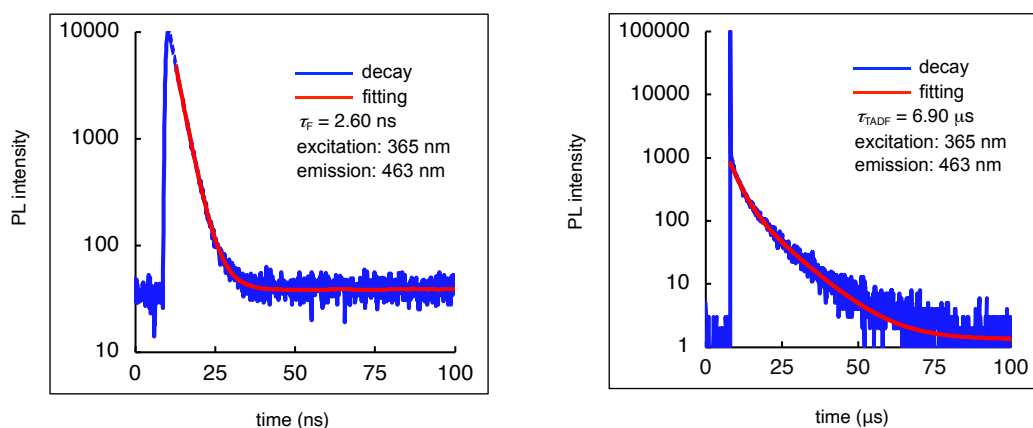
Supplementary Figure 11: Normalized PL spectra at 77 K with/without delay time of 25 ms (green/red). The spectra of (a) v-DABNA-M and (b) v-DABNA-M-B-Mes in 1 wt% doped PMMA film with emission maxima (nm, eV) and Singlet–triplet energy gap (meV).



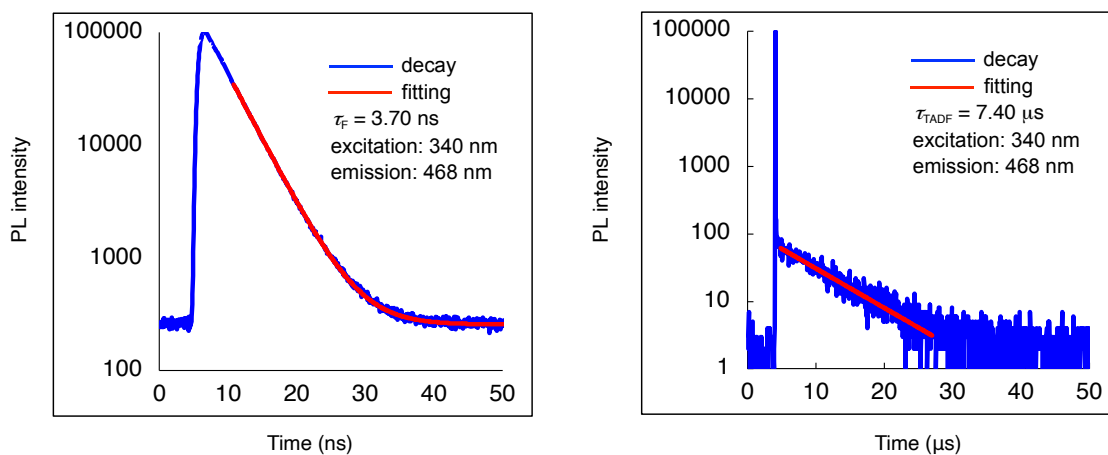
Supplementary Figure 12: Normalized absorption (black) and fluorescence (blue) spectra at 298 K. The spectra of (a) v-DABNA-M and (b) v-DABNA-M-B-Mes in toluene with absorption/emission maxima (nm, eV), absolute quantum yield (Φ), and full width at half maximum (nm, meV).



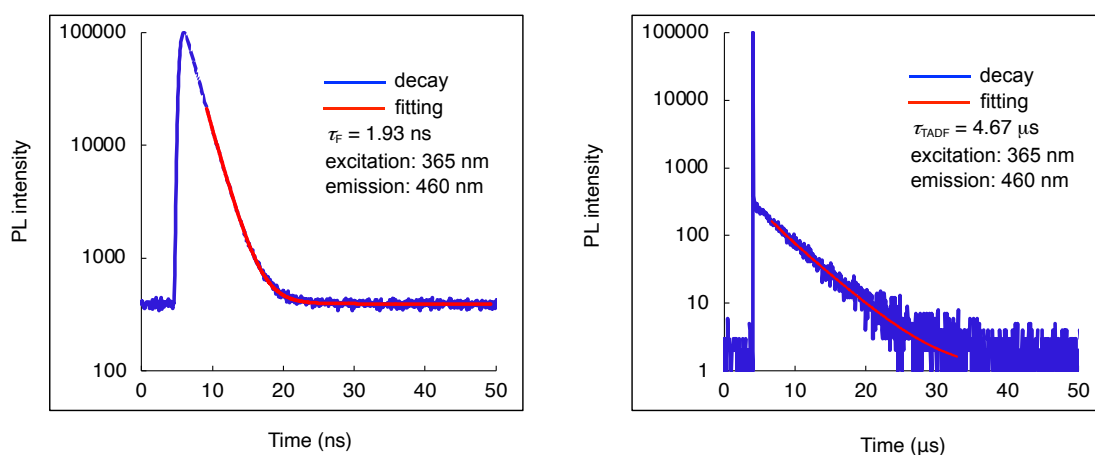
Supplementary Figure 13: Transient decay spectra of 1 wt% v-DABNA-M doped in PMMA film. The red curves are single exponential fitting data.



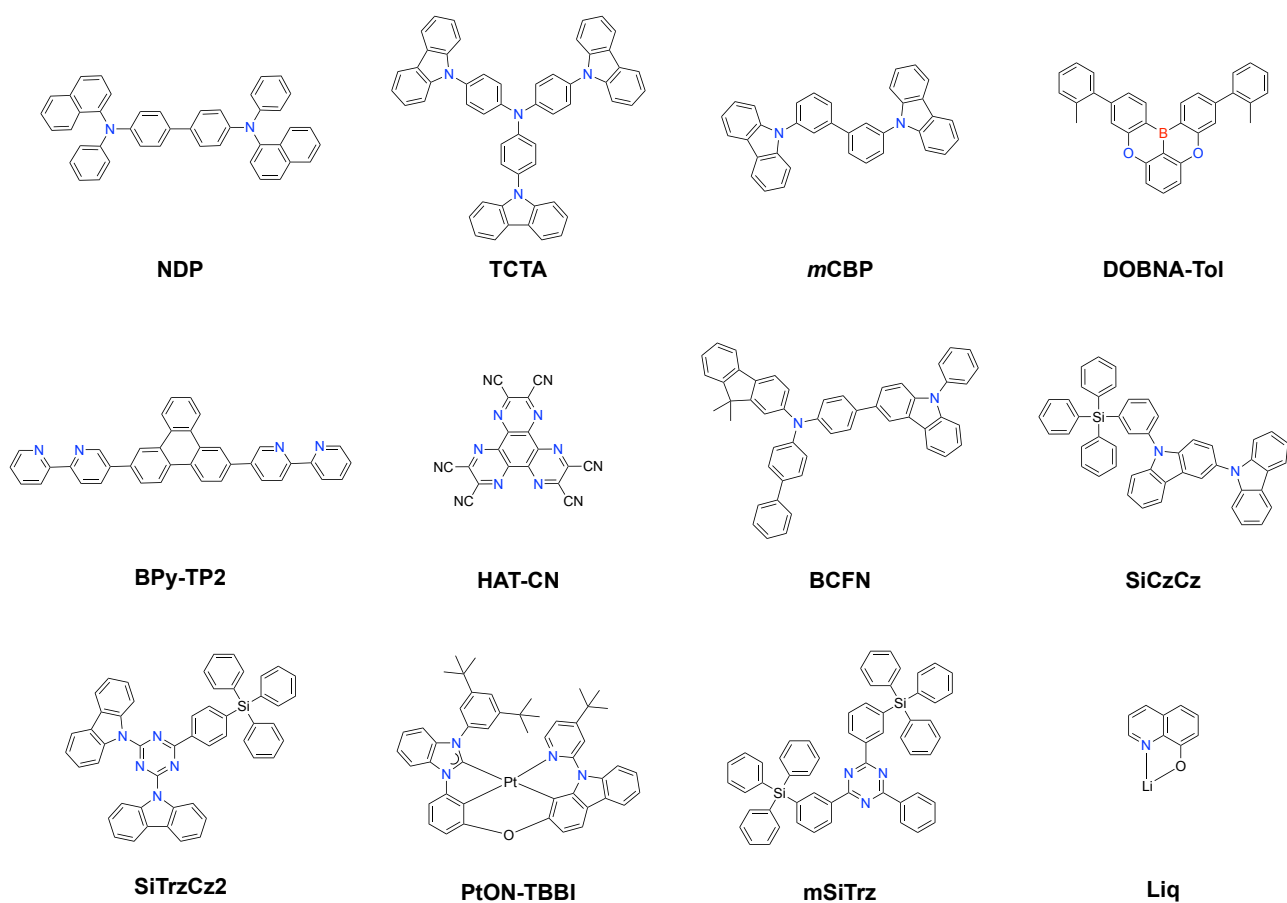
Supplementary Figure 14: Transient decay spectra of 1 wt% v-DABNA-M-B-Mes doped in PMMA film. The red curves are single exponential fitting data.



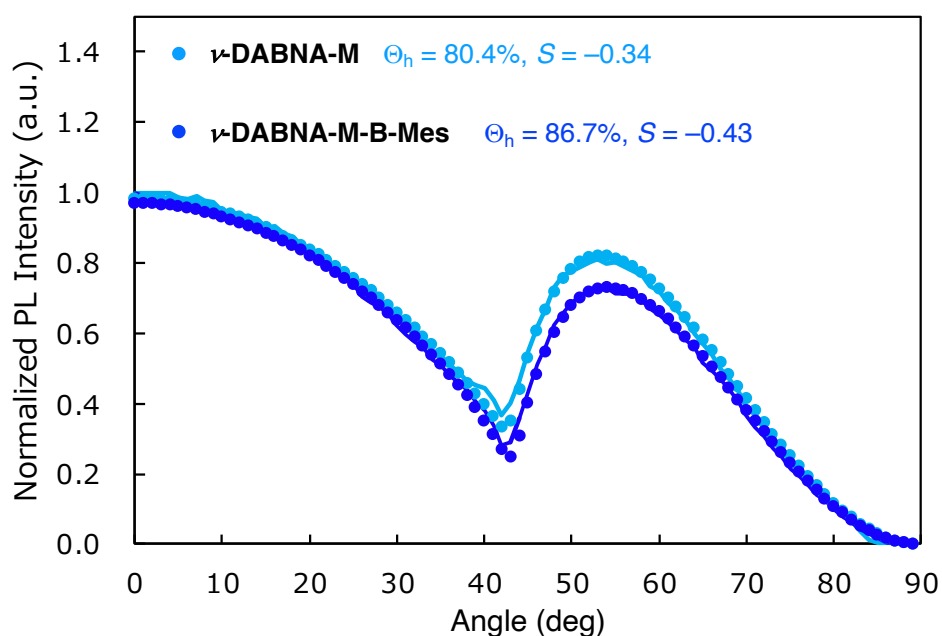
Supplementary Figure 15: Transient decay spectra of v-DABNA-M in toluene (10^{-6} M). The red curves are single exponential fitting data.



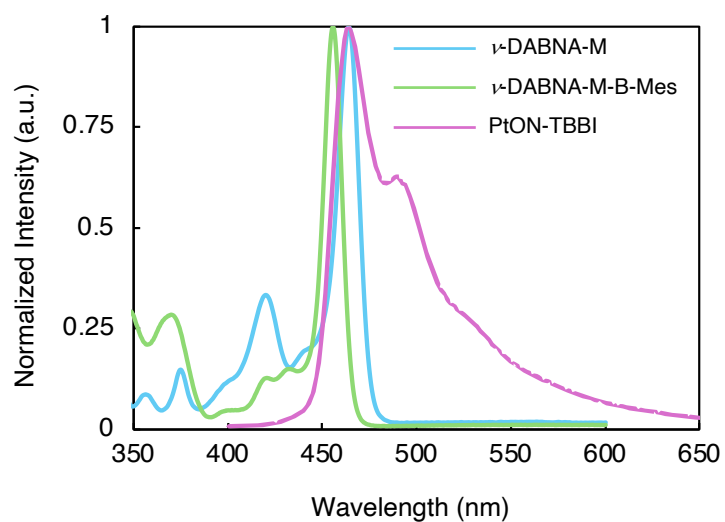
Supplementary Figure 16: Transient decay spectra of v-DABNA-M-B-Mes in toluene (10^{-6} M). The red curves are single exponential fitting data.



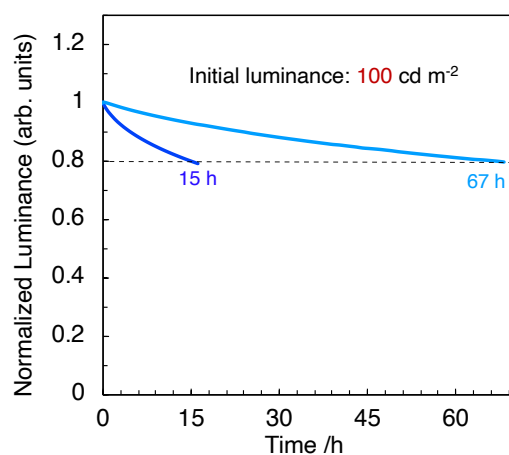
Supplementary Figure 17: Molecular structures of the OLED materials employed in this work.



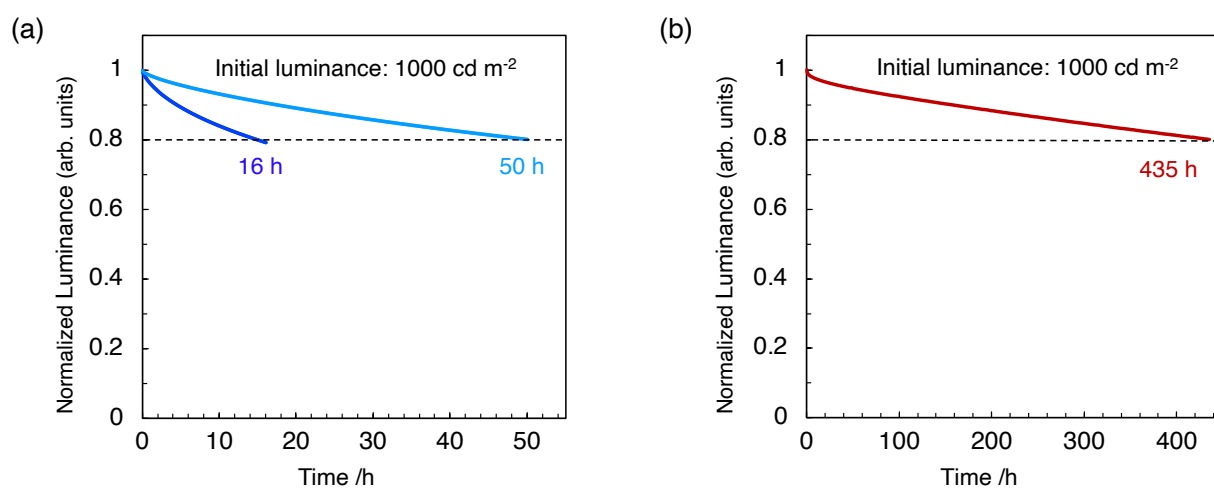
Supplementary Figure 18: Angular-dependent PL measurements of ν -DABNA-M and ν -DABNA-M-B-Mes. The ν -DABNA-M and ν -DABNA-M-B-Mes were doped into co-deposited mCBP: DOBNA-Tol films.



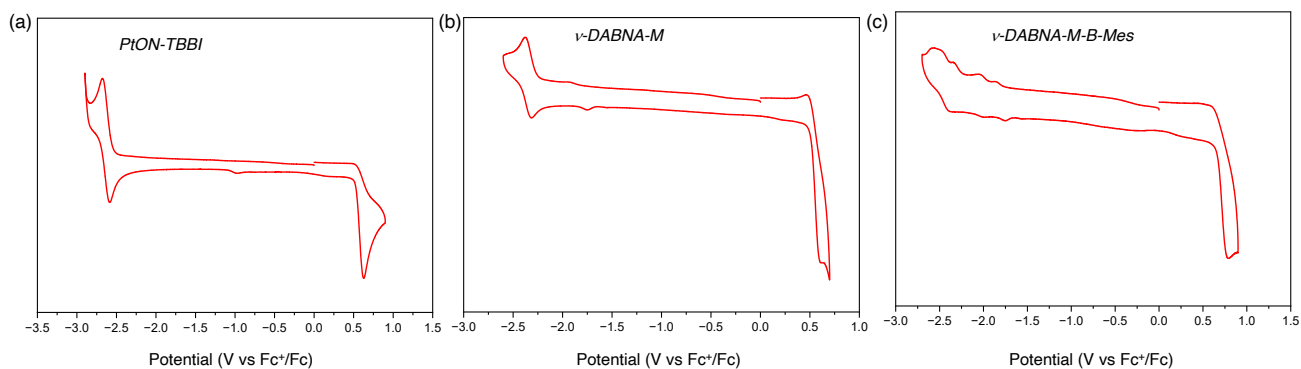
Supplementary Figure 19: Spectral overlap between the sensitizer and emitters. UV-vis absorption spectra of ν -DABNA-M and ν -DABNA-M-B-Mes in toluene solution, and fluorescence spectra of PtON-TBBI in co-deposited films of Si-CzCz and SiTrzCz2.



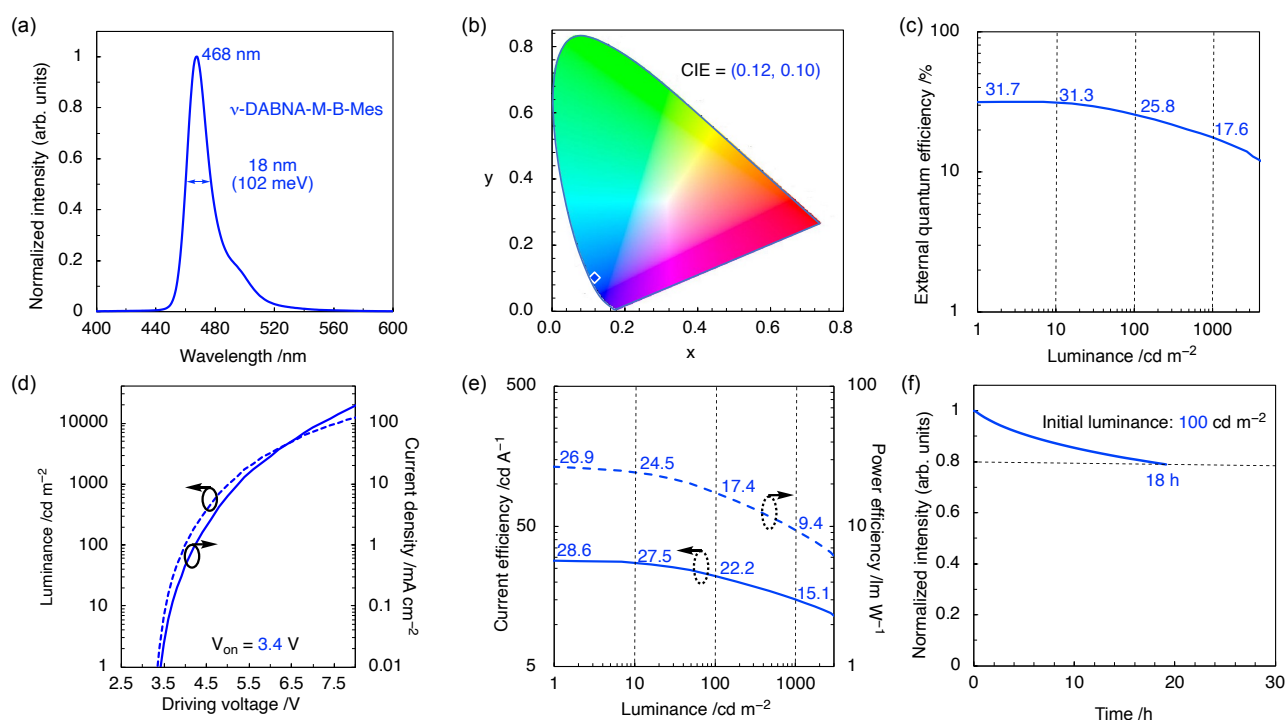
Supplementary Figure 20: Change in luminance vs. operational time at an initial luminance of 100 cd m^{-2} for TADF-devices. Deep-blue line for v-DABNA-M-B-Mes, the sky-blue line for v-DABNA-M.



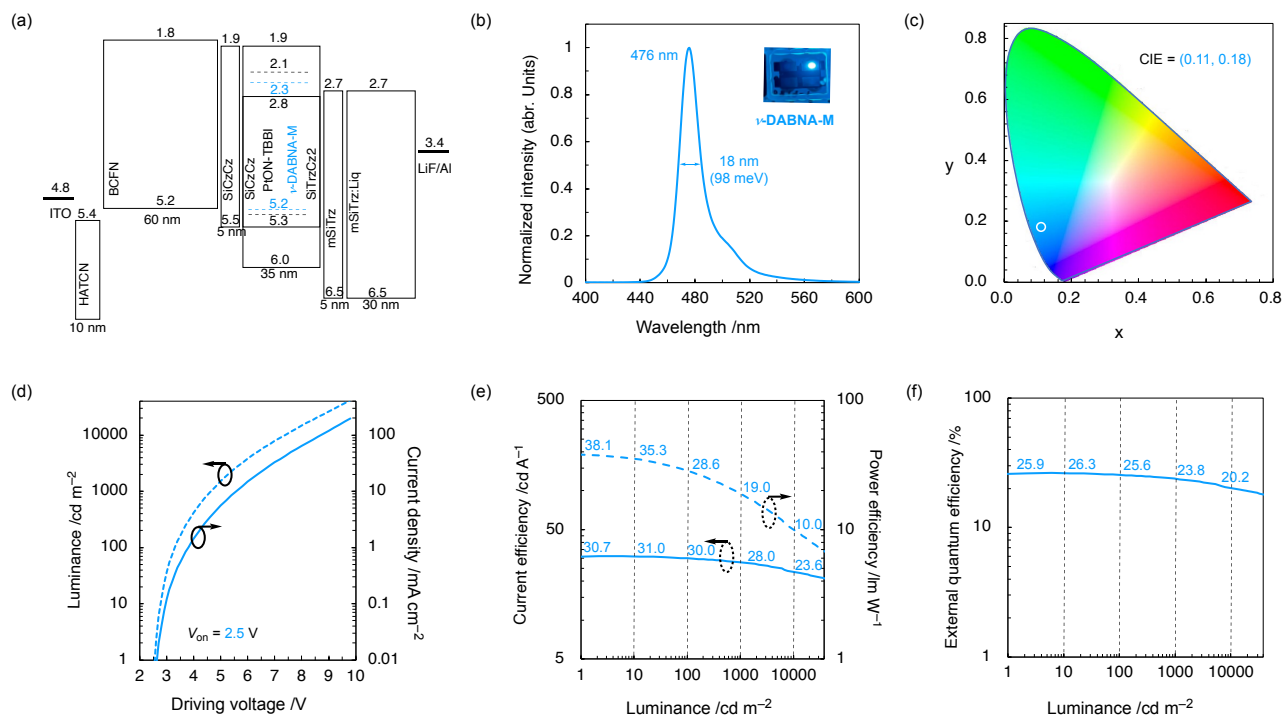
Supplementary Figure 21: Change in luminance vs. operational time at an initial luminance of 1000 cd m^{-2} . (a) PSF-device based on v-DABNA-M-B-Mes (blue) and v-DABNA-M (sky-blue); (b) Phosphorescent-only (PtON-TBBI) device.



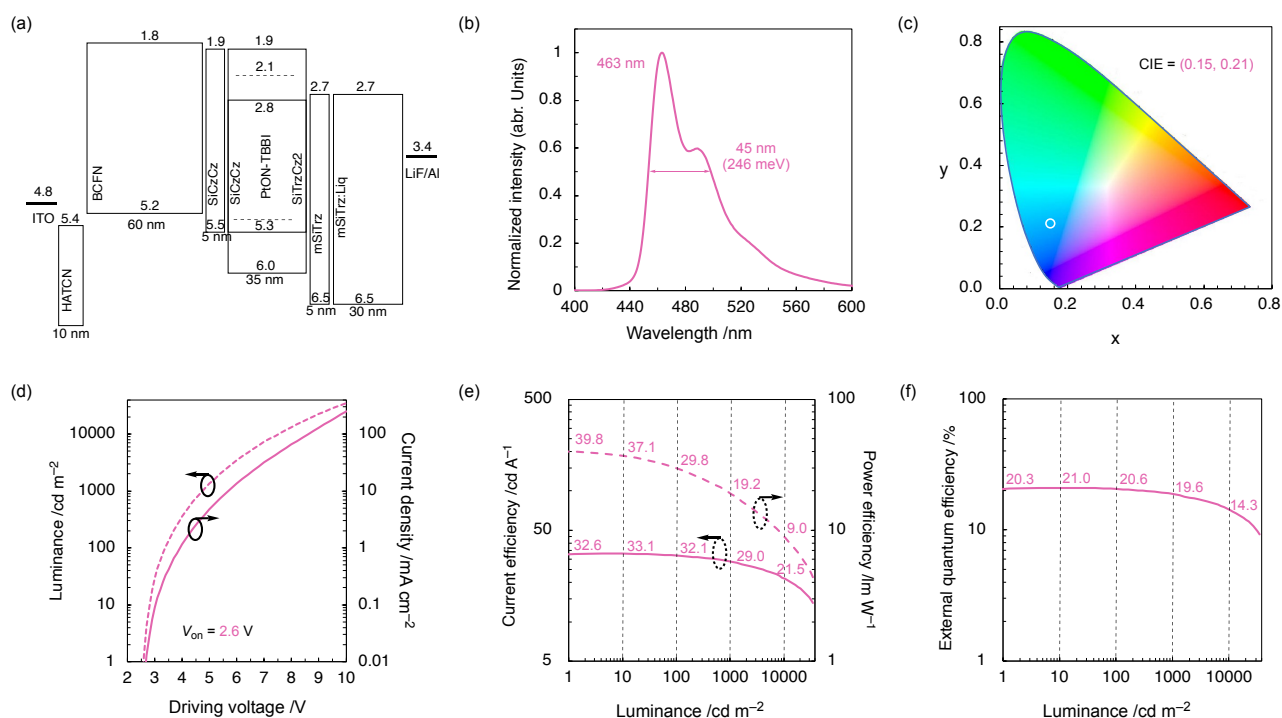
Supplementary Figure 22: Cyclic voltammetry curves of the sensitizer and emitters. (a) PtON-TBBI, (b) v-DABNA-M, and (c) v-DABNA-M-B-Mes.



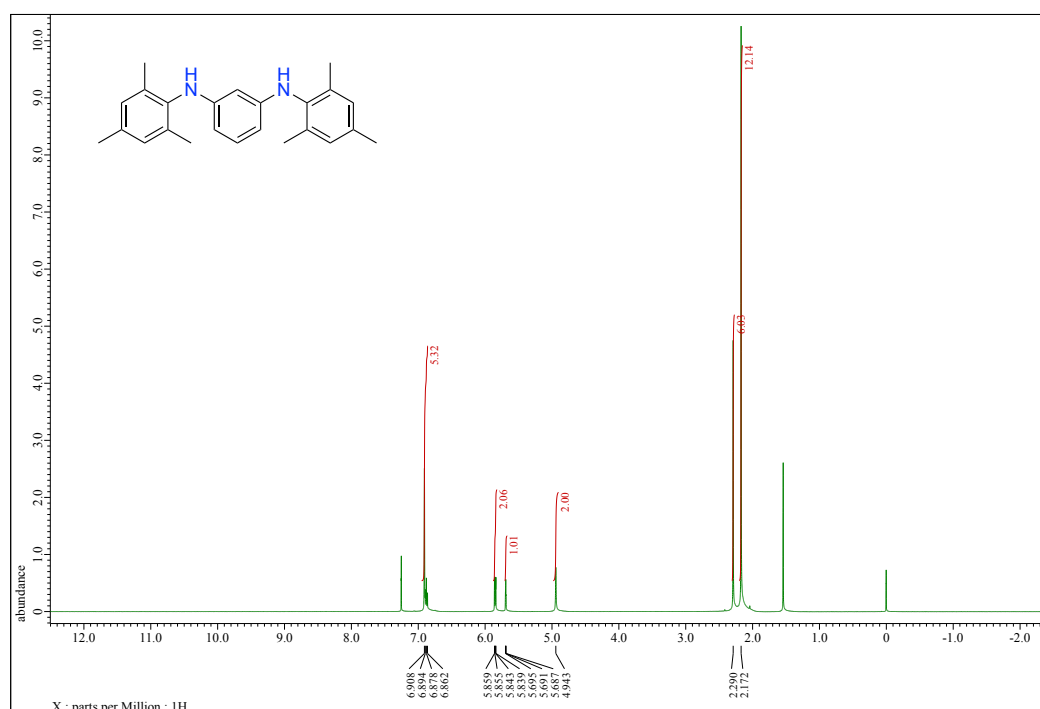
Supplementary Figure 23: Characteristics of fabricated TADF-based device using v-DABNA-M-B-Mes as emitter with 2 wt% doping concentration. (a) Normalized EL spectra of the devices in operation. Inset: Electroluminescence and FWHM of the fabricated device. (b) Commission Internationale d'Éclairage (CIE) (x,y) coordinates. (c) External quantum efficiency (EQE) vs. luminance. (d) Current density (solid) and luminance (dashed) vs. driving voltage. (e) Current efficiency (solid) and Power efficiency (dashed) vs. luminance. (f) Change in luminance vs. operational time at an initial luminance of 100 cd m⁻² for TADF-device.



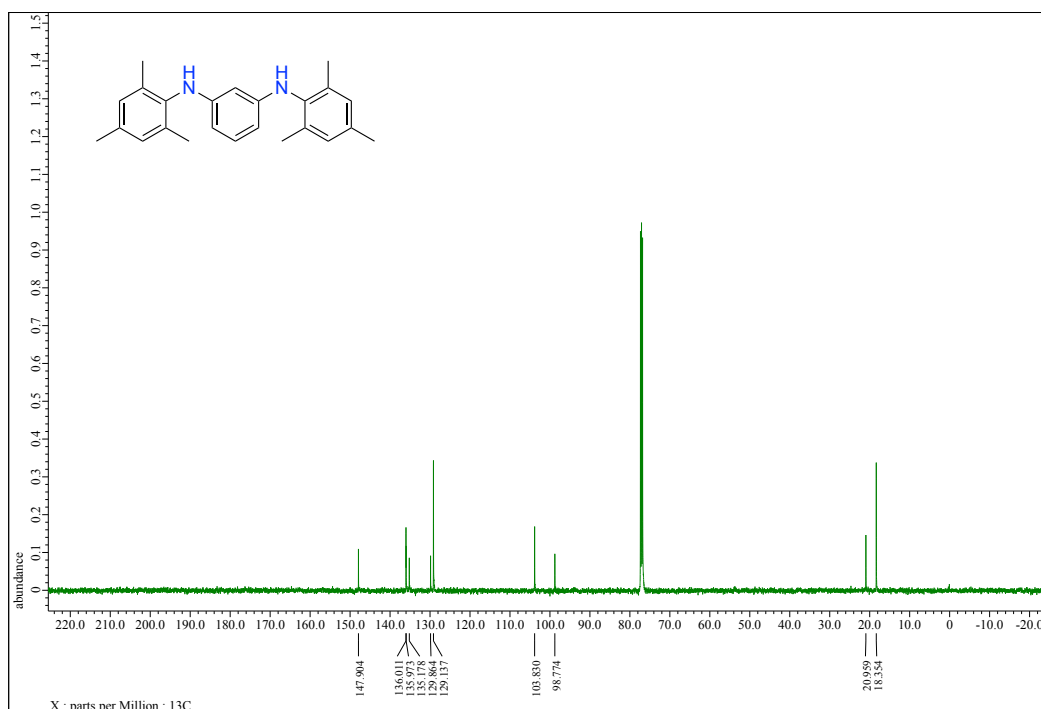
Supplementary Figure 24: Characteristics of fabricated PSF-based OLED device using v-DABNA-M as emitter. (a) Device structure with the estimated energy levels of each component in eV. (b) Normalized EL spectra of the PSF device in operation. Inset: Electroluminescence, FWHM and the image of the fabricated device. (c) Commission Internationale d'Éclairage (CIE) (x,y) coordinates. (d) Current density (solid) and luminance (dashed) vs. driving voltage. (e) Current efficiency (solid) and Power efficiency (dashed) vs. luminance. (f) External quantum efficiency (EQE) vs. luminance.



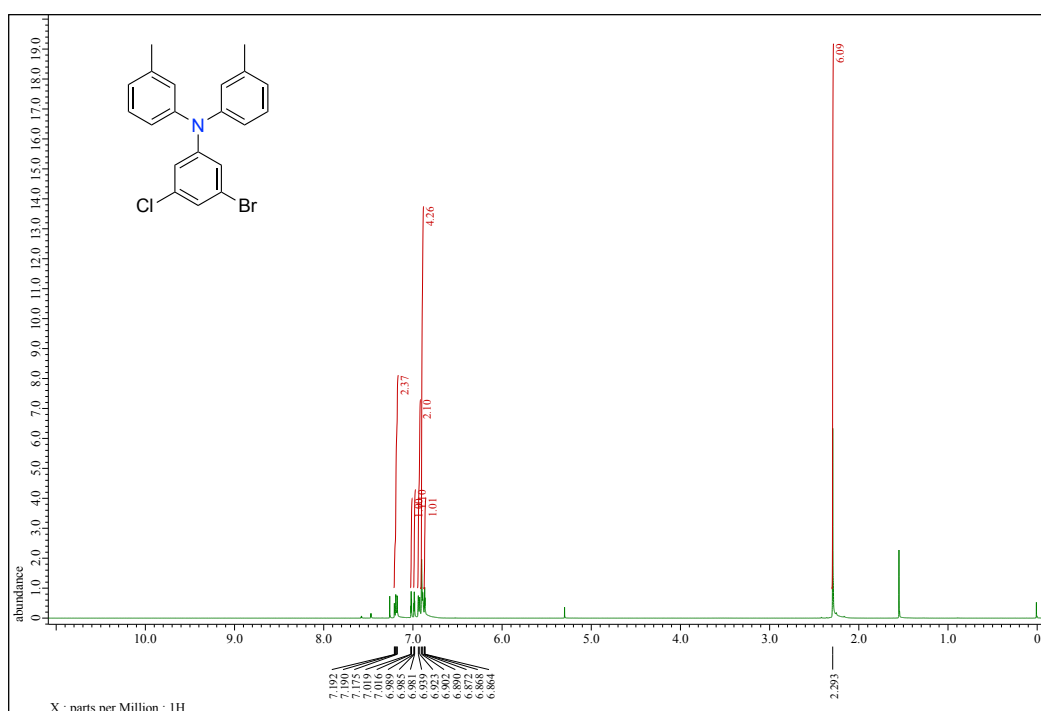
Supplementary Figure 25: Characteristics of the fabricated phosphor only device using PtON-TBBI as emitter. (a) Device structure with the estimated energy levels of each component in eV. (b) Normalized EL spectra of the phosphor only device in operation. Inset: Electroluminescence and FWHM. (c) Commission Internationale d’Éclairage (CIE) (x,y) coordinates. (d) Current density (solid) and luminance (dashed) vs. driving voltage. (e) Current efficiency (solid) and Power efficiency (dashed) vs. luminance. (f) External quantum efficiency (EQE) vs. luminance.



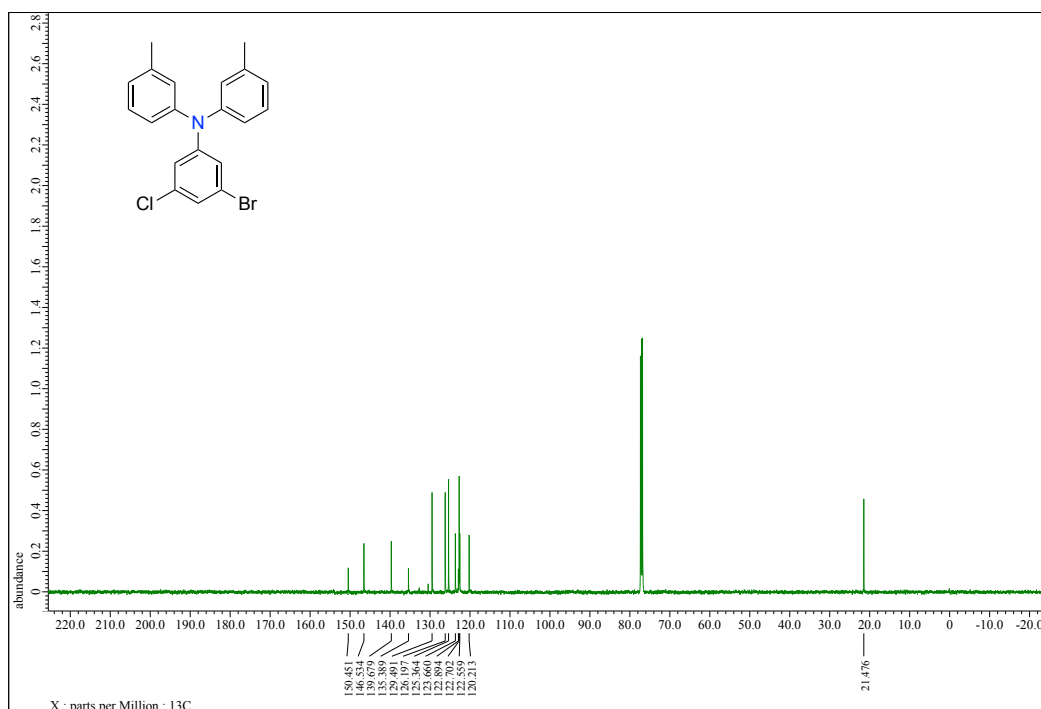
Supplementary Figure 26: NMR data. ¹H NMR spectrum of **1** in CDCl₃ at 25 °C.



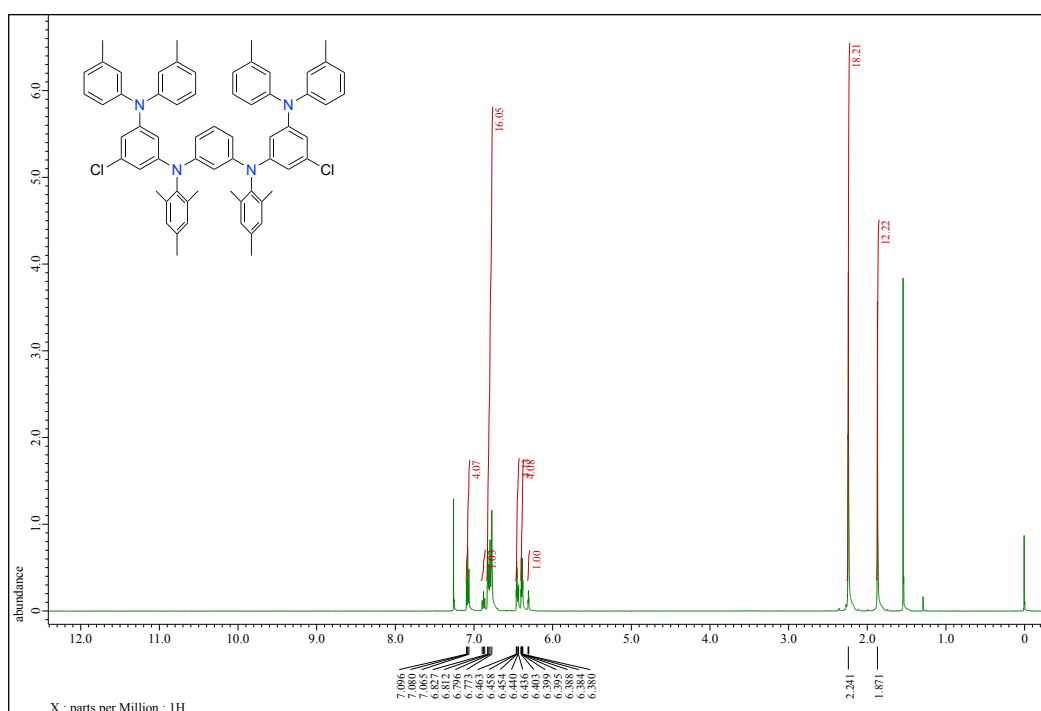
Supplementary Figure 27: NMR data. ¹³C NMR spectrum of **1** in CDCl₃ at 25 °C.



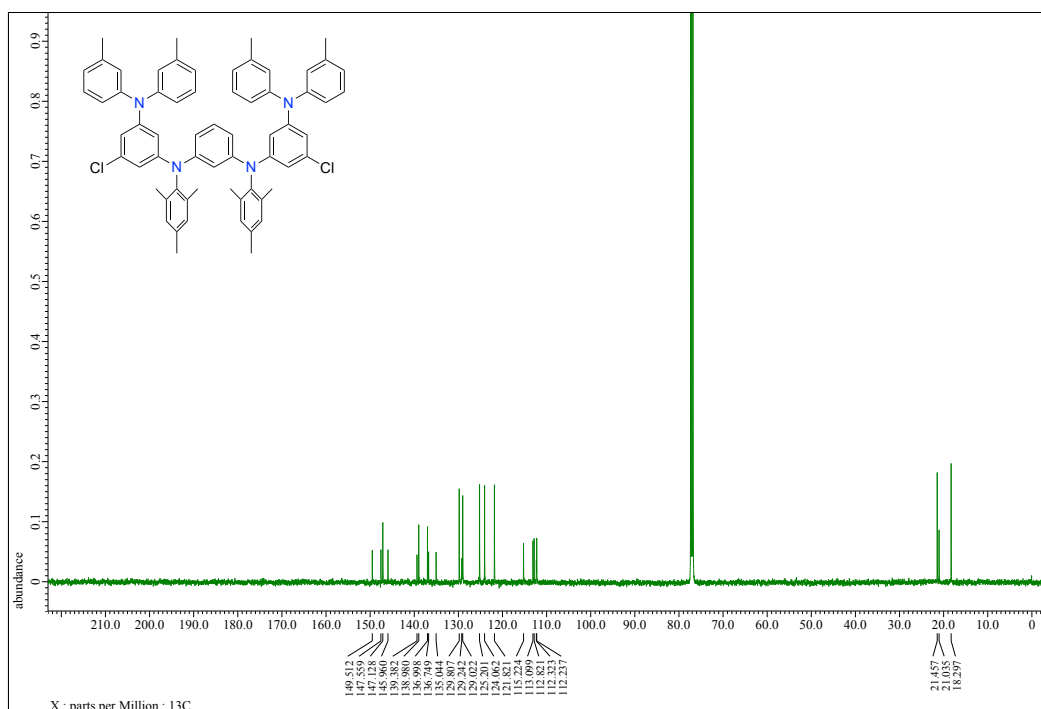
Supplementary Figure 28: NMR data. ¹H NMR spectrum of **2** in CDCl₃ at 25 °C.



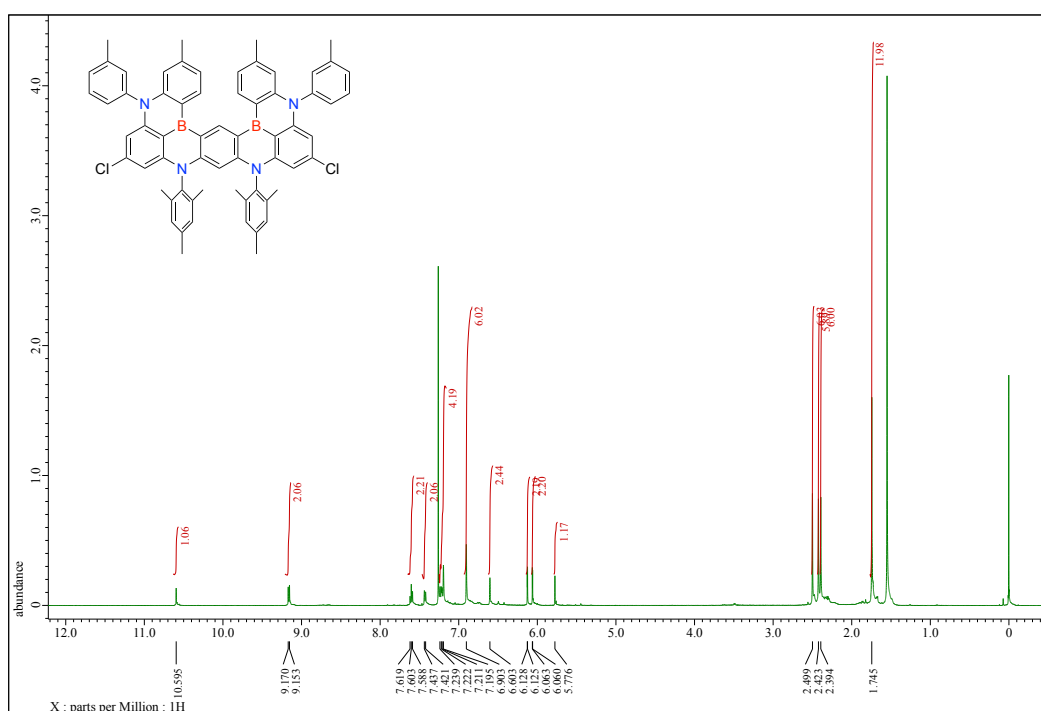
Supplementary Figure 29: NMR data. ¹³C NMR spectrum of **2** in CDCl₃ at 25 °C.



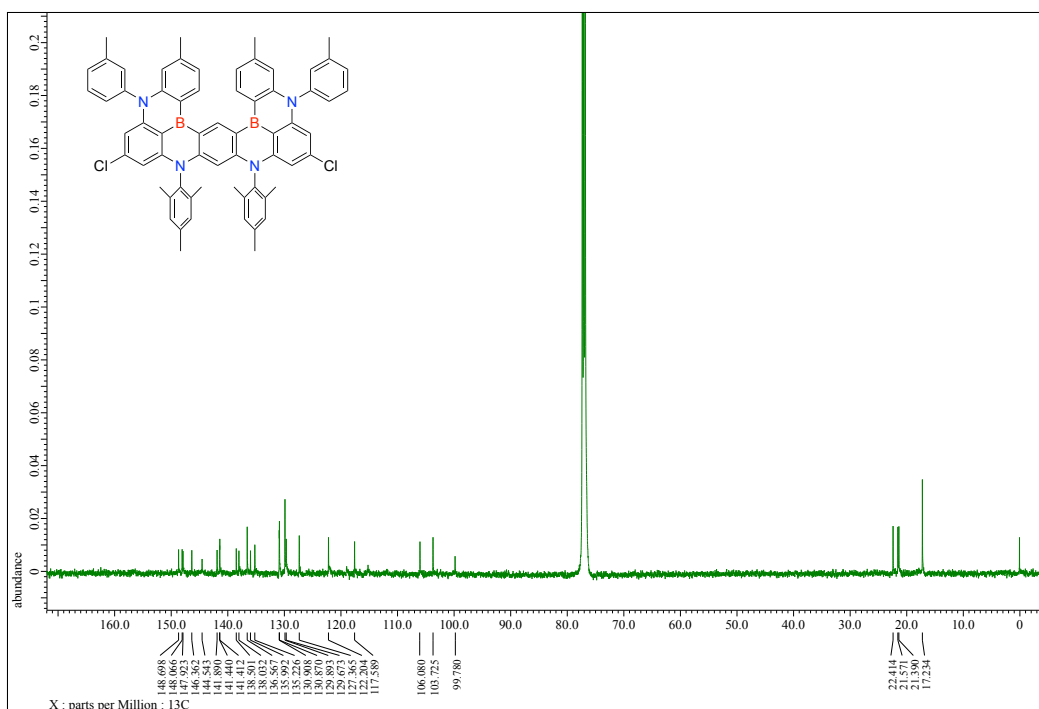
Supplementary Figure 30: NMR data. ¹H NMR spectrum of **3** in CDCl₃ at 25 °C.



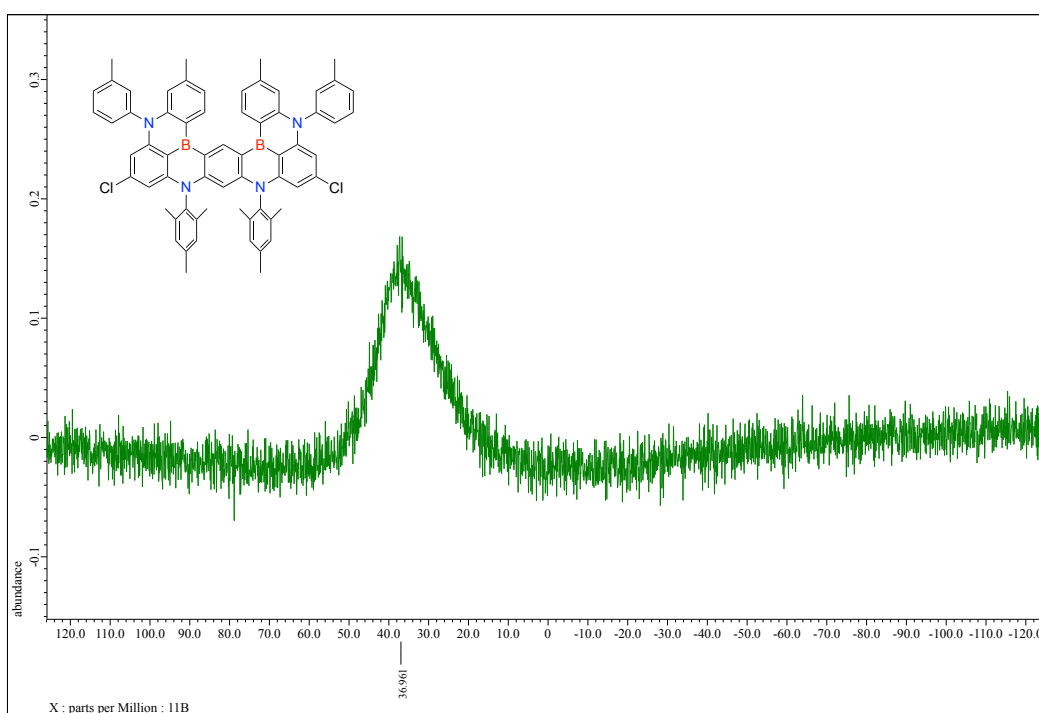
Supplementary Figure 31: NMR data. ¹³C NMR spectrum of **3** in CDCl₃ at 25 °C.



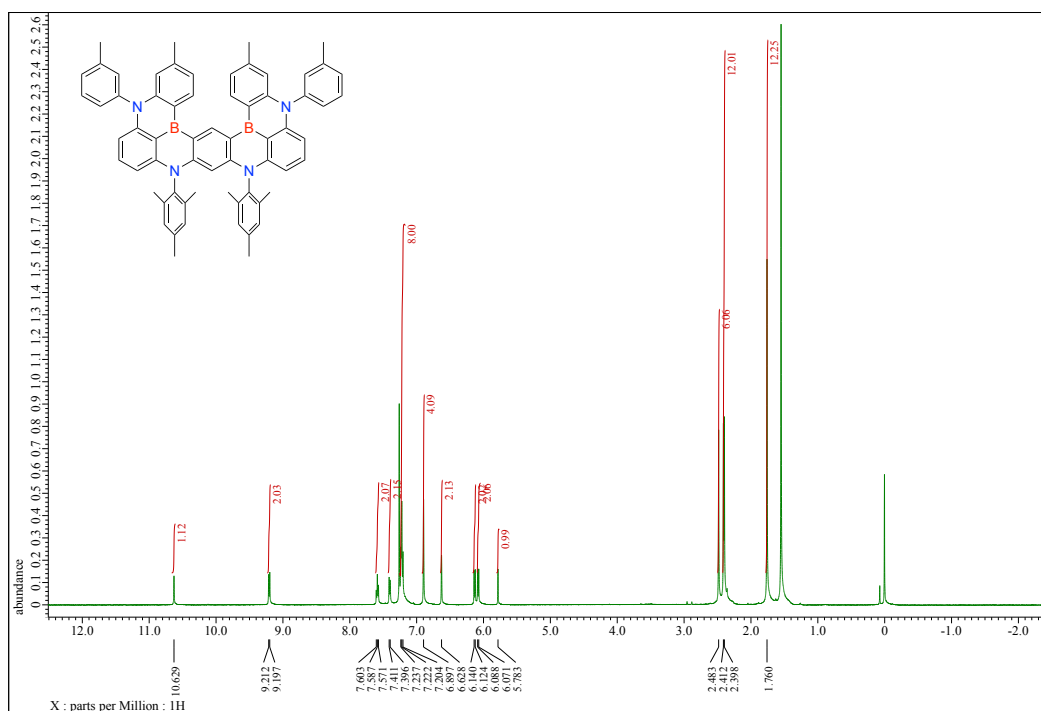
Supplementary Figure 32: NMR data. ¹H NMR spectrum of v-DABNA-M-Cl in CDCl₃ at 25 °C.



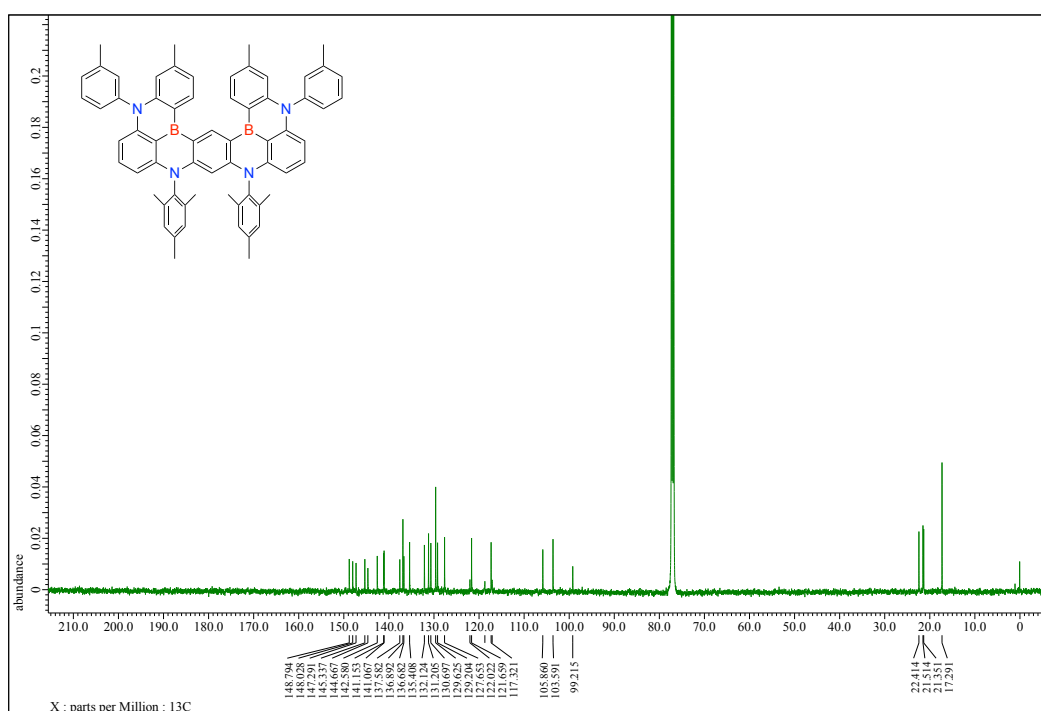
Supplementary Figure 33: NMR data. ^{13}C NMR spectrum of **v-DABNA-M-Cl** in CDCl_3 at 25 °C.



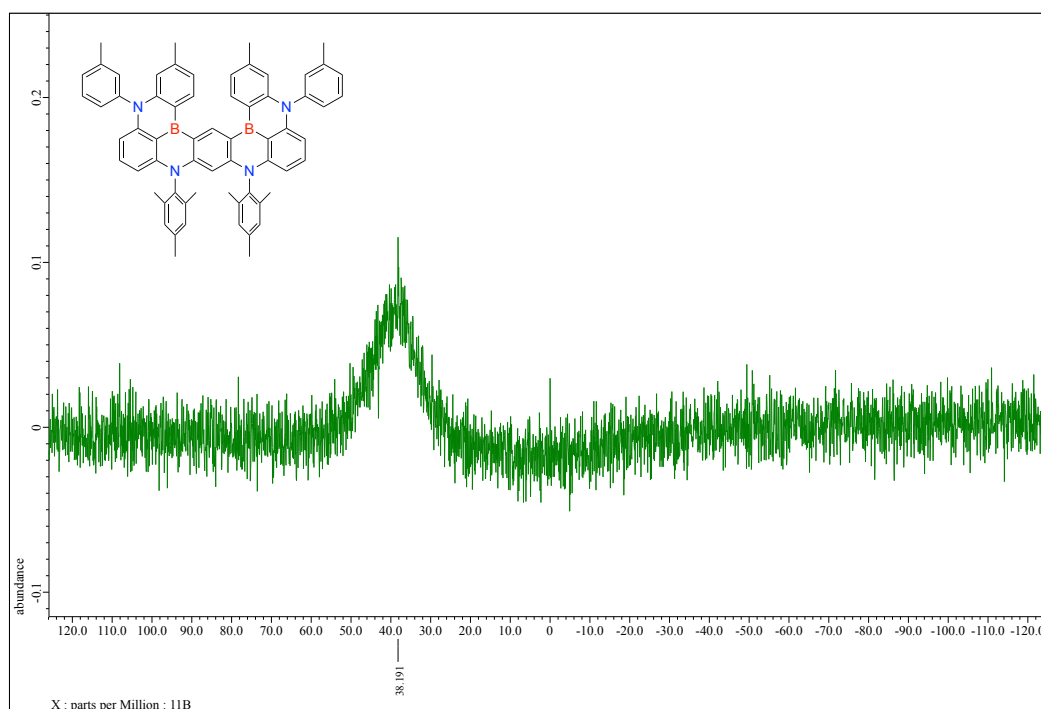
Supplementary Figure 34: NMR data. ^{11}B NMR spectrum of **v-DABNA-M-Cl** in CDCl_3 at 25 °C.



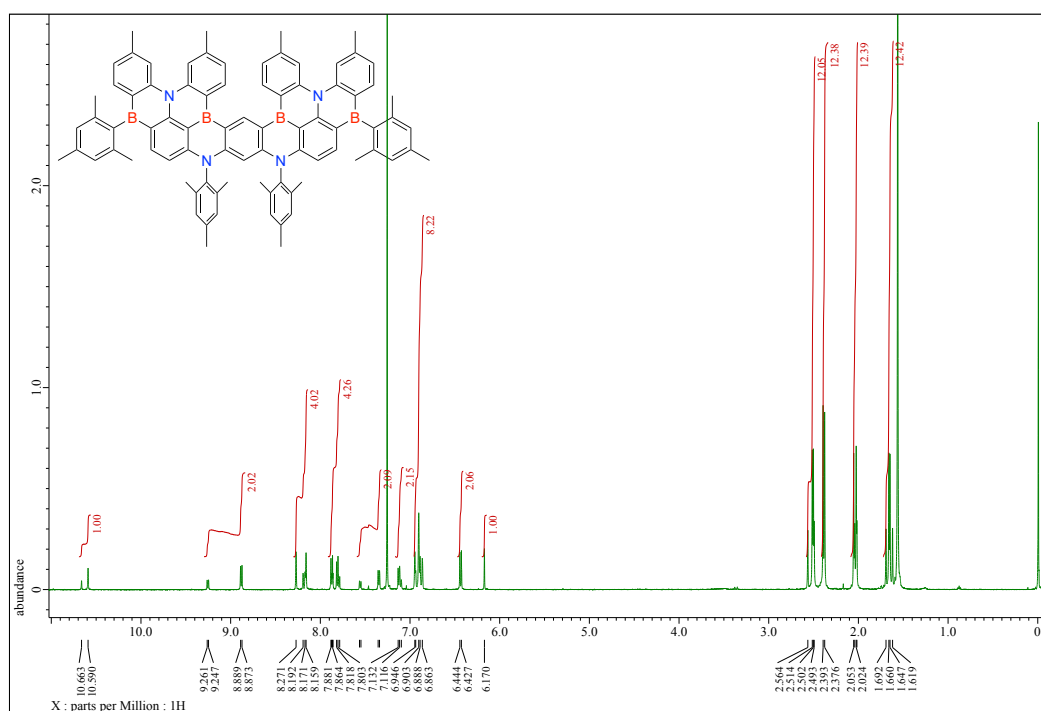
Supplementary Figure 35: NMR data. ¹H NMR spectrum of **v-DABNA-M** in CDCl₃ at 25 °C.



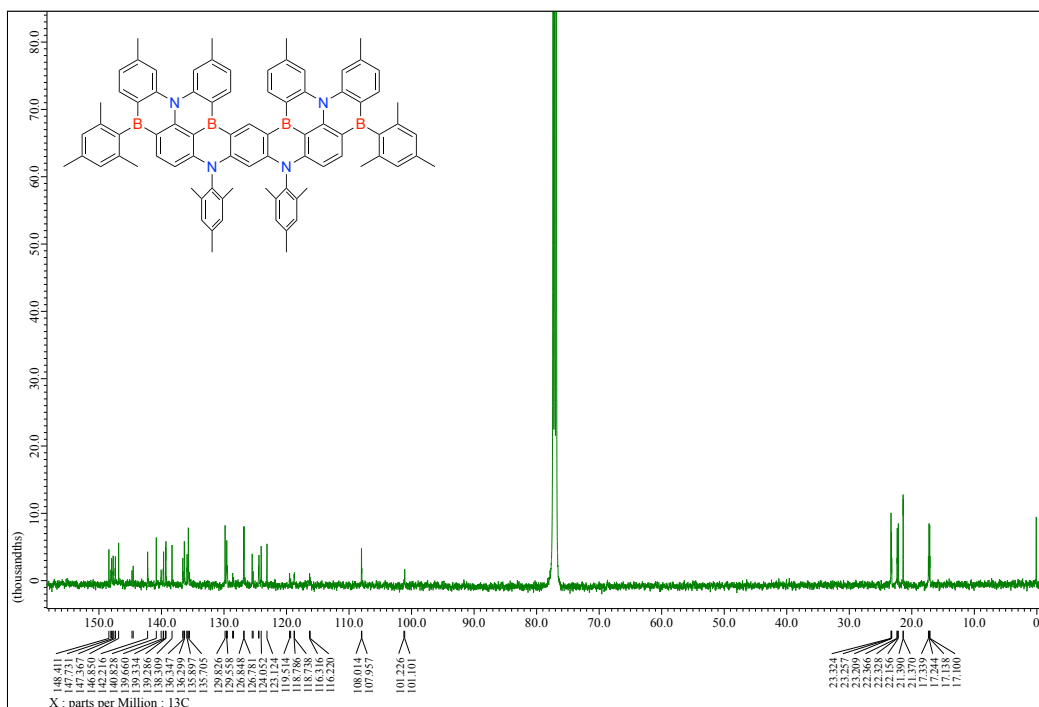
Supplementary Figure 36: NMR data. ¹³C NMR spectrum of **v-DABNA-M** in CDCl₃ at 25 °C.



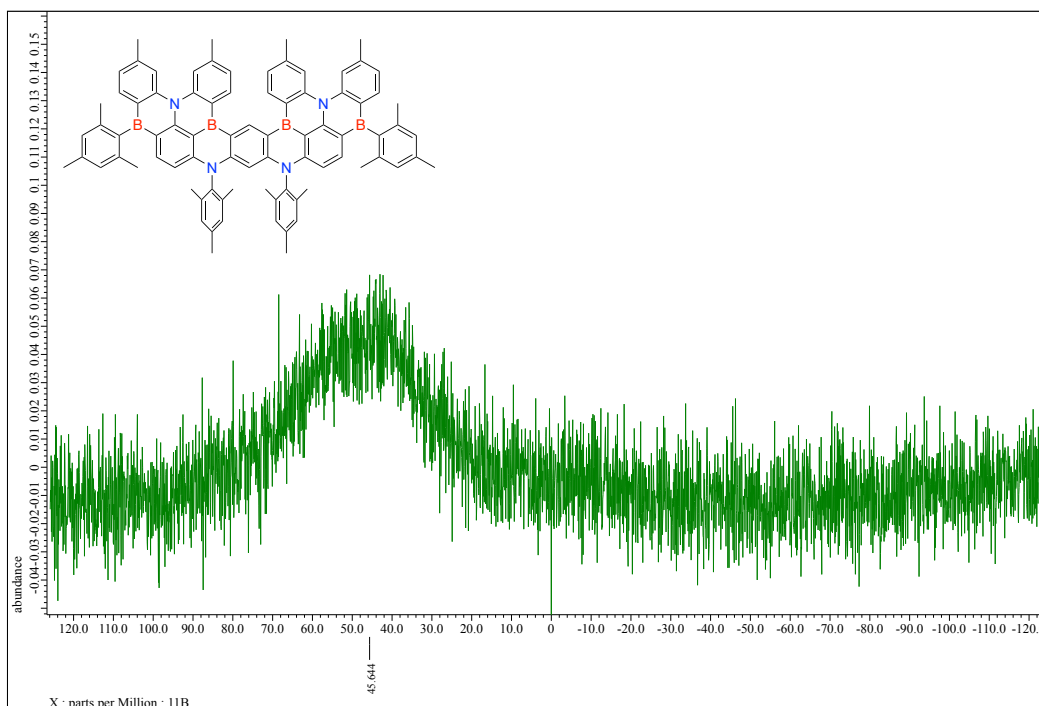
Supplementary Figure 37: NMR data. ^{11}B NMR spectrum of v-DABNA-M in CDCl_3 at 25 °C.



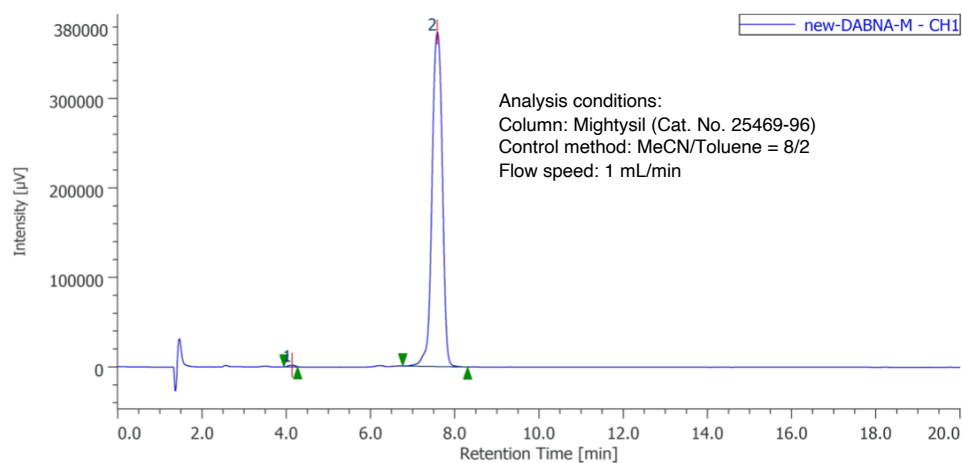
Supplementary Figure 38: NMR data. ^1H NMR spectrum of v-DABNA-M-B-Mes in CDCl_3 at 25 °C.



Supplementary Figure 39: NMR data. ^{13}C NMR spectrum of **v-DABNA-M-B-Mes** in CDCl_3 at 25°C .

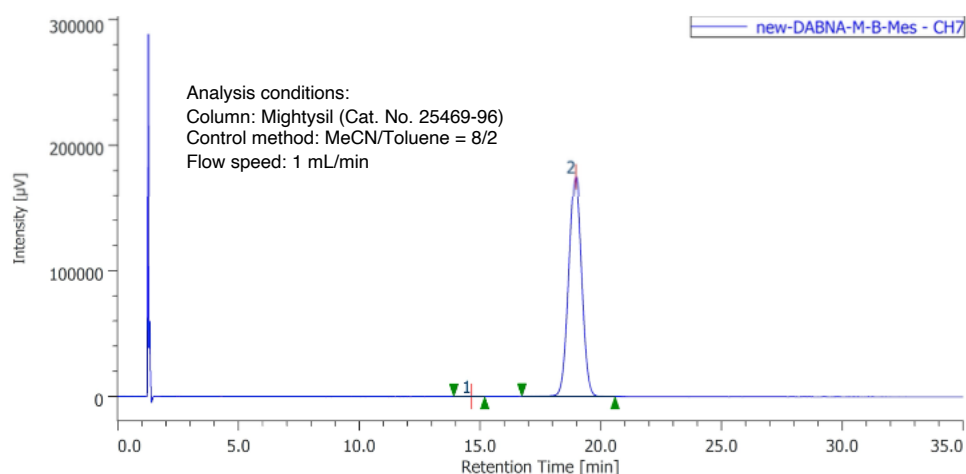


Supplementary Figure 40: NMR data. ^{11}B NMR spectrum of **v-DABNA-M-B-Mes** in CDCl_3 at 25°C .



#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	1	4.142	21251	1822	0.334	0.485	N/A	2405	8.727	0.822	
2	Unknown	1	7.585	6340274	373564	99.666	99.515	N/A	4478	N/A	0.946	

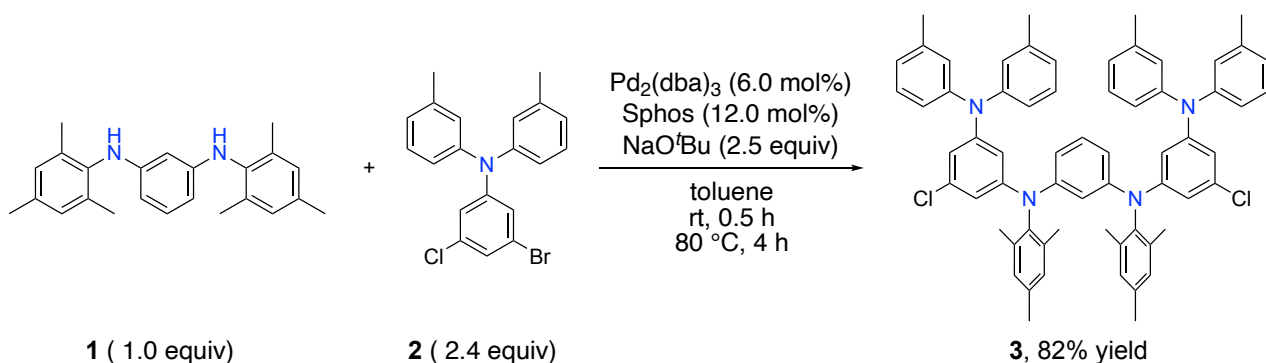
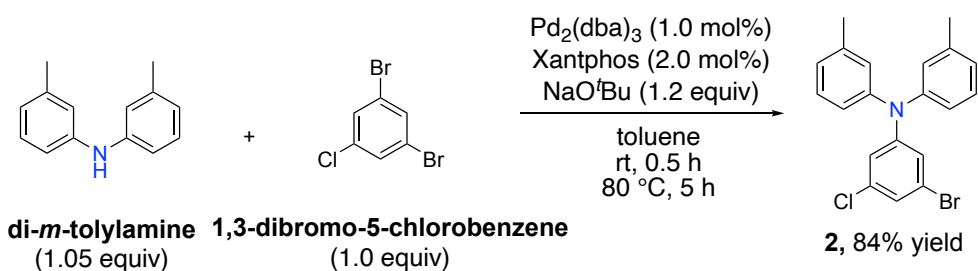
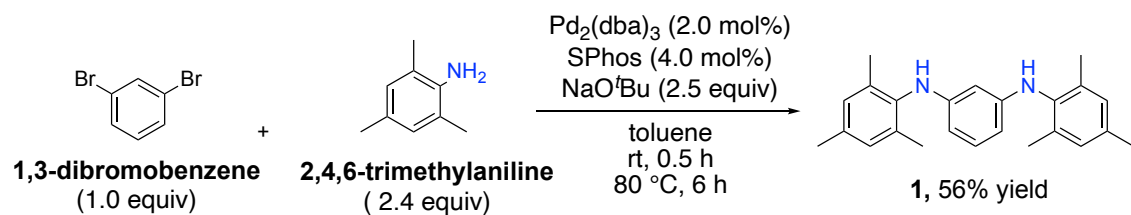
Supplementary Figure 41: HPLC data. HPLC analysis of v-DABNA-M (5).



#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	7	14.647	8191	301	0.125	0.172	N/A	4749	4.666	0.919	
2	Unknown	7	18.938	6558830	174950	99.875	99.828	N/A	5806	N/A	1.021	

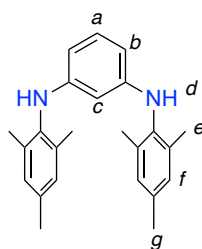
Supplementary Figure 42: HPLC data. HPLC analysis of v-DABNA-M-B-Mes (6).

Supplementary Methods



Supplementary Figure 43: Synthesis. Synthetic route of precursor compound **3**.

Synthesis of *N*¹,*N*³-dimesitylbenzene-1,3-diamine (**1**).

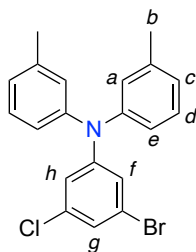


A 300 mL three-neck round bottle flask was charged with tris(dibenzylideneacetone)dipalladium(0) (916 mg, 1.0 mmol), Sphos (821 mg, 2.0 mmol), 1,3-dibromobenzene (11.8 g, 50.0 mmol), 2,4,6-trimethylaniline (16.2 g, 120.0 mmol), and sodium *tert*-butoxide (12.0 g, 125 mmol). After being

evacuated and backfilled with N₂ (3 times), dry toluene (100 mL) was added under a nitrogen atmosphere. The reaction mixture was stirred at 80 °C for 6 hours. Upon cooling, the resulting suspension was filtered through silica gel, then washed with dichloromethane to yield a dark brown solution. Then, the solution was concentrated under vacuum and followed by purification through silica gel column chromatography (eluent: hexane/dichloromethane = 3/1, v/v) to obtain the title compound as a white solid (9.6 g, 56% yield).

IR(neat): cm⁻¹ 3378, 2945, 2910, 2852, 1615, 1599, 1582, 1502, 1479, 1377, 1327, 1297, 1274, 1248, 1225, 1183, 1159, 1089, 1009, 988, 976, 955, 851, 842, 763, 716, 699, 646, 626, 577, 518, 447, 405; ¹H NMR (CDCl₃, 495 MHz) δ 6.91-6.86 (m, 5H, *f*, *a*), 5.85 (dd, *J* = 7.9, 2.0 Hz, 2H, *b*), 5.69 (t, *J* = 2.1 Hz, 1H, *c*), 4.94 (s, 2H, *d*), 2.29 (s, 6H, *g*), 2.17 (s, 12H, *e*); ¹³C NMR (125 MHz, CDCl₃) δ 147.9 (2C), 136.0 (4C), 135.9 (2C), 135.2 (2C), 129.9 (1C), 129.1 (4C), 103.8 (2C), 98.8 (1C), 21.0 (2C), 18.4 (4C).

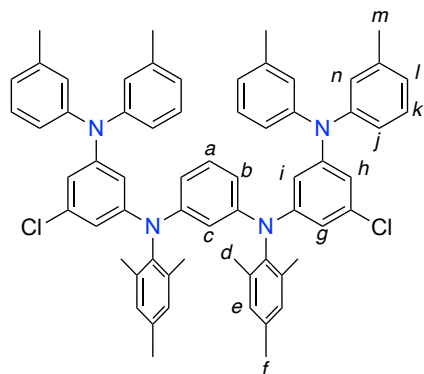
Synthesis of 3-bromo-5-chloro-*N,N*-di-*m*-tolylaniline (2).



A 300 mL three-neck round bottle flask was charged with tris(dibenzylideneacetone)dipalladium(0) (275 mg, 0.3 mmol), Xantphos (347 mg, 0.6 mmol), di-*m*-tolylamine (6.21 g, 31.5 mmol), 1,3-dibromo-5-chlorobenzene (8.11 g, 30 mmol), and sodium *tert*-butoxide (3.5 g, 36 mol). After being evacuated and backfilled with N₂ (3 times), dry toluene (80 mL) was added under a nitrogen atmosphere. The reaction mixture was stirred at 80 °C for 5 hours. The reaction mixture was allowed to cool to room temperature, followed by filtration with a pad of silica gel (eluent: toluene), the organic layer was concentrated in vacuo. The resulting crude product was purified by silica gel column chromatography (eluent: hexane) to provide the title compound as a bright oil (9.7 g, 84% yield).

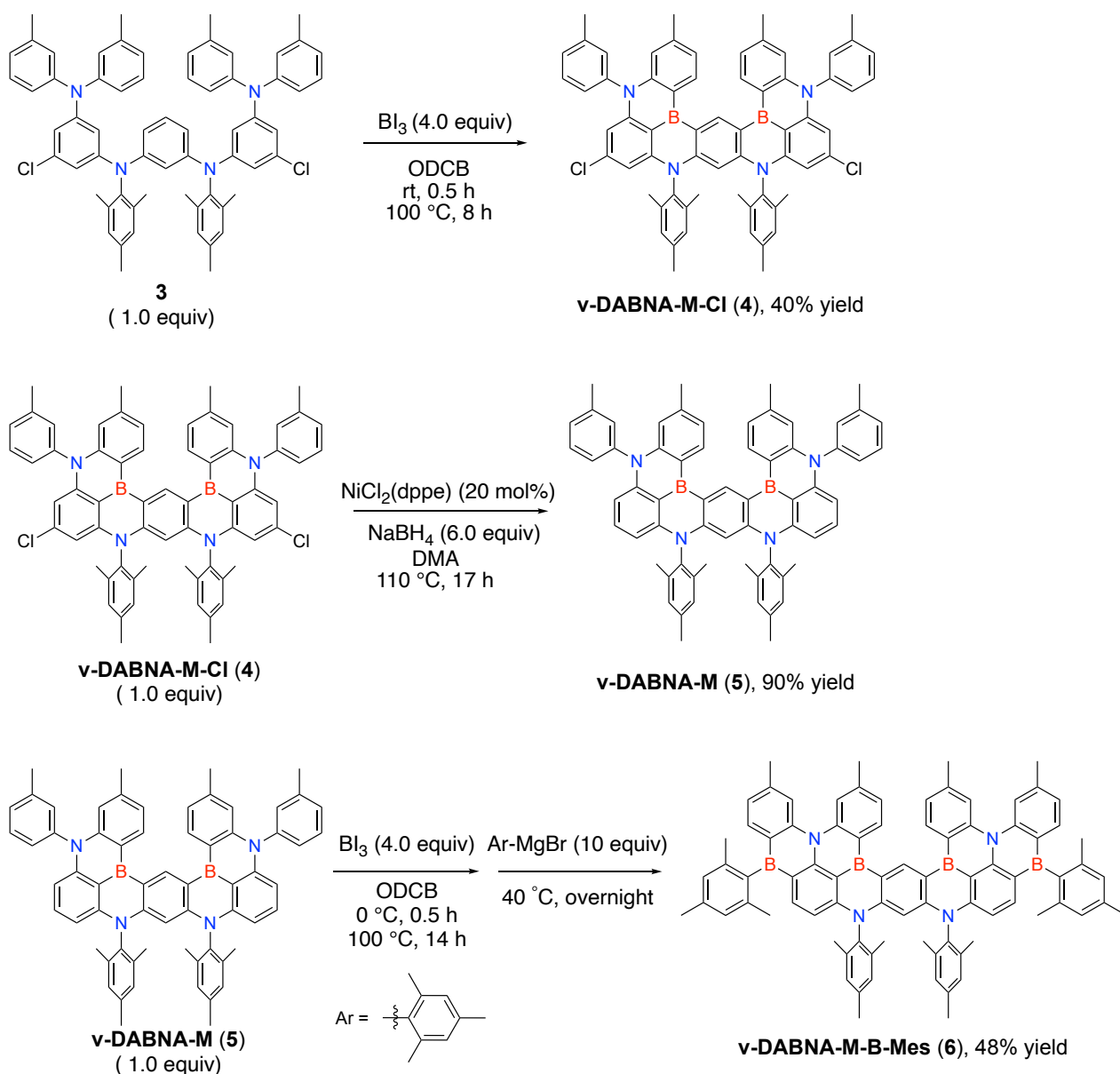
¹H NMR (495 MHz, CDCl₃) δ 7.21-7.18 (m, 2H, *d*), 7.02 (t, *J* = 1.8 Hz, 1H, *g*), 6.98 (t, *J* = 2.0 Hz, 1H, *h*), 6.93 (d, *J* = 7.7 Hz, 2H, *c*), 6.90 (m, 4H, *a*, *e*), 6.87 (t, *J* = 2.0 Hz, 1H, *f*), 2.29 (s, 6H, *b*); ¹³C NMR (125 MHz, CDCl₃) δ 150.5 (1C), 146.5 (2C), 139.7 (2C), 135.4 (1C), 129.5 (2C), 126.2 (2C), 125.4 (2C), 123.7 (1C), 122.9 (1C), 122.7 (2C), 122.6 (1C), 120.2 (1C), 21.5 (2C).

Synthesis of $N^1,N^{1'}$ -(1,3-phenylene)bis(5-chloro- N^1 -mesityl- N^3,N^3 -di-*m*-tolylbenzene-1,3-diamine) (3).



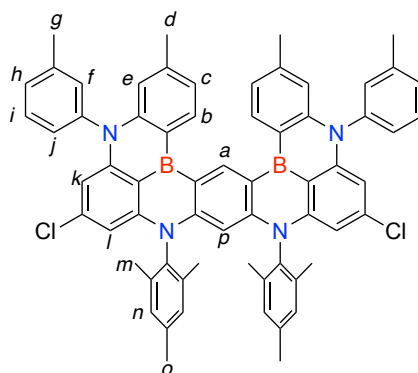
A tris(dibenzylideneacetone)dipalladium(0) (138 mg, 0.15 mmol), SPhos (123 mg, 0.3 mmol), N^1,N^3 -dimesitylbenzene-1,3-diamine (860 mg, 2.5 mmol), 3-bromo-5-chloro- N,N -di-*m*-tolylaniline (2.32 g, 6.0 mmol), and sodium *tert*-butoxide (961 mg, 10.0 mol) were dissolved in toluene (20 mL) under a nitrogen atmosphere and stirred at 80 °C for 4 hours. After cooling to room temperature, the reaction mixture was filtered through a silica gel pad (eluent: toluene), and the organic solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography (eluent: hexane/ toluene = 6/1, v/v) followed by washing with methanol to obtain the title compound as a white solid (1.95 g, 82% yield).

IR(neat): cm^{-1} 2916, 1575, 1559, 1486, 1447, 1375, 1340, 1301, 1258, 1212, 1185, 1166, 1148, 1102, 1033, 1010, 987, 966, 945, 877, 852, 824, 794, 773, 759, 729, 699, 679, 654, 636, 613, 569, 557, 520, 500, 477, 458, 444, 418, 402; ^1H NMR (495 MHz, CDCl_3) δ 7.08 (t, J = 7.8 Hz, 4H, *k*), 6.88 (t, J = 8.1 Hz, 1H, *a*), 6.83-6.77 (m, 16H, *l, j, n, e*), 6.46-6.44 (m, 4H, *b, i*), 6.39 (dt, J = 7.4, 2.0 Hz, 4H, *h, g*), 6.31 (t, J = 2.3 Hz, 1H, *c*), 2.24 (s, 18H, *m, f*), 1.87 (s, 12H, *d*); ^{13}C NMR (125 MHz, CDCl_3) δ 149.5 (2C), 147.6 (2C), 147.1 (4C), 146.0 (2C), 139.4 (2C), 139.0 (4C), 137.0 (4C), 136.7 (2C), 135.0 (2C), 129.8 (4C), 129.2 (1C), 129.0 (4C), 125.2 (4C), 124.1 (4C), 121.8 (4C), 115.2 (2C), 113.1 (2C), 112.8 (2C), 112.3 (1C), 112.2 (2C), 21.5 (4C), 21.0 (2C), 18.3 (4C).



Supplementary Figure 44: Synthesis. Synthetic route of **v-DABNA-M** and **v-DABNA-M-B-Mes**.

Synthesis of 7,13-dichloro-9,11-dimesityl-3,17-dimethyl-5,15-di-*m*-tolyl-5,9,11,15-tetrahydro-5,9,11,15-tetraaza-19b,20b-diboradinaphtho[3,2,1-*de*:1',2',3'-*jk*]pentacene (4).

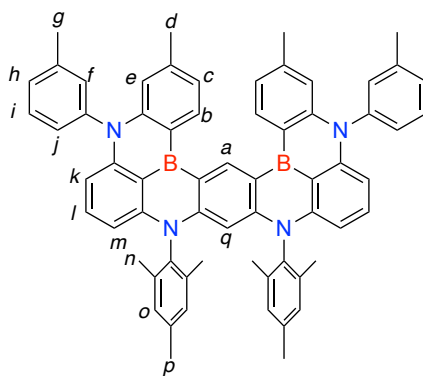


A 25 mL Schlenk tube with a magnetic stir bar was charged with the borylative precursor **3** (1.43 g,

1.5 mmol) and BI_3 (2.35 g, 6.0 mmol). After being evacuated and backfilled with N_2 (3 times), dry *o*-dichlorobenzene (10 mL) was added under N_2 atmosphere. The reaction mixture was stirred at 100 °C for 8 hours. After the reaction mixture cooled down to room temperature, it was quenched with phosphate buffer solution and extracted with toluene. The organic solvent was then removed under reduced pressure, and the crude product was purified by silica gel column chromatography (hexane/dichloromethane =5:1, v/v) to obtain the title product **v-DABNA-M-Cl** as a yellow solid (580 mg, 40%).

IR(neat): cm^{-1} 2915, 1599, 1563, 1557, 1496, 1484, 1456, 1407, 1357, 1307, 1234, 1218, 1195, 1162, 1132, 1107, 1003, 958, 948, 931, 912, 894, 877, 849, 808, 771, 761, 732, 723, 695, 644, 630, 609, 556, 505, 477, 458, 445, 427, 418, 401; ^1H NMR (495 MHz, CDCl_3) δ 10.59 (s, 1H, *a*), 9.16 (d, J = 7.9 Hz, 2H, *b*), 7.60 (t, J = 7.8 Hz, 2H, *i*), 7.43 (d, J = 7.9 Hz, 2H, *c*), 7.19-7.23 (m, 4H, *h*, *e*), 6.90 (s, 6H, *n*, *j*), 6.60 (s, 2H, *f*), 6.13 (d, J = 1.4 Hz, 2H, *k*), 6.06 (d, J = 1.4 Hz, 2H, *l*), 5.78 (s, 1H, *p*), 2.50 (s, 6H, *o*), 2.42 (s, 6H, *d*), 2.39 (s, 6H, *g*), 1.74 (s, 12H, *m*); ^{13}C NMR (125 MHz, CDCl_3) δ 148.7 (2C), 148.1 (2C), 147.9 (2C), 146.4 (2C), 144.5 (1C), 141.9 (2C), 141.5 (2C), 141.4 (2C), 138.5 (2C), 138.0 (2C), 136.6 (4C), 136.0 (2C), 135.2 (2C), 131.0 (2C), 130.9 (2C), 129.9 (4C), 129.7 (2C), 127.4 (2C), 122.2 (2C), 117.6 (2C), 106.1 (2C), 103.7 (2C), 99.8 (1C), 22.4 (2C), 21.6 (2C), 21.4 (2C), 17.2 (4C). The NMR signal of the carbon α to the boron was not observed.; ^{11}B NMR (159 MHz, CDCl_3) δ 37.0.

Synthesis of 9,11-dimesityl-3,17-dimethyl-5,15-di-*m*-tolyl-5,9,11,15-tetrahydro-5,9,11,15-tetraaza-19b,20b-diboradinaphtho[3,2,1-*de*:1',2',3'-*jk*]pentacene (5).

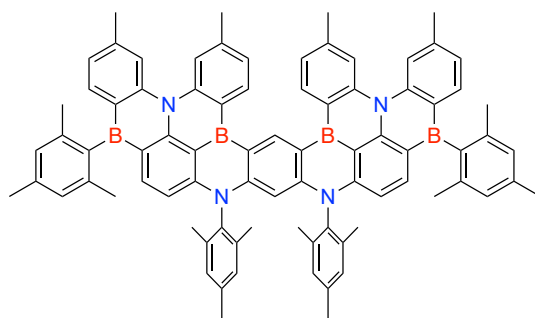


A 50 mL two-neck round flask was charged with **v-DABNA-M-Cl** (240 mg, 0.25 mmol), 1,2-bis(diphenylphosphino)ethane]dichloronickel(II) (27 mg, 0.05 mmol), and NaBH_4 (60 mg, 1.5 mmol). After being evacuated and backfilled with N_2 (3 times), dry dimethylacetamide (5 mL) was added under N_2 atmosphere. The reaction mixture was stirred at 110 °C for 17 hours. After the reaction mixture cooled down to room temperature, it was quenched with NH_4Cl solution and extracted with toluene. The organic solvent was then removed under reduced pressure, and the crude product was purified by silica gel column chromatography (hexane/dichloromethane =5:1, v/v) to obtain the title product **v-DABNA-M** as a yellow solid (203 mg, 90%).

IR(neat): cm^{-1} 2913, 1583, 1567, 1520, 1496, 1443, 1407, 1375, 1351, 1330, 1304, 1285, 1221, 1193, 1176, 1129, 1057, 1003, 960, 927, 900, 855, 801, 788, 746, 738, 713, 697, 640, 606, 589, 553, 508,

455, 401; ^1H NMR (495 MHz, CDCl_3) δ 10.63 (s, 1H, *a*), 9.20 (d, $J = 7.7$ Hz, 2H, *b*), 7.59 (t, $J = 7.9$ Hz, 2H, *i*), 7.40 (d, $J = 7.7$ Hz, 2H, *c*), 7.24-7.20 (m, 8H, *h, j, e, l*), 6.90 (s, 4H, *o*), 6.63 (s, 2H, *f*), 6.13 (d, $J = 8.2$ Hz, 2H, *k*), 6.08 (d, $J = 8.2$ Hz, 2H, *m*), 5.78 (s, 1H, *q*), 2.48 (s, 6H, *p*), 2.40 (d, $J = 7.1$ Hz, 12H, *d, g*), 1.76 (s, 12H, *n*); ^{13}C NMR (125 MHz, CDCl_3) δ 148.8 (2C), 148.0 (2C), 147.3 (2C), 145.3 (2C), 144.7 (1C), 142.6 (2C), 141.2 (2C), 141.1 (2C), 137.6 (2C), 136.9 (4C), 136.7 (2C), 135.4 (2C), 132.1 (2C), 131.2 (2C), 130.7 (2C), 129.6 (4C), 129.2 (2C), 127.7 (2C), 122.0 (2C), 121.7 (2C), 118.7 (2C), 117.3 (2C), 117.1 (2C), 105.9 (2C), 103.6 (2C), 99.2 (1C), 22.4 (2C), 21.5 (2C), 21.4 (2C), 17.3 (4C); ^{11}B NMR (159 MHz, CDCl_3) δ 38.2; HRMS (MALDI) m/z $[\text{M}]^+$ calcd for $\text{C}_{64}\text{H}_{56}\text{B}_2\text{N}_4$ 902.4705; observed 902.4772; HPLC analysis: 99.66% purity, retention time 7.585 min in 80% MeCN and 20% toluene.

Synthesis of 5,8,10,13-tetramesityl-2,16,19,25-tetramethyl-5,8,10,13-tetrahydro-8,10,17b,26b-tetraaza-5,13,21b,22b-tetraboranaphtho[1,2,3,4-*vw*]*x*naphtho[3',2',1':4,10]anthra[1,9-*pq*]hexaphene (6).



A 25 mL Schlenk tube equipped with a magnetic stir bar was charged with v-DABNA-M (136 mg, 0.15 mmol) and BI_3 (235 mg, 0.6 mmol). The tube was evacuated and backfilled with nitrogen three times, then dry *o*-dichlorobenzene (3.0 mL) was added under a nitrogen atmosphere. The reaction mixture was stirred at 100 °C for 14 hours. After cooling to room temperature, the mixture was placed under vacuum to remove HI for 10 minutes. Mesityl Grignard reagent (1.5 mL, 1.5 mmol) was then added dropwise, and the mixture was stirred at 40 °C overnight. Upon completion of the reaction, the mixture was quenched with phosphate buffer solution and extracted with toluene. The solvent was removed under reduced pressure, and the crude product was purified by silica gel column chromatography (hexane/dichloromethane = 6:1, v/v), yielding the title product **v-DABNA-M-B-Mes** as a yellow solid (85 mg, 48%).

IR(neat): cm^{-1} 2915, 1608, 1575, 1557, 1539, 1500, 1397, 1378, 1298, 1285, 1262, 1223, 1189, 1179, 1149, 1040, 966, 887, 869, 847, 814, 788, 761, 728, 669, 657, 609, 556, 524, 434, 411, 402; ^1H NMR (CDCl_3 , 495 MHz) δ 10.60 (s, 1H), 8.89 (d, $J = 7.7$ Hz, 2H), 8.28 (s, 2H), 8.17 (s, 2H), 7.88 (d, $J = 7.7$ Hz, 2H), 7.82 (d, $J = 7.9$ Hz, 2H), 7.36 (d, $J = 7.7$ Hz, 2H), 7.13 (d, $J = 7.9$ Hz, 2H), 6.95-6.87 (m, 7H), 6.44 (d, $J = 8.5$ Hz, 2H), 6.18 (s, 1H), 2.52 (s, 6H), 2.51 (s, 6H), 2.40 (s, 6H), 2.38 (s, 6H), 2.06 (s, 6H), 2.03 (s, 6H), 1.67 (s, 6H), 1.65 (s, 6H); The signals are not assignable because of conformational isomerism; ^{13}C NMR (125 MHz, CDCl_3) δ 148.41, 148.09, 147.97, 147.78, 147.73, 147.41, 147.37, 146.85, 144.72, 144.52, 142.22, 140.83, 140.05, 139.72, 139.66, 139.33, 139.29, 138.31, 136.59, 136.55, 136.35, 136.30, 135.94, 135.90, 135.71, 135.52, 129.83, 129.62, 129.56,

129.47, 128.62, 128.48, 126.85, 126.78, 125.49, 125.34, 124.47, 124.41, 124.05, 123.12, 119.51, 119.34, 118.79, 118.74, 116.32, 116.22, 108.01, 107.96, 101.23, 101.10, 23.32, 23.26, 23.21, 22.37, 22.33, 22.15, 21.39, 21.37, 17.34, 17.24, 17.14, 17.10; The signals display two distinct digits to clearly identify them because of conformational isomerism. ^{11}B NMR (159 MHz, CDCl_3) δ 45.6; HRMS (MALDI) m/z $[\text{M}]^+$ calcd for $\text{C}_{82}\text{H}_{74}\text{B}_4\text{N}_4$ 1158.6321; observed 1158.6314; HPLC analysis: 99.87% purity, retention time 18.928 min in 80% MeCN and 20% toluene.

Computational Method

All calculations were performed with Gaussian 16 (Revision B.01)^[1], ADF2021^[2] and PySCF^[3–6] packages unless otherwise noted. The DFT method was employed using the B3LYP^[7] or M062X^[8] hybrid functional. Structures were optimized with the 6-31G(d)^[9] basis set. The time-dependent density functional theory (TD-DFT) calculation^[10] was conducted at the B3LYP/6-31G(d) level or the M062X/TZP^[11] level. Coupled-cluster (CC2) calculations were performed using the TURBOMOLE package^[12] with def2-TZVP basis set at the structures optimized at the (TD) M062X/TZP level.

Spin-orbit coupling calculations

Using the optimized geometries in the S_1 state, the spin-orbit coupling (SOC) matrix elements $\langle S_1 | \hat{H}_{\text{SOC}} | T_n \rangle$ between S_1 and T_n ($n = 1, 2$) were obtained performing TD-DFT calculations with the M062X functional and the TZP basis set as implemented in the ADF2021 program. Taking into account the contributions from the three degenerate triplet states ($T_{n,x}$, $T_{n,y}$, and $T_{n,z}$), $\langle S_1 | \hat{H}_{\text{SOC}} | T_n \rangle$ were calculated by the square root of the sum of squares of the real and imaginary parts (Re and Im) of the matrix elements (eq. S1).

$$\langle S_1 | \hat{H}_{\text{SOC}} | T_n \rangle = \sum_{\alpha=x,y,z} \left[(Re \langle S_1 | \hat{H}_{\text{SOC}} | T_{n,\alpha} \rangle)^2 + (Im \langle S_1 | \hat{H}_{\text{SOC}} | T_{n,\alpha} \rangle)^2 \right]^{\frac{1}{2}} \quad (\text{S1})$$

Supplementary Notes

Estimation of rate constant for reverse intersystem crossing.

Rate constants (k_F , k_{IC} , k_{ISC} , and k_{RISC}) were determined from the measurements of quantum yields (Φ_F and Φ_{TADF}) and lifetimes (τ_F and τ_{TADF}) and of the prompt fluorescence and delayed TADF components according to Adachi's method (equations 1–2^[13], 3–5^[14] and 6^[15]).

ν -DABNA-M doped PMMA film (1 wt%)

$$\Phi = 0.920$$

$$\Phi_F = 0.755$$

$$\Phi_{TADF} = 0.165$$

$$\tau_F = 4.60 \text{ ns}$$

$$\tau_{TADF} = 10.0 \text{ } \mu\text{s}$$

$$k_p = 2.17 \times 10^8 \text{ s}^{-1} \quad k_p = 1/\tau_F \quad (1)$$

$$k_d = 1.00 \times 10^5 \text{ s}^{-1} \quad k_d = 1/\tau_{TADF} \quad (2)$$

$$k_F = 1.64 \times 10^8 \text{ s}^{-1} \quad k_F = \Phi_F/\tau_F \quad (3)$$

$$k_{IC} = 1.43 \times 10^7 \text{ s}^{-1} \quad \Phi = k_F/(k_F + k_{IC}) \quad (4)$$

$$k_{ISC} = 3.89 \times 10^7 \text{ s}^{-1} \quad \Phi_F = k_F/(k_F + k_{IC} + k_{ISC}) \quad (5)$$

$$k_{RISC} = 1.22 \times 10^5 \text{ s}^{-1} \quad k_{RISC} = k_p k_d / (k_p - k_{ISC}) \quad (6)$$

ν -DABNA-M-B-Mes doped PMMA film (1 wt%)

$$\Phi = 0.931$$

$$\Phi_F = 0.659$$

$$\Phi_{TADF} = 0.272$$

$$\tau_F = 2.60 \text{ ns}$$

$$\tau_{TADF} = 6.90 \text{ } \mu\text{s}$$

$$k_p = 3.89 \times 10^8 \text{ s}^{-1} \quad k_p = 1/\tau_F \quad (1)$$

$$k_d = 1.45 \times 10^5 \text{ s}^{-1} \quad k_d = 1/\tau_{TADF} \quad (2)$$

$$k_F = 2.57 \times 10^8 \text{ s}^{-1} \quad k_F = \Phi_F/\tau_F \quad (3)$$

$$k_{IC} = 1.90 \times 10^7 \text{ s}^{-1} \quad \Phi = k_F/(k_F + k_{IC}) \quad (4)$$

$$k_{ISC} = 1.14 \times 10^8 \text{ s}^{-1} \quad \Phi_F = k_F/(k_F + k_{IC} + k_{ISC}) \quad (5)$$

$$k_{RISC} = 2.05 \times 10^5 \text{ s}^{-1} \quad k_{RISC} = k_p k_d / (k_p - k_{ISC}) \quad (6)$$

ν -DABNA-M in toluene (10^{-6}M)

$$\Phi = 0.941$$

$$\Phi_F = 0.855$$

$$\Phi_{\text{TADF}} = 0.086$$

$$\tau_F = 3.70 \text{ ns}$$

$$\tau_{\text{TADF}} = 7.40 \text{ }\mu\text{s}$$

$$k_p = 2.68 \times 10^8 \text{ s}^{-1} \quad k_p = 1/\tau_F \quad (1)$$

$$k_d = 1.34 \times 10^5 \text{ s}^{-1} \quad k_d = 1/\tau_{\text{TADF}} \quad (2)$$

$$k_F = 2.29 \times 10^8 \text{ s}^{-1} \quad k_F = \Phi_F/\tau_F \quad (3)$$

$$k_{\text{IC}} = 1.44 \times 10^7 \text{ s}^{-1} \quad \Phi = k_F/(k_F + k_{\text{IC}}) \quad (4)$$

$$k_{\text{ISC}} = 0.25 \times 10^8 \text{ s}^{-1} \quad \Phi_F = k_F/(k_F + k_{\text{IC}} + k_{\text{ISC}}) \quad (5)$$

$$k_{\text{RISC}} = 1.48 \times 10^5 \text{ s}^{-1} \quad k_{\text{RISC}} = k_p k_d/(k_p - k_{\text{ISC}}) \quad (6)$$

ν -DABNA-M-B-Mes in toluene (10^{-6}M)

$$\Phi = 0.985$$

$$\Phi_F = 0.771$$

$$\Phi_{\text{TADF}} = 0.214$$

$$\tau_F = 1.93 \text{ ns}$$

$$\tau_{\text{TADF}} = 4.67 \text{ }\mu\text{s}$$

$$k_p = 5.19 \times 10^8 \text{ s}^{-1} \quad k_p = 1/\tau_F \quad (1)$$

$$k_d = 2.14 \times 10^5 \text{ s}^{-1} \quad k_d = 1/\tau_{\text{TADF}} \quad (2)$$

$$k_F = 3.99 \times 10^8 \text{ s}^{-1} \quad k_F = \Phi_F/\tau_F \quad (3)$$

$$k_{\text{IC}} = 0.61 \times 10^7 \text{ s}^{-1} \quad \Phi = k_F/(k_F + k_{\text{IC}}) \quad (4)$$

$$k_{\text{ISC}} = 1.12 \times 10^8 \text{ s}^{-1} \quad \Phi_F = k_F/(k_F + k_{\text{IC}} + k_{\text{ISC}}) \quad (5)$$

$$k_{\text{RISC}} = 2.73 \times 10^5 \text{ s}^{-1} \quad k_{\text{RISC}} = k_p k_d/(k_p - k_{\text{ISC}}) \quad (6)$$

Cartesian coordinates.

v-DABNA-core (S_0 , C_1 symmetry)

$E(M06-2X/6-31G(d)) = -2347.344298$ hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.800959	2.411956	-0.207270
2	6	0	3.678083	1.592903	-0.034846
3	6	0	3.817436	0.186895	0.072792
4	6	0	5.113232	-0.375632	-0.018645
5	6	0	6.235115	0.444263	-0.219296
6	6	0	6.052500	1.816672	-0.301015
7	1	0	4.706050	3.487443	-0.280780
8	1	0	6.922506	2.450983	-0.445686
9	5	0	2.600206	-0.699190	0.280364
10	7	0	2.403226	2.163190	0.038801
11	7	0	5.266566	-1.760203	0.082363
12	6	0	0.000012	2.116936	0.000030
13	6	0	-1.214713	1.426411	-0.052398
14	6	0	-1.238244	0.006864	-0.128858
15	6	0	0.000014	-0.631472	0.000023
16	6	0	1.238265	0.006869	0.128899
17	6	0	1.214725	1.426405	0.052454
18	1	0	0.000007	3.195379	0.000054
19	1	0	0.000015	-1.712631	0.000008
20	6	0	7.016410	-2.675767	-1.356039
21	6	0	6.586684	-2.294418	-0.088352
22	6	0	7.430425	-2.422442	1.012799
23	6	0	8.712089	-2.937493	0.842313
24	6	0	9.147144	-3.321608	-0.424864
25	6	0	8.299737	-3.190473	-1.522537
26	1	0	7.069681	-2.116339	1.990299
27	1	0	9.371245	-3.038724	1.698706
28	1	0	10.147057	-3.722950	-0.556418
29	1	0	8.637025	-3.488971	-2.510077
30	6	0	2.905020	-2.181802	0.598463
31	6	0	1.956391	-3.112574	1.069558
32	6	0	2.259304	-4.442226	1.296826
33	6	0	3.561105	-4.886260	1.049316
34	6	0	4.541324	-4.005759	0.632063
35	6	0	4.234722	-2.642525	0.432533
36	1	0	0.953682	-2.763876	1.290773
37	1	0	1.500951	-5.127418	1.661058
38	1	0	3.821325	-5.929585	1.203030
39	1	0	5.548493	-4.370627	0.473970
40	5	0	-2.600173	-0.699206	-0.280327
41	7	0	-2.403227	2.163168	-0.038749
42	6	0	-4.800963	2.411928	0.207302
43	6	0	-6.052497	1.816637	0.301036
44	6	0	-6.235095	0.444229	0.219320
45	6	0	-5.113209	-0.375672	0.018679
46	6	0	-3.817408	0.186864	-0.072755
47	6	0	-3.678078	1.592881	0.034896
48	1	0	-4.706045	3.487413	0.280816
49	1	0	-6.922521	2.450925	0.445687
50	7	0	-5.266550	-1.760231	-0.082354

51	6	0	-2.904991	-2.181821	-0.598437
52	6	0	-4.234697	-2.642533	-0.432546
53	6	0	-4.541287	-4.005783	-0.632074
54	6	0	-3.561062	-4.886266	-1.049304
55	6	0	-2.259252	-4.442239	-1.296809
56	6	0	-1.956356	-3.112587	-1.069529
57	1	0	-5.548462	-4.370634	-0.473975
58	1	0	-3.821257	-5.929603	-1.203031
59	1	0	-1.500905	-5.127437	-1.661036
60	1	0	-0.953646	-2.763862	-1.290725
61	6	0	-7.016402	-2.675847	1.356008
62	6	0	-8.299733	-3.190571	1.522479
63	6	0	-9.147106	-3.321675	0.424783
64	6	0	-8.712042	-2.937535	-0.842381
65	6	0	-7.430372	-2.422470	-1.012833
66	6	0	-6.586655	-2.294468	0.088349
67	1	0	-8.637032	-3.489085	2.510008
68	1	0	-10.147027	-3.723023	0.556295
69	1	0	-9.371187	-3.038760	-1.698778
70	1	0	-7.069611	-2.116337	-1.990314
71	6	0	-1.970759	6.353042	0.020985
72	6	0	-1.995404	5.640190	1.218170
73	6	0	-2.159930	4.258335	1.203661
74	6	0	-2.296703	3.593654	-0.012985
75	6	0	-2.281440	4.301757	-1.211109
76	6	0	-2.118025	5.684439	-1.192013
77	1	0	-1.836251	7.430213	0.033955
78	1	0	-1.880523	6.159723	2.164306
79	1	0	-2.168768	3.680144	2.122817
80	1	0	-2.385120	3.757522	-2.144842
81	1	0	-2.099867	6.238226	-2.125441
82	6	0	1.970613	6.353033	-0.021055
83	6	0	1.995208	5.640140	-1.218218
84	6	0	2.159789	4.258287	-1.203667
85	6	0	2.296668	3.593669	0.013000
86	6	0	2.281451	4.301808	1.211101
87	6	0	2.117986	5.684488	1.191955
88	1	0	1.836061	7.430196	-0.034069
89	1	0	1.880246	6.159639	-2.164363
90	1	0	2.168594	3.680065	-2.122802
91	1	0	2.385221	3.757616	2.144848
92	1	0	2.099860	6.238310	2.125366
93	1	0	6.339018	-2.563588	-2.197037
94	1	0	7.230188	0.027041	-0.298865
95	1	0	-7.230165	0.026994	0.298861
96	1	0	-6.339042	-2.563698	2.197036

v-DABNA-core (S_0 , C_2 symmetry)
E(M06-2X/6-31G(d)) = -2347.344319 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.727044	4.751793	2.408953
2	6	0	-0.428661	3.653603	1.592609
3	6	0	-0.322758	3.804135	0.187646
4	6	0	-0.543468	5.083371	-0.376896
5	6	0	-0.869433	6.177622	0.440067

6	6	0	-0.945971	5.986721	1.811673
7	1	0	-0.801224	4.649462	3.483722
8	1	0	-1.187726	6.836472	2.443872
9	5	0	0.016033	2.615045	-0.695868
10	7	0	-0.225224	2.393453	2.164402
11	7	0	-0.444052	5.246934	-1.760433
12	6	0	0.000000	0.000000	2.119453
13	6	0	0.078785	-1.213231	1.428584
14	6	0	0.000000	-1.244689	0.009328
15	6	0	0.000000	0.000000	-0.629413
16	6	0	0.000000	1.244689	0.009328
17	6	0	-0.078785	1.213231	1.428584
18	1	0	0.000000	0.000000	3.197973
19	1	0	0.000000	0.000000	-1.710840
20	6	0	-2.049038	6.830904	-2.699832
21	6	0	-0.748233	6.541221	-2.298503
22	6	0	0.257054	7.499109	-2.412080
23	6	0	-0.043359	8.754212	-2.933148
24	6	0	-1.344121	9.049072	-3.337657
25	6	0	-2.345633	8.087990	-3.220629
26	1	0	1.263142	7.246476	-2.090663
27	1	0	0.738105	9.502106	-3.023426
28	1	0	-1.576683	10.028340	-3.744068
29	1	0	-3.359193	8.316106	-3.534883
30	6	0	0.316527	2.951323	-2.175048
31	6	0	0.893752	2.056299	-3.099040
32	6	0	1.106510	2.382276	-4.425605
33	6	0	0.733742	3.652712	-4.873076
34	6	0	0.206962	4.584449	-3.998639
35	6	0	0.021543	4.257571	-2.638152
36	1	0	1.210903	1.080904	-2.746778
37	1	0	1.555238	1.665996	-5.105930
38	1	0	0.874282	3.928461	-5.914280
39	1	0	-0.047825	5.570714	-4.365888
40	5	0	-0.016033	-2.615045	-0.695868
41	7	0	0.225224	-2.393453	2.164402
42	6	0	0.727044	-4.751793	2.408953
43	6	0	0.945971	-5.986721	1.811673
44	6	0	0.869433	-6.177622	0.440067
45	6	0	0.543468	-5.083371	-0.376896
46	6	0	0.322758	-3.804135	0.187646
47	6	0	0.428661	-3.653603	1.592609
48	1	0	0.801224	-4.649462	3.483722
49	1	0	1.187726	-6.836472	2.443872
50	7	0	0.444052	-5.246934	-1.760433
51	6	0	-0.316527	-2.951323	-2.175048
52	6	0	-0.021543	-4.257571	-2.638152
53	6	0	-0.206962	-4.584449	-3.998639
54	6	0	-0.733742	-3.652712	-4.873076
55	6	0	-1.106510	-2.382276	-4.425605
56	6	0	-0.893752	-2.056299	-3.099040
57	1	0	0.047825	-5.570714	-4.365888
58	1	0	-0.874282	-3.928461	-5.914280
59	1	0	-1.555238	-1.665996	-5.105930
60	1	0	-1.210903	-1.080904	-2.746778
61	6	0	2.049038	-6.830904	-2.699832
62	6	0	2.345633	-8.087990	-3.220629
63	6	0	1.344121	-9.049072	-3.337657
64	6	0	0.043359	-8.754212	-2.933148

65	6	0	-0.257054	-7.499109	-2.412080
66	6	0	0.748233	-6.541221	-2.298503
67	1	0	3.359193	-8.316106	-3.534883
68	1	0	1.576683	-10.028340	-3.744068
69	1	0	-0.738105	-9.502106	-3.023426
70	1	0	-1.263142	-7.246476	-2.090663
71	6	0	0.306892	-1.953338	6.353177
72	6	0	1.486760	-1.843817	5.619615
73	6	0	1.466777	-2.009991	4.238084
74	6	0	0.261902	-2.283092	3.594359
75	6	0	-0.917927	-2.402025	4.323079
76	6	0	-0.893205	-2.236421	5.705498
77	1	0	0.323313	-1.817387	7.430112
78	1	0	2.422862	-1.622968	6.122805
79	1	0	2.370964	-1.915967	3.644080
80	1	0	-1.843398	-2.610868	3.795219
81	1	0	-1.813063	-2.322794	6.275355
82	6	0	-0.306892	1.953338	6.353177
83	6	0	-1.486760	1.843817	5.619615
84	6	0	-1.466777	2.009991	4.238084
85	6	0	-0.261902	2.283092	3.594359
86	6	0	0.917927	2.402025	4.323079
87	6	0	0.893205	2.236421	5.705498
88	1	0	-0.323313	1.817387	7.430112
89	1	0	-2.422862	1.622968	6.122805
90	1	0	-2.370964	1.915967	3.644080
91	1	0	1.843398	2.610868	3.795219
92	1	0	1.813063	2.322794	6.275355
93	1	0	-2.813254	6.066346	-2.598917
94	1	0	-1.048829	7.158994	0.021327
95	1	0	1.048829	-7.158994	0.021327
96	1	0	2.813254	-6.066346	-2.598917

ν -DABNA-core (S_1 , C_2 symmetry)
 $E(\text{M06-2X/6-31G(d)}) = -2347.221295 \text{ hartree}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.068067	4.838250	2.392657
2	6	0	0.097498	3.694758	1.594579
3	6	0	0.261456	3.815235	0.186794
4	6	0	0.243417	5.112971	-0.393713
5	6	0	0.051503	6.251259	0.410101
6	6	0	-0.093615	6.089087	1.782576
7	1	0	-0.189201	4.763390	3.464912
8	1	0	-0.232481	6.971272	2.402906
9	5	0	0.440167	2.580323	-0.679228
10	7	0	0.109510	2.418045	2.186884
11	7	0	0.409023	5.250392	-1.780877
12	6	0	0.000000	0.000000	2.146162
13	6	0	-0.096111	-1.217871	1.456462
14	6	0	-0.192226	-1.234658	0.031981
15	6	0	0.000000	0.000000	-0.606346
16	6	0	0.192226	1.234658	0.031981
17	6	0	0.096111	1.217871	1.456462
18	1	0	0.000000	0.000000	3.224673
19	1	0	0.000000	0.000000	-1.687489

20	6	0	-0.974561	7.005730	-2.794462
21	6	0	0.274494	6.569281	-2.346083
22	6	0	1.387042	7.410262	-2.442881
23	6	0	1.247883	8.686684	-2.989712
24	6	0	0.000000	9.124556	-3.439267
25	6	0	-1.110006	8.283041	-3.340915
26	1	0	2.351090	7.056633	-2.089607
27	1	0	2.114226	9.338230	-3.064317
28	1	0	-0.106679	10.118560	-3.864949
29	1	0	-2.082601	8.619572	-3.689295
30	6	0	0.841260	2.852801	-2.148221
31	6	0	1.316978	1.870528	-3.046716
32	6	0	1.633021	2.145829	-4.368381
33	6	0	1.473738	3.453583	-4.840872
34	6	0	1.051909	4.464938	-3.991632
35	6	0	0.761972	4.188698	-2.635929
36	1	0	1.463488	0.861539	-2.677981
37	1	0	1.997197	1.360592	-5.024832
38	1	0	1.698944	3.693741	-5.877167
39	1	0	0.963377	5.473041	-4.375951
40	5	0	-0.440167	-2.580323	-0.679228
41	7	0	-0.109510	-2.418045	2.186884
42	6	0	0.068067	-4.838250	2.392657
43	6	0	0.093615	-6.089087	1.782576
44	6	0	-0.051503	-6.251259	0.410101
45	6	0	-0.243417	-5.112971	-0.393713
46	6	0	-0.261456	-3.815235	0.186794
47	6	0	-0.097498	-3.694758	1.594579
48	1	0	0.189201	-4.763390	3.464912
49	1	0	0.232481	-6.971272	2.402906
50	7	0	-0.409023	-5.250392	-1.780877
51	6	0	-0.841260	-2.852801	-2.148221
52	6	0	-0.761972	-4.188698	-2.635929
53	6	0	-1.051909	-4.464938	-3.991632
54	6	0	-1.473738	-3.453583	-4.840872
55	6	0	-1.633021	-2.145829	-4.368381
56	6	0	-1.316978	-1.870528	-3.046716
57	1	0	-0.963377	-5.473041	-4.375951
58	1	0	-1.698944	-3.693741	-5.877167
59	1	0	-1.997197	-1.360592	-5.024832
60	1	0	-1.463488	-0.861539	-2.677981
61	6	0	0.974561	-7.005730	-2.794462
62	6	0	1.110006	-8.283041	-3.340915
63	6	0	0.000000	-9.124556	-3.439267
64	6	0	-1.247883	-8.686684	-2.989712
65	6	0	-1.387042	-7.410262	-2.442881
66	6	0	-0.274494	-6.569281	-2.346083
67	1	0	2.082601	-8.619572	-3.689295
68	1	0	0.106679	-10.118560	-3.864949
69	1	0	-2.114226	-9.338230	-3.064317
70	1	0	-2.351090	-7.056633	-2.089607
71	6	0	0.038568	-2.244174	6.414131
72	6	0	1.222292	-2.221056	5.673279
73	6	0	1.177557	-2.274399	4.279627
74	6	0	-0.055423	-2.349880	3.625458
75	6	0	-1.240696	-2.372018	4.364520
76	6	0	-1.191865	-2.319533	5.758410
77	1	0	0.075260	-2.204131	7.499370
78	1	0	2.181940	-2.162952	6.179548

79	1	0	2.089751	-2.259028	3.690776
80	1	0	-2.189922	-2.433013	3.840687
81	1	0	-2.115226	-2.338262	6.330874
82	6	0	-0.038568	2.244174	6.414131
83	6	0	-1.222292	2.221056	5.673279
84	6	0	-1.177557	2.274399	4.279627
85	6	0	0.055423	2.349880	3.625458
86	6	0	1.240696	2.372018	4.364520
87	6	0	1.191865	2.319533	5.758410
88	1	0	-0.075260	2.204131	7.499370
89	1	0	-2.181940	2.162952	6.179548
90	1	0	-2.089751	2.259028	3.690776
91	1	0	2.189922	2.433013	3.840687
92	1	0	2.115226	2.338262	6.330874
93	1	0	-1.828843	6.340582	-2.711309
94	1	0	0.027359	7.244231	-0.018349
95	1	0	-0.027359	-7.244231	-0.018349
96	1	0	1.828843	-6.340582	-2.711309

v-DABNA-B-Mes (S_0 , C_1 symmetry)
 $E(M06-2X/6-31G(d)) = -3093.608325$ hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.809927	2.077327	-0.164573
2	6	0	-3.667438	1.247625	-0.224136
3	6	0	-3.802149	-0.155098	-0.295873
4	6	0	-5.100431	-0.722875	-0.222503
5	6	0	-6.250787	0.088059	-0.104768
6	6	0	-6.050385	1.485285	-0.111180
7	1	0	-4.715878	3.155485	-0.144120
8	1	0	-6.935271	2.116897	-0.057078
9	5	0	-2.572748	-1.032372	-0.422876
10	7	0	-2.397762	1.817887	-0.211803
11	7	0	-5.221772	-2.117187	-0.247712
12	6	0	0.000023	1.776708	-0.000052
13	6	0	1.206923	1.083396	0.130484
14	6	0	1.224777	-0.336711	0.193254
15	6	0	0.000003	-0.983792	-0.000033
16	6	0	-1.224773	-0.336695	-0.193338
17	6	0	-1.206877	1.083394	-0.130590
18	1	0	0.000038	2.855190	-0.000074
19	1	0	0.000000	-2.069759	-0.000010
20	5	0	-7.632655	-0.535361	0.055261
21	6	0	-7.600964	-2.043348	0.361274
22	6	0	-6.377634	-2.740569	0.284620
23	6	0	-6.288247	-4.044321	0.808462
24	6	0	-7.410800	-4.666142	1.324633
25	6	0	-8.650974	-4.016248	1.343428
26	6	0	-8.725916	-2.717930	0.877248
27	1	0	-5.334141	-4.558007	0.826617
28	1	0	-7.315512	-5.667694	1.733661
29	1	0	-9.526870	-4.516825	1.743060
30	1	0	-9.665590	-2.171170	0.921000
31	6	0	-2.871358	-2.470461	-0.903608
32	6	0	-1.934518	-3.275112	-1.579905
33	6	0	-2.286628	-4.466901	-2.188478

34	6	0	-3.625304	-4.864357	-2.168918
35	6	0	-4.580716	-4.091981	-1.531007
36	6	0	-4.211403	-2.909707	-0.867046
37	1	0	-0.911589	-2.921810	-1.663384
38	1	0	-1.542673	-5.064292	-2.705340
39	1	0	-3.934722	-5.769363	-2.683071
40	1	0	-5.621523	-4.390859	-1.568626
41	5	0	2.572742	-1.032402	0.422824
42	7	0	2.397810	1.817852	0.211699
43	6	0	4.809975	2.077235	0.164437
44	6	0	6.050435	1.485161	0.111083
45	6	0	6.250822	0.087953	0.104714
46	6	0	5.100425	-0.722969	0.222444
47	6	0	3.802165	-0.155160	0.295799
48	6	0	3.667496	1.247585	0.224024
49	1	0	4.715997	3.155402	0.143933
50	1	0	6.935319	2.116777	0.056967
51	7	0	5.221746	-2.117285	0.247699
52	6	0	2.871340	-2.470464	0.903619
53	6	0	4.211383	-2.909755	0.867044
54	6	0	4.580646	-4.092032	1.531026
55	6	0	3.625200	-4.864376	2.168961
56	6	0	2.286551	-4.466865	2.188521
57	6	0	1.934490	-3.275065	1.579931
58	1	0	5.621429	-4.390969	1.568667
59	1	0	3.934605	-5.769380	2.683114
60	1	0	1.542562	-5.064206	2.705400
61	1	0	0.911569	-2.921727	1.663426
62	6	0	7.600945	-2.043489	-0.361286
63	6	0	8.725887	-2.718072	-0.877280
64	6	0	8.650922	-4.016367	-1.343514
65	6	0	7.410729	-4.666230	-1.324742
66	6	0	6.288193	-4.044414	-0.808546
67	6	0	6.377608	-2.740679	-0.284651
68	1	0	9.665570	-2.171321	-0.920999
69	1	0	9.526805	-4.516953	-1.743181
70	1	0	7.315445	-5.667772	-1.733807
71	1	0	5.334071	-4.558073	-0.826723
72	5	0	7.632691	-0.535503	-0.055267
73	6	0	9.454879	0.906734	-1.210459
74	6	0	10.634644	1.651266	-1.169734
75	6	0	11.352292	1.814954	0.013862
76	6	0	10.858784	1.215682	1.172960
77	6	0	9.683756	0.466263	1.159961
78	6	0	8.965742	0.304446	-0.038192
79	1	0	11.002016	2.115101	-2.083767
80	1	0	11.402783	1.336489	2.108543
81	6	0	-10.634654	1.651230	1.169991
82	6	0	-9.454812	0.906822	1.210593
83	6	0	-8.965737	0.304554	0.038289
84	6	0	-9.683898	0.466282	-1.159778
85	6	0	-10.859012	1.215585	-1.172676
86	6	0	-11.352452	1.814822	-0.013530
87	1	0	-11.001986	2.115043	2.084055
88	1	0	-11.403111	1.336315	-2.108202
89	6	0	1.955872	6.007093	0.180541
90	6	0	2.080103	5.312904	-1.021477
91	6	0	2.248713	3.931493	-1.014655
92	6	0	2.289844	3.251144	0.199757

93	6	0	2.173802	3.938678	1.403965
94	6	0	2.007256	5.321075	1.391662
95	1	0	1.819949	7.084029	0.172751
96	1	0	2.041221	5.846468	-1.965816
97	1	0	2.335612	3.367941	-1.938830
98	1	0	2.204733	3.381428	2.335261
99	1	0	1.913150	5.860791	2.328629
100	6	0	-1.955612	6.007107	-0.180726
101	6	0	-2.079914	5.312951	1.021313
102	6	0	-2.248609	3.931553	1.014502
103	6	0	-2.289758	3.251178	-0.199883
104	6	0	-2.173660	3.938672	-1.404114
105	6	0	-2.007029	5.321059	-1.391826
106	1	0	-1.819610	7.084027	-0.172952
107	1	0	-2.041016	5.846524	1.965643
108	1	0	-2.335561	3.368023	1.938695
109	1	0	-2.204611	3.381408	-2.335396
110	1	0	-1.912878	5.860745	-2.328806
111	6	0	-8.699234	0.747800	2.509292
112	1	0	-8.587928	-0.310539	2.773341
113	1	0	-7.688012	1.164290	2.432515
114	1	0	-9.211580	1.250617	3.333893
115	6	0	-9.168926	-0.173778	-2.427104
116	1	0	-8.164159	0.190644	-2.671216
117	1	0	-9.096448	-1.262035	-2.314584
118	1	0	-9.822371	0.036086	-3.278135
119	6	0	-12.642612	2.595297	-0.037504
120	1	0	-13.506735	1.930645	0.075275
121	1	0	-12.680152	3.324829	0.776256
122	1	0	-12.764325	3.131918	-0.982951
123	6	0	9.168694	-0.173841	2.427225
124	1	0	8.163860	0.190466	2.671203
125	1	0	9.096366	-1.262107	2.314726
126	1	0	9.822021	0.036118	3.278328
127	6	0	8.699461	0.747625	-2.509236
128	1	0	8.588284	-0.310729	-2.773288
129	1	0	7.688199	1.164015	-2.432575
130	1	0	9.211858	1.250469	-3.333782
131	6	0	12.642375	2.595552	0.037979
132	1	0	13.506554	1.931006	-0.074913
133	1	0	12.679856	3.325259	-0.775620
134	1	0	12.764017	3.131991	0.983547

v-DABNA-B-Mes (S_0 , C_2 symmetry)
E(M06-2X/6-31G(d)) = -3093.608308 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.361929	4.617310	2.079215
2	6	0	-0.945015	3.551098	1.250601
3	6	0	-0.919812	3.700538	-0.152259
4	6	0	-1.400422	4.908140	-0.721403
5	6	0	-1.874940	5.963371	0.088597
6	6	0	-1.804387	5.776866	1.485974
7	1	0	-1.351026	4.522948	3.157498
8	1	0	-2.134645	6.600179	2.116852
9	5	0	-0.410975	2.573817	-1.028669

10	7	0	-0.555946	2.342645	1.821699
11	7	0	-1.416631	5.029233	-2.115937
12	6	0	0.000000	0.000000	1.781276
13	6	0	0.256759	-1.186534	1.087837
14	6	0	0.202633	-1.223085	-0.332201
15	6	0	0.000000	0.000000	-0.979311
16	6	0	-0.202633	1.223085	-0.332201
17	6	0	-0.256759	1.186534	1.087837
18	1	0	0.000000	0.000000	2.859793
19	1	0	0.000000	0.000000	-2.065278
20	5	0	-2.463617	7.223193	-0.536028
21	6	0	-2.747077	7.093534	-2.043270
22	6	0	-2.288999	5.955895	-2.739170
23	6	0	-2.760993	5.702302	-4.041115
24	6	0	-3.607725	6.602312	-4.662692
25	6	0	-4.016397	7.774197	-4.014317
26	6	0	-3.594421	7.995841	-2.717595
27	1	0	-2.477862	4.790302	-4.553582
28	1	0	-3.968426	6.380196	-5.662730
29	1	0	-4.674168	8.477386	-4.514690
30	1	0	-3.931798	8.874594	-2.171882
31	6	0	-0.050644	3.007310	-2.467455
32	6	0	0.886818	2.331270	-3.271458
33	6	0	1.350952	2.855274	-4.464997
34	6	0	0.906955	4.117510	-4.865157
35	6	0	0.000000	4.823345	-4.093343
36	6	0	-0.510575	4.265787	-2.908715
37	1	0	1.290646	1.388445	-2.916280
38	1	0	2.076370	2.312275	-5.061997
39	1	0	1.294922	4.571673	-5.771970
40	1	0	-0.295149	5.821377	-4.394727
41	5	0	0.410975	-2.573817	-1.028669
42	7	0	0.555946	-2.342645	1.821699
43	6	0	1.361929	-4.617310	2.079215
44	6	0	1.804387	-5.776866	1.485974
45	6	0	1.874940	-5.963371	0.088597
46	6	0	1.400422	-4.908140	-0.721403
47	6	0	0.919812	-3.700538	-0.152259
48	6	0	0.945015	-3.551098	1.250601
49	1	0	1.351026	-4.522948	3.157498
50	1	0	2.134645	-6.600179	2.116852
51	7	0	1.416631	-5.029233	-2.115937
52	6	0	0.050644	-3.007310	-2.467455
53	6	0	0.510575	-4.265787	-2.908715
54	6	0	0.000000	-4.823345	-4.093343
55	6	0	-0.906955	-4.117510	-4.865157
56	6	0	-1.350952	-2.855274	-4.464997
57	6	0	-0.886818	-2.331270	-3.271458
58	1	0	0.295149	-5.821377	-4.394727
59	1	0	-1.294922	-4.571673	-5.771970
60	1	0	-2.076370	-2.312275	-5.061997
61	1	0	-1.290646	-1.388445	-2.916280
62	6	0	2.747077	-7.093534	-2.043270
63	6	0	3.594421	-7.995841	-2.717595
64	6	0	4.016397	-7.774197	-4.014317
65	6	0	3.607725	-6.602312	-4.662692
66	6	0	2.760993	-5.702302	-4.041115
67	6	0	2.288999	-5.955895	-2.739170
68	1	0	3.931798	-8.874594	-2.171882

69	1	0	4.674168	-8.477386	-4.514690
70	1	0	3.968426	-6.380196	-5.662730
71	1	0	2.477862	-4.790302	-4.553582
72	5	0	2.463617	-7.223193	-0.536028
73	6	0	4.128922	-8.593122	0.909063
74	6	0	4.459261	-9.729131	1.649533
75	6	0	3.562079	-10.784554	1.803735
76	6	0	2.309281	-10.679239	1.199153
77	6	0	1.954097	-9.556406	0.453748
78	6	0	2.865046	-8.496135	0.301304
79	1	0	5.440322	-9.791439	2.117727
80	1	0	1.592723	-11.491316	1.312685
81	6	0	-4.459261	9.729131	1.649533
82	6	0	-4.128922	8.593122	0.909063
83	6	0	-2.865046	8.496135	0.301304
84	6	0	-1.954097	9.556406	0.453748
85	6	0	-2.309281	10.679239	1.199153
86	6	0	-3.562079	10.784554	1.803735
87	1	0	-5.440322	9.791439	2.117727
88	1	0	-1.592723	11.491316	1.312685
89	6	0	0.468803	-1.909144	6.011030
90	6	0	1.647120	-1.657170	5.310913
91	6	0	1.685675	-1.820257	3.929409
92	6	0	0.540068	-2.235149	3.254966
93	6	0	-0.637728	-2.495975	3.948449
94	6	0	-0.670771	-2.332002	5.330837
95	1	0	0.439518	-1.776634	7.088013
96	1	0	2.536185	-1.329005	5.839932
97	1	0	2.588716	-1.618155	3.361171
98	1	0	-1.516791	-2.813140	3.395783
99	1	0	-1.588471	-2.530854	5.875162
100	6	0	-0.468803	1.909144	6.011030
101	6	0	-1.647120	1.657170	5.310913
102	6	0	-1.685675	1.820257	3.929409
103	6	0	-0.540068	2.235149	3.254966
104	6	0	0.637728	2.495975	3.948449
105	6	0	0.670771	2.332002	5.330837
106	1	0	-0.439518	1.776634	7.088013
107	1	0	-2.536185	1.329005	5.839932
108	1	0	-2.588716	1.618155	3.361171
109	1	0	1.516791	2.813140	3.395783
110	1	0	1.588471	2.530854	5.875162
111	6	0	-5.123641	7.465765	0.759476
112	1	0	-5.343316	7.271787	-0.297084
113	1	0	-4.730174	6.532317	1.178736
114	1	0	-6.065717	7.694281	1.265019
115	6	0	-0.592103	9.465069	-0.192475
116	1	0	-0.042593	8.588698	0.170758
117	1	0	-0.681068	9.359140	-1.280169
118	1	0	0.011127	10.353367	0.013207
119	6	0	-3.943060	12.020244	2.579704
120	1	0	-4.326431	12.800978	1.912887
121	1	0	-4.723348	11.802668	3.314319
122	1	0	-3.081866	12.437302	3.109822
123	6	0	0.592103	-9.465069	-0.192475
124	1	0	0.042593	-8.588698	0.170758
125	1	0	0.681068	-9.359140	-1.280169
126	1	0	-0.011127	-10.353367	0.013207
127	6	0	5.123641	-7.465765	0.759476

128	1	0	5.343316	-7.271787	-0.297084
129	1	0	4.730174	-6.532317	1.178736
130	1	0	6.065717	-7.694281	1.265019
131	6	0	3.943060	-12.020244	2.579704
132	1	0	4.326431	-12.800978	1.912887
133	1	0	4.723348	-11.802668	3.314319
134	1	0	3.081866	-12.437302	3.109822

v-DABNA-B-Mes (S_1 , C_2 symmetry)
 $E(M06-2X/6-31G(d)) = -3093.485495$ hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.487523	4.581405	2.076634
2	6	0	-1.043290	3.533518	1.248900
3	6	0	-0.985524	3.689406	-0.153232
4	6	0	-1.462543	4.902312	-0.710166
5	6	0	-1.961470	5.954433	0.101273
6	6	0	-1.924905	5.760223	1.495357
7	1	0	-1.496802	4.473300	3.154389
8	1	0	-2.268729	6.572778	2.131057
9	5	0	-0.458107	2.576661	-1.030746
10	7	0	-0.645813	2.313956	1.813022
11	7	0	-1.442546	5.045609	-2.100596
12	6	0	0.000000	0.000000	1.779816
13	6	0	0.300525	-1.179417	1.086397
14	6	0	0.238497	-1.221273	-0.344668
15	6	0	0.000000	0.000000	-0.992250
16	6	0	-0.238497	1.221273	-0.344668
17	6	0	-0.300525	1.179417	1.086397
18	1	0	0.000000	0.000000	2.857459
19	1	0	0.000000	0.000000	-2.077152
20	5	0	-2.525994	7.229060	-0.535886
21	6	0	-2.779766	7.106255	-2.046457
22	6	0	-2.312337	5.968336	-2.738594
23	6	0	-2.767269	5.705022	-4.042427
24	6	0	-3.607426	6.602911	-4.680999
25	6	0	-4.018684	7.777801	-4.041212
26	6	0	-3.613513	8.006711	-2.737744
27	1	0	-2.476391	4.789496	-4.544358
28	1	0	-3.956506	6.376719	-5.683888
29	1	0	-4.667913	8.481436	-4.552230
30	1	0	-3.957042	8.889661	-2.202819
31	6	0	-0.072824	3.026994	-2.452975
32	6	0	0.857172	2.358174	-3.276059
33	6	0	1.330229	2.905300	-4.454703
34	6	0	0.907086	4.183545	-4.836132
35	6	0	0.000000	4.878855	-4.056585
36	6	0	-0.522738	4.298261	-2.886984
37	1	0	1.247472	1.401641	-2.944176
38	1	0	2.050516	2.364635	-5.060615
39	1	0	1.308202	4.650712	-5.730073
40	1	0	-0.287062	5.885689	-4.336163
41	5	0	0.458107	-2.576661	-1.030746
42	7	0	0.645813	-2.313956	1.813022
43	6	0	1.487523	-4.581405	2.076634
44	6	0	1.924905	-5.760223	1.495357

45	6	0	1.961470	-5.954433	0.101273
46	6	0	1.462543	-4.902312	-0.710166
47	6	0	0.985524	-3.689406	-0.153232
48	6	0	1.043290	-3.533518	1.248900
49	1	0	1.496802	-4.473300	3.154389
50	1	0	2.268729	-6.572778	2.131057
51	7	0	1.442546	-5.045609	-2.100596
52	6	0	0.072824	-3.026994	-2.452975
53	6	0	0.522738	-4.298261	-2.886984
54	6	0	0.000000	-4.878855	-4.056585
55	6	0	-0.907086	-4.183545	-4.836132
56	6	0	-1.330229	-2.905300	-4.454703
57	6	0	-0.857172	-2.358174	-3.276059
58	1	0	0.287062	-5.885689	-4.336163
59	1	0	-1.308202	-4.650712	-5.730073
60	1	0	-2.050516	-2.364635	-5.060615
61	1	0	-1.247472	-1.401641	-2.944176
62	6	0	2.779766	-7.106255	-2.046457
63	6	0	3.613513	-8.006711	-2.737744
64	6	0	4.018684	-7.777801	-4.041212
65	6	0	3.607426	-6.602911	-4.680999
66	6	0	2.767269	-5.705022	-4.042427
67	6	0	2.312337	-5.968336	-2.738594
68	1	0	3.957042	-8.889661	-2.202819
69	1	0	4.667913	-8.481436	-4.552230
70	1	0	3.956506	-6.376719	-5.683888
71	1	0	2.476391	-4.789496	-4.544358
72	5	0	2.525994	-7.229060	-0.535886
73	6	0	4.200638	-8.581911	0.910542
74	6	0	4.541333	-9.713523	1.652904
75	6	0	3.653867	-10.776960	1.808709
76	6	0	2.400472	-10.684591	1.203103
77	6	0	2.035258	-9.566822	0.455038
78	6	0	2.936019	-8.497779	0.301683
79	1	0	5.522913	-9.766009	2.121249
80	1	0	1.691231	-11.502802	1.318582
81	6	0	-4.541333	9.713523	1.652904
82	6	0	-4.200638	8.581911	0.910542
83	6	0	-2.936019	8.497779	0.301683
84	6	0	-2.035258	9.566822	0.455038
85	6	0	-2.400472	10.684591	1.203103
86	6	0	-3.653867	10.776960	1.808709
87	1	0	-5.522913	9.766009	2.121249
88	1	0	-1.691231	11.502802	1.318582
89	6	0	0.664590	-1.846041	5.998839
90	6	0	1.818537	-1.579090	5.264696
91	6	0	1.822250	-1.752060	3.883743
92	6	0	0.666465	-2.193963	3.245666
93	6	0	-0.487158	-2.471255	3.972441
94	6	0	-0.485369	-2.295082	5.353612
95	1	0	0.662175	-1.704851	7.075115
96	1	0	2.715836	-1.231116	5.766475
97	1	0	2.704785	-1.537385	3.288695
98	1	0	-1.374937	-2.808188	3.446079
99	1	0	-1.384225	-2.505141	5.924513
100	6	0	-0.664590	1.846041	5.998839
101	6	0	-1.818537	1.579090	5.264696
102	6	0	-1.822250	1.752060	3.883743
103	6	0	-0.666465	2.193963	3.245666

104	6	0	0.487158	2.471255	3.972441
105	6	0	0.485369	2.295082	5.353612
106	1	0	-0.662175	1.704851	7.075115
107	1	0	-2.715836	1.231116	5.766475
108	1	0	-2.704785	1.537385	3.288695
109	1	0	1.374937	2.808188	3.446079
110	1	0	1.384225	2.505141	5.924513
111	6	0	-5.185965	7.447067	0.755816
112	1	0	-5.413438	7.264725	-0.301177
113	1	0	-4.779433	6.512434	1.159854
114	1	0	-6.125601	7.660147	1.272591
115	6	0	-0.672283	9.489356	-0.190950
116	1	0	-0.117512	8.613601	0.165978
117	1	0	-0.759523	9.392012	-1.279507
118	1	0	-0.074629	10.379531	0.023047
119	6	0	-4.045722	12.007387	2.587536
120	1	0	-4.435014	12.786638	1.922380
121	1	0	-4.824756	11.781432	3.320942
122	1	0	-3.188421	12.430246	3.119369
123	6	0	0.672283	-9.489356	-0.190950
124	1	0	0.117512	-8.613601	0.165978
125	1	0	0.759523	-9.392012	-1.279507
126	1	0	0.074629	-10.379531	0.023047
127	6	0	5.185965	-7.447067	0.755816
128	1	0	5.413438	-7.264725	-0.301177
129	1	0	4.779433	-6.512434	1.159854
130	1	0	6.125601	-7.660147	1.272591
131	6	0	4.045722	-12.007387	2.587536
132	1	0	4.435014	-12.786638	1.922380
133	1	0	4.824756	-11.781432	3.320942
134	1	0	3.188421	-12.430246	3.119369

v-DABNA-M (S₀, C₂ symmetry)
E(M06-2X/6-31G(d)) = -2740.331175 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.199298	4.779226	2.280858
2	6	0	-0.052369	3.667507	1.441774
3	6	0	0.000000	3.820758	0.033563
4	6	0	-0.123597	5.122115	-0.509253
5	6	0	-0.301654	6.233444	0.331387
6	6	0	-0.327127	6.037005	1.704089
7	1	0	-0.228668	4.663844	3.357606
8	1	0	-0.453781	6.899410	2.352509
9	5	0	0.201022	2.615331	-0.873255
10	7	0	0.048918	2.391697	1.998292
11	7	0	-0.072304	5.292893	-1.894195
12	6	0	0.000000	0.000000	1.933033
13	6	0	-0.044607	-1.215183	1.245970
14	6	0	-0.097106	-1.243032	-0.174500
15	6	0	0.000000	0.000000	-0.811740
16	6	0	0.097106	1.243032	-0.174500
17	6	0	0.044607	1.215183	1.245970
18	1	0	0.000000	0.000000	3.012362
19	1	0	0.000000	0.000000	-1.892399
20	6	0	-1.566676	7.030474	-2.731813

21	6	0	-0.279889	6.617333	-2.405978
22	6	0	0.804611	7.475999	-2.570259
23	6	0	0.585462	8.755596	-3.068959
24	6	0	-0.704286	9.168752	-3.396492
25	6	0	-1.796895	8.315381	-3.230314
26	1	0	1.799881	7.128624	-2.310556
27	1	0	1.422151	9.433396	-3.206476
28	6	0	0.460611	2.944510	-2.359930
29	6	0	0.907263	2.019677	-3.328058
30	6	0	1.077453	2.347688	-4.657017
31	6	0	0.798006	3.652688	-5.092149
32	6	0	0.402234	4.601678	-4.165718
33	6	0	0.259013	4.275045	-2.799141
34	1	0	1.158561	1.014019	-3.009526
35	1	0	1.427114	1.603618	-5.367916
36	1	0	0.215238	5.613411	-4.506458
37	5	0	-0.201022	-2.615331	-0.873255
38	7	0	-0.048918	-2.391697	1.998292
39	6	0	0.199298	-4.779226	2.280858
40	6	0	0.327127	-6.037005	1.704089
41	6	0	0.301654	-6.233444	0.331387
42	6	0	0.123597	-5.122115	-0.509253
43	6	0	0.000000	-3.820758	0.033563
44	6	0	0.052369	-3.667507	1.441774
45	1	0	0.228668	-4.663844	3.357606
46	1	0	0.453781	-6.899410	2.352509
47	7	0	0.072304	-5.292893	-1.894195
48	6	0	-0.460611	-2.944510	-2.359930
49	6	0	-0.259013	-4.275045	-2.799141
50	6	0	-0.402234	-4.601678	-4.165718
51	6	0	-0.798006	-3.652688	-5.092149
52	6	0	-1.077453	-2.347688	-4.657017
53	6	0	-0.907263	-2.019677	-3.328058
54	1	0	-0.215238	-5.613411	-4.506458
55	1	0	-1.427114	-1.603618	-5.367916
56	1	0	-1.158561	-1.014019	-3.009526
57	6	0	1.566676	-7.030474	-2.731813
58	6	0	1.796895	-8.315381	-3.230314
59	6	0	0.704286	-9.168752	-3.396492
60	6	0	-0.585462	-8.755596	-3.068959
61	6	0	-0.804611	-7.475999	-2.570259
62	6	0	0.279889	-6.617333	-2.405978
63	1	0	-1.422151	-9.433396	-3.206476
64	1	0	-1.799881	-7.128624	-2.310556
65	6	0	-0.635394	-1.834812	6.141553
66	6	0	0.652662	-1.850874	5.608071
67	6	0	0.878321	-2.063572	4.246823
68	6	0	-0.229156	-2.264442	3.419579
69	6	0	-1.536139	-2.261575	3.920300
70	6	0	-1.717012	-2.047957	5.284588
71	1	0	1.506220	-1.687639	6.263459
72	1	0	-2.727660	-2.041343	5.688397
73	6	0	0.635394	1.834812	6.141553
74	6	0	-0.652662	1.850874	5.608071
75	6	0	-0.878321	2.063572	4.246823
76	6	0	0.229156	2.264442	3.419579
77	6	0	1.536139	2.261575	3.920300
78	6	0	1.717012	2.047957	5.284588
79	1	0	-1.506220	1.687639	6.263459

80	1	0	2.727660	2.041343	5.688397
81	1	0	-2.390298	6.334533	-2.592678
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83	1	0	0.404426	-7.232033	-0.072145
84	1	0	2.390298	-6.334533	-2.592678
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86	1	0	-0.250181	-3.438157	-7.165286
87	1	0	-0.754734	-5.075845	-6.718612
88	1	0	-1.958045	-3.788487	-6.904354
89	6	0	0.947698	4.013916	-6.547565
90	1	0	0.250181	3.438157	-7.165286
91	1	0	0.754734	5.075845	-6.718612
92	1	0	1.958045	3.788487	-6.904354
93	6	0	-2.263585	2.034175	3.659655
94	1	0	-3.018503	1.964560	4.446369
95	1	0	-2.457903	2.931977	3.063700
96	1	0	-2.377870	1.169880	2.994357
97	6	0	2.699337	2.466354	2.986930
98	1	0	2.629119	3.435824	2.481724
99	1	0	3.646283	2.425184	3.530155
100	1	0	2.711891	1.697183	2.206294
101	6	0	0.870700	1.570181	7.606591
102	1	0	1.217458	0.542031	7.763858
103	1	0	1.635163	2.239416	8.012396
104	1	0	-0.044644	1.704840	8.189402
105	6	0	2.263585	-2.034175	3.659655
106	1	0	3.018503	-1.964560	4.446369
107	1	0	2.457903	-2.931977	3.063700
108	1	0	2.377870	-1.169880	2.994357
109	6	0	-2.699337	-2.466354	2.986930
110	1	0	-2.629119	-3.435824	2.481724
111	1	0	-3.646283	-2.425184	3.530155
112	1	0	-2.711891	-1.697183	2.206294
113	6	0	-0.870700	-1.570181	7.606591
114	1	0	-1.217458	-0.542031	7.763858
115	1	0	-1.635163	-2.239416	8.012396
116	1	0	0.044644	-1.704840	8.189402
117	1	0	0.866589	-10.169357	-3.788713
118	1	0	-0.866589	10.169357	-3.788713
119	6	0	3.197180	-8.769305	-3.555908
120	1	0	3.721711	-9.093532	-2.650434
121	1	0	3.188686	-9.610308	-4.253987
122	1	0	3.782004	-7.959875	-4.001415
123	6	0	-3.197180	8.769305	-3.555908
124	1	0	-3.721711	9.093532	-2.650434
125	1	0	-3.188686	9.610308	-4.253987
126	1	0	-3.782004	7.959875	-4.001415

v-DABNA-M-B-Mes (S_0 , C_2 symmetry)
E(M06-2X/6-31G(d)) = -3486.595716 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.007992	4.801229	2.048727
2	6	0	0.103938	3.666109	1.212055
3	6	0	0.218974	3.810860	-0.187149
4	6	0	0.150801	5.113466	-0.746330

5	6	0	0.000000	6.256771	0.070022
6	6	0	-0.035499	6.046506	1.465222
7	1	0	-0.043160	4.692137	3.125386
8	1	0	-0.113903	6.926486	2.101158
9	5	0	0.374540	2.588107	-1.072089
10	7	0	0.083888	2.396272	1.777153
11	7	0	0.211461	5.247063	-2.139066
12	6	0	0.000000	0.000000	1.722729
13	6	0	-0.078776	-1.211498	1.031625
14	6	0	-0.159672	-1.231072	-0.387324
15	6	0	0.000000	0.000000	-1.034449
16	6	0	0.159672	1.231072	-0.387324
17	6	0	0.078776	1.211498	1.031625
18	1	0	0.000000	0.000000	2.802040
19	1	0	0.000000	0.000000	-2.120731
20	5	0	-0.155211	7.642449	-0.547361
21	6	0	-0.416644	7.619378	-2.061165
22	6	0	-0.313955	6.404279	-2.765864
23	6	0	-0.805113	6.320160	-4.083293
24	6	0	-1.320155	7.432137	-4.729540
25	6	0	-1.355167	8.666407	-4.055900
26	6	0	-0.924810	8.741657	-2.748542
27	1	0	-0.801773	5.366248	-4.599696
28	1	0	-1.749220	9.543398	-4.562949
29	1	0	-0.991362	9.680646	-2.202717
30	6	0	0.878494	2.902209	-2.496579
31	6	0	1.575528	1.979806	-3.302109
32	6	0	2.209186	2.350656	-4.471570
33	6	0	2.209931	3.695860	-4.868801
34	6	0	1.544809	4.627241	-4.085971
35	6	0	0.852130	4.244221	-2.924053
36	1	0	1.654458	0.951107	-2.964588
37	1	0	2.742738	1.613655	-5.066230
38	1	0	1.586025	5.673805	-4.367725
39	5	0	-0.374540	-2.588107	-1.072089
40	7	0	-0.083888	-2.396272	1.777153
41	6	0	-0.007992	-4.801229	2.048727
42	6	0	0.035499	-6.046506	1.465222
43	6	0	0.000000	-6.256771	0.070022
44	6	0	-0.150801	-5.113466	-0.746330
45	6	0	-0.218974	-3.810860	-0.187149
46	6	0	-0.103938	-3.666109	1.212055
47	1	0	0.043160	-4.692137	3.125386
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49	7	0	-0.211461	-5.247063	-2.139066
50	6	0	-0.878494	-2.902209	-2.496579
51	6	0	-0.852130	-4.244221	-2.924053
52	6	0	-1.544809	-4.627241	-4.085971
53	6	0	-2.209931	-3.695860	-4.868801
54	6	0	-2.209186	-2.350656	-4.471570
55	6	0	-1.575528	-1.979806	-3.302109
56	1	0	-1.586025	-5.673805	-4.367725
57	1	0	-2.742738	-1.613655	-5.066230
58	1	0	-1.654458	-0.951107	-2.964588
59	6	0	0.416644	-7.619378	-2.061165
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62	6	0	1.320155	-7.432137	-4.729540
63	6	0	0.805113	-6.320160	-4.083293

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65	1	0	0.991362	-9.680646	-2.202717
66	1	0	1.749220	-9.543398	-4.562949
67	1	0	0.801773	-5.366248	-4.599696
68	5	0	0.155211	-7.642449	-0.547361
69	6	0	1.374437	-9.435446	0.879375
70	6	0	1.373492	-10.615160	1.624763
71	6	0	0.206874	-11.352864	1.819603
72	6	0	-0.973029	-10.886254	1.240222
73	6	0	-0.999548	-9.711546	0.490200
74	6	0	0.179657	-8.969119	0.303293
75	1	0	2.306150	-10.968339	2.061880
76	1	0	-1.893172	-11.452904	1.374616
77	6	0	-2.288398	-9.228532	-0.131561
78	1	0	-2.545227	-8.224841	0.227003
79	1	0	-2.197537	-9.165198	-1.222364
80	1	0	-3.122374	-9.896052	0.101364
81	6	0	2.656421	-8.660370	0.682824
82	1	0	2.888257	-8.545711	-0.382650
83	1	0	2.575713	-7.650069	1.100871
84	1	0	3.502730	-9.159398	1.162507
85	6	0	0.213636	-12.608028	2.655489
86	1	0	1.197725	-13.085033	2.647325
87	1	0	-0.036361	-12.386893	3.699469
88	1	0	-0.519871	-13.332428	2.289871
89	6	0	-1.373492	10.615160	1.624763
90	6	0	-1.374437	9.435446	0.879375
91	6	0	-0.179657	8.969119	0.303293
92	6	0	0.999548	9.711546	0.490200
93	6	0	0.973029	10.886254	1.240222
94	6	0	-0.206874	11.352864	1.819603
95	1	0	-2.306150	10.968339	2.061880
96	1	0	1.893172	11.452904	1.374616
97	6	0	2.288398	9.228532	-0.131561
98	1	0	2.545227	8.224841	0.227003
99	1	0	2.197537	9.165198	-1.222364
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101	6	0	-2.656421	8.660370	0.682824
102	1	0	-2.888257	8.545711	-0.382650
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106	1	0	0.519871	13.332428	2.289871
107	1	0	-1.197725	13.085033	2.647325
108	1	0	0.036361	12.386893	3.699469
109	6	0	0.569478	-1.836641	5.911307
110	6	0	1.640777	-2.040208	5.038249
111	6	0	1.443832	-2.253335	3.676692
112	6	0	0.128214	-2.268314	3.197081
113	6	0	-0.968637	-2.070442	4.037155
114	6	0	-0.725137	-1.857001	5.395633
115	1	0	2.656732	-2.026760	5.428084
116	1	0	-1.570349	-1.698875	6.062670
117	6	0	-0.569478	1.836641	5.911307
118	6	0	-1.640777	2.040208	5.038249
119	6	0	-1.443832	2.253335	3.676692
120	6	0	-0.128214	2.268314	3.197081
121	6	0	0.968637	2.070442	4.037155
122	6	0	0.725137	1.857001	5.395633

123	1	0	-2.656732	2.026760	5.428084
124	1	0	1.570349	1.698875	6.062670
125	6	0	-1.855157	7.325225	-6.134381
126	1	0	-1.290790	7.971021	-6.815545
127	1	0	-1.794090	6.300811	-6.509432
128	1	0	-2.901773	7.643342	-6.178978
129	6	0	2.947908	4.121201	-6.112071
130	1	0	3.983722	3.768130	-6.093577
131	1	0	2.476991	3.700063	-7.006983
132	1	0	2.959551	5.208748	-6.217447
133	6	0	-2.947908	-4.121201	-6.112071
134	1	0	-2.476991	-3.700063	-7.006983
135	1	0	-2.959551	-5.208748	-6.217447
136	1	0	-3.983722	-3.768130	-6.093577
137	6	0	1.855157	-7.325225	-6.134381
138	1	0	1.290790	-7.971021	-6.815545
139	1	0	1.794090	-6.300811	-6.509432
140	1	0	2.901773	-7.643342	-6.178978
141	6	0	2.362028	2.042841	3.469251
142	1	0	2.484188	1.185525	2.796177
143	1	0	2.570537	2.945866	2.886661
144	1	0	3.105104	1.961771	4.265780
145	6	0	-2.598811	2.448178	2.730952
146	1	0	-3.550928	2.360794	3.259169
147	1	0	-2.555722	3.434769	2.256273
148	1	0	-2.576872	1.701665	1.928965
149	6	0	-0.825893	1.583554	7.374644
150	1	0	0.093118	1.662175	7.961434
151	1	0	-1.549737	2.298041	7.778001
152	1	0	-1.236600	0.578914	7.528274
153	6	0	0.825893	-1.583554	7.374644
154	1	0	1.236600	-0.578914	7.528274
155	1	0	-0.093118	-1.662175	7.961434
156	1	0	1.549737	-2.298041	7.778001
157	6	0	-2.362028	-2.042841	3.469251
158	1	0	-2.570537	-2.945866	2.886661
159	1	0	-3.105104	-1.961771	4.265780
160	1	0	-2.484188	-1.185525	2.796177
161	6	0	2.598811	-2.448178	2.730952
162	1	0	3.550928	-2.360794	3.259169
163	1	0	2.555722	-3.434769	2.256273
164	1	0	2.576872	-1.701665	1.928965

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