Supporting Information of

Deep-Blue Electroluminescence from Nondoped and Doped Organic Light-Emitting Diodes (OLEDs) Based on a New Monoaza[6]helicene†

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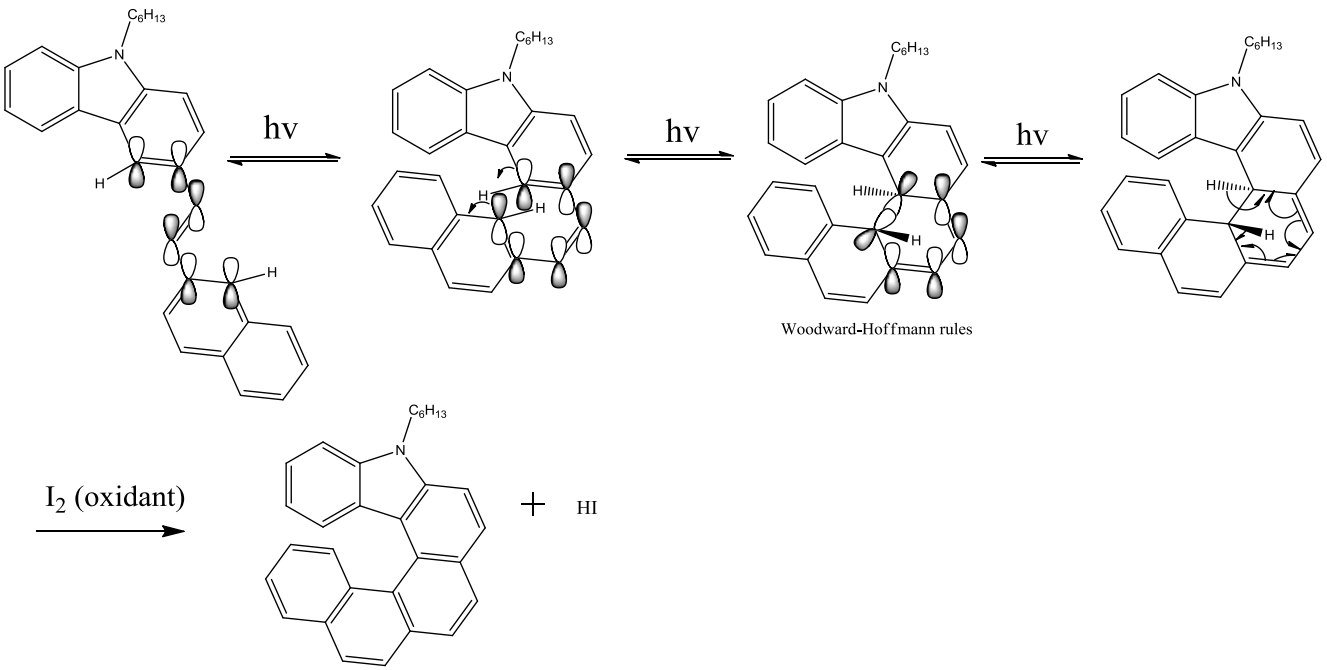

Scheme S1. Photochemical reaction mechanism involved in the synthesis of **1**

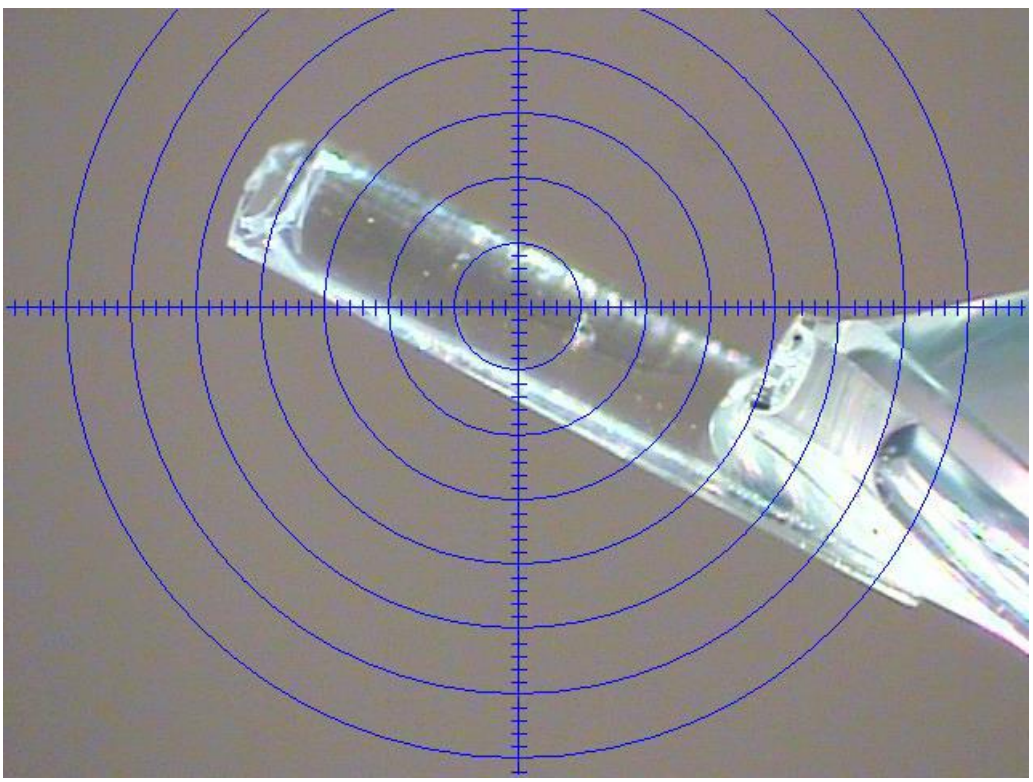

Fig. S1 Single-crystal of compound 1 used for X-ray diffraction test.

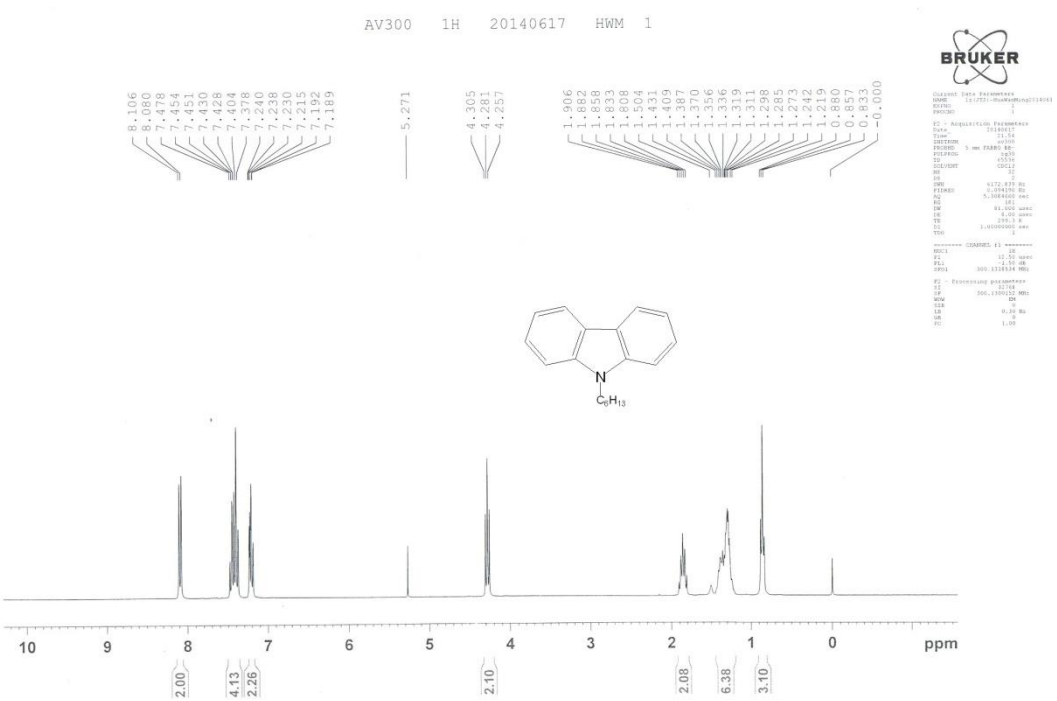

Fig. S2 ^{1}H NMR spectrum of compound **5**

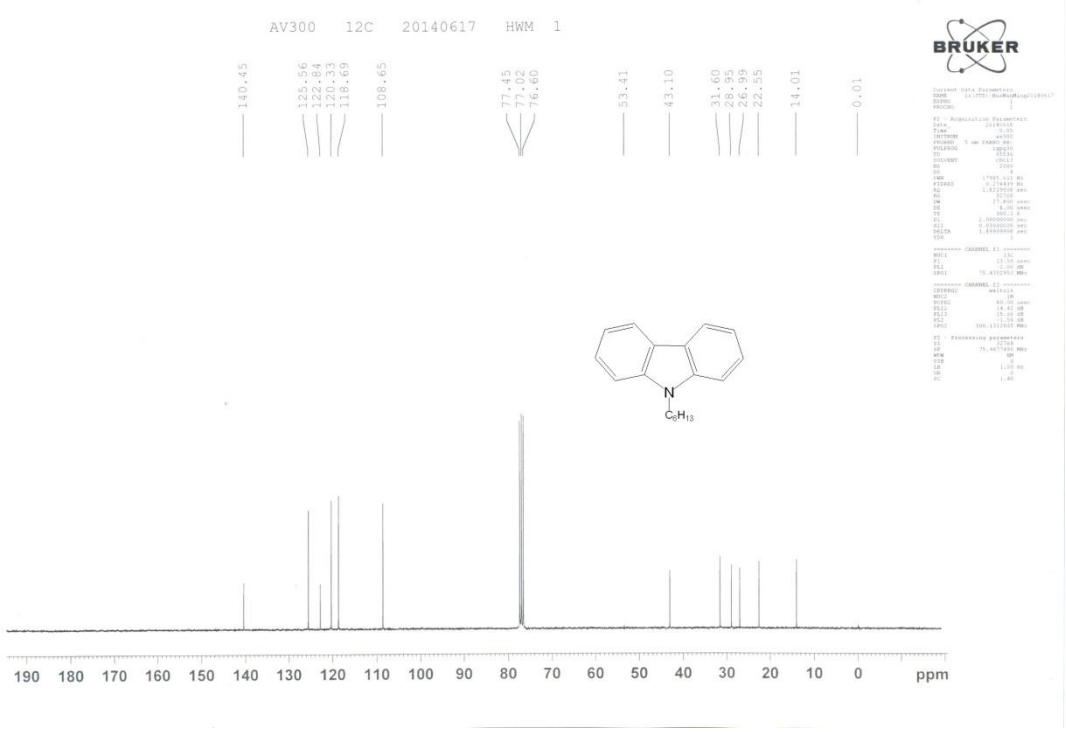

Fig. S3 ^{13} C NMR spectrum of compound **5**

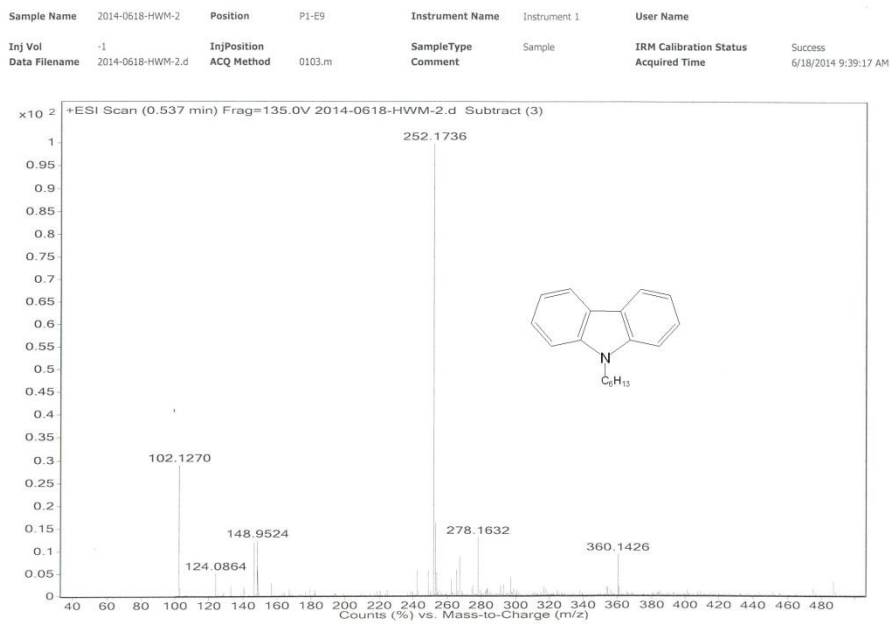

Fig. S4 HRMS spectrum of compound **5**

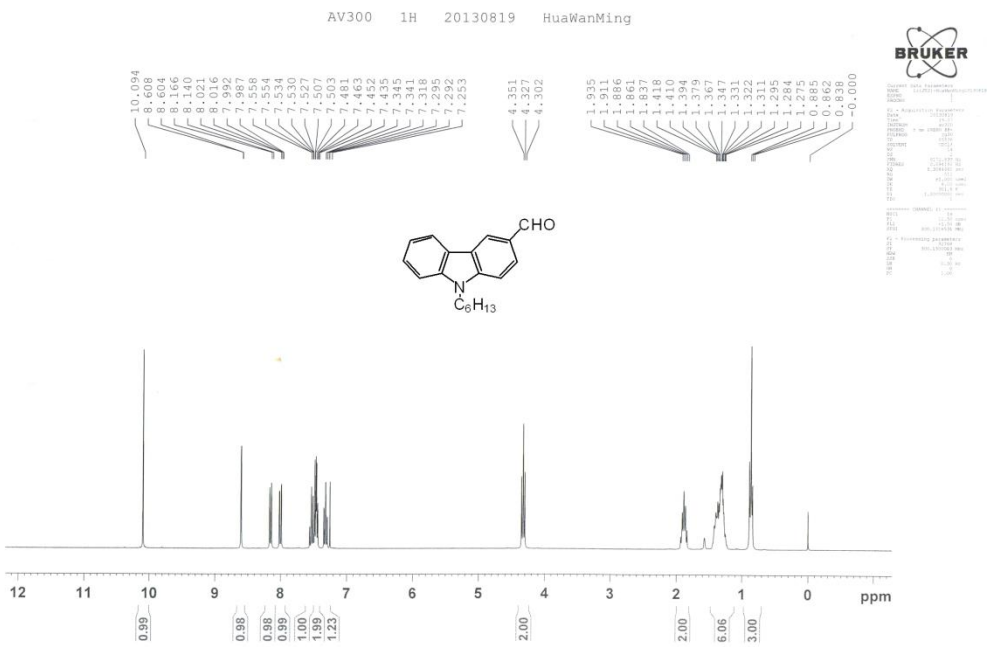

Fig. S5 ^{1}H NMR spectrum of compound **4.**

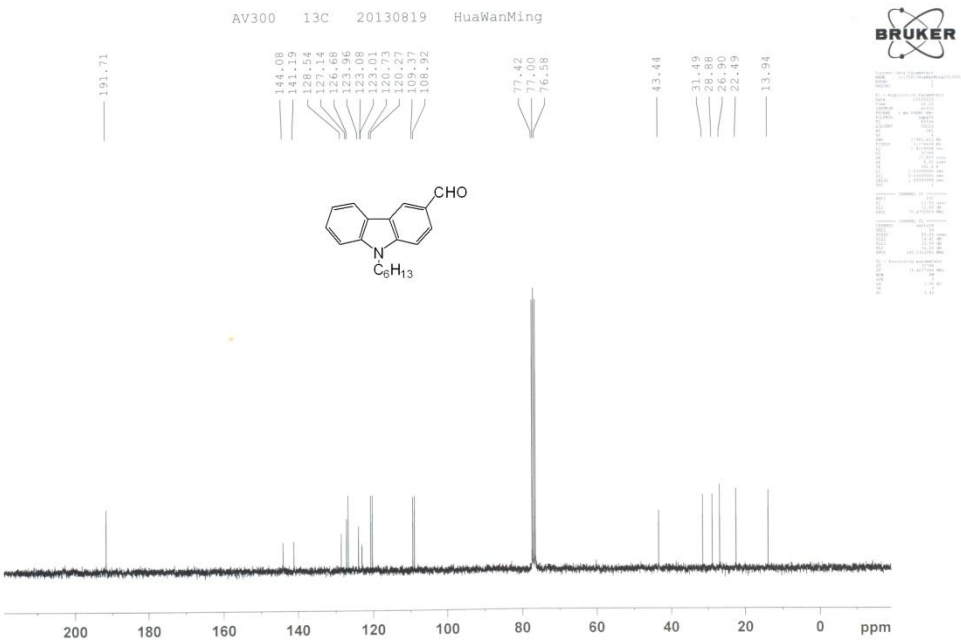

Fig. S6 ^{13}C NMR spectrum of compound **4.**

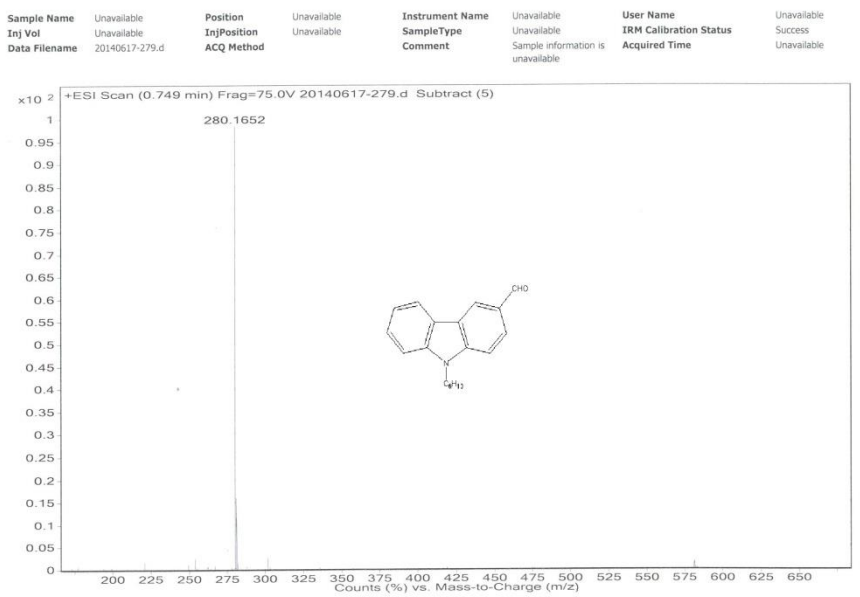

Fig. S7 HRMS spectrum of compound **4**

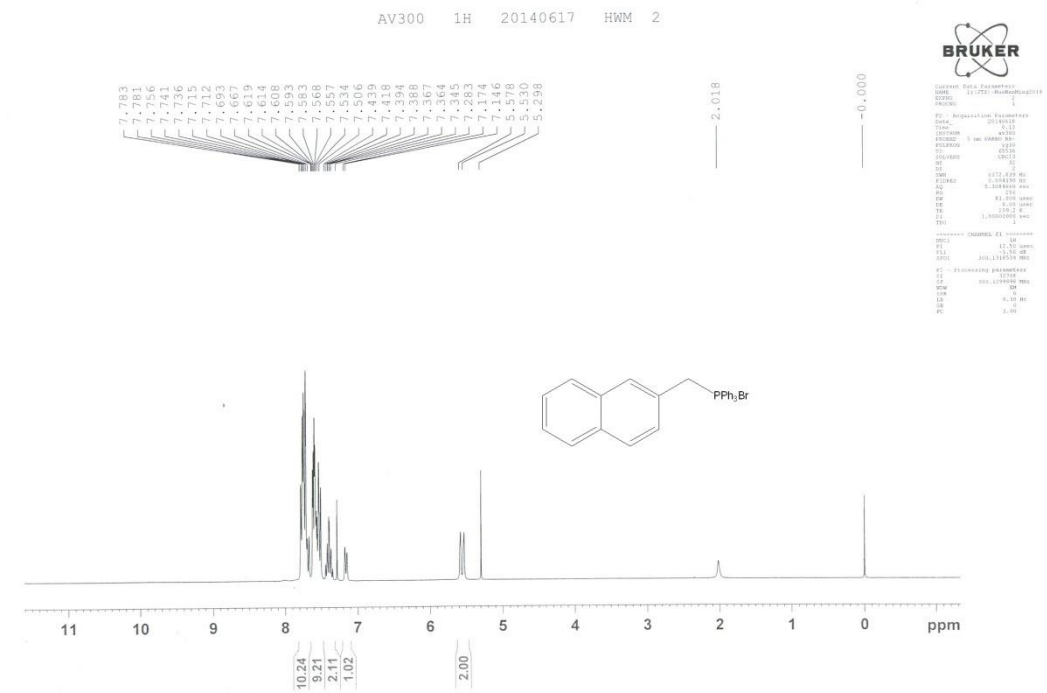

Fig. S8 [1]H NMR spectrum of compound **3**

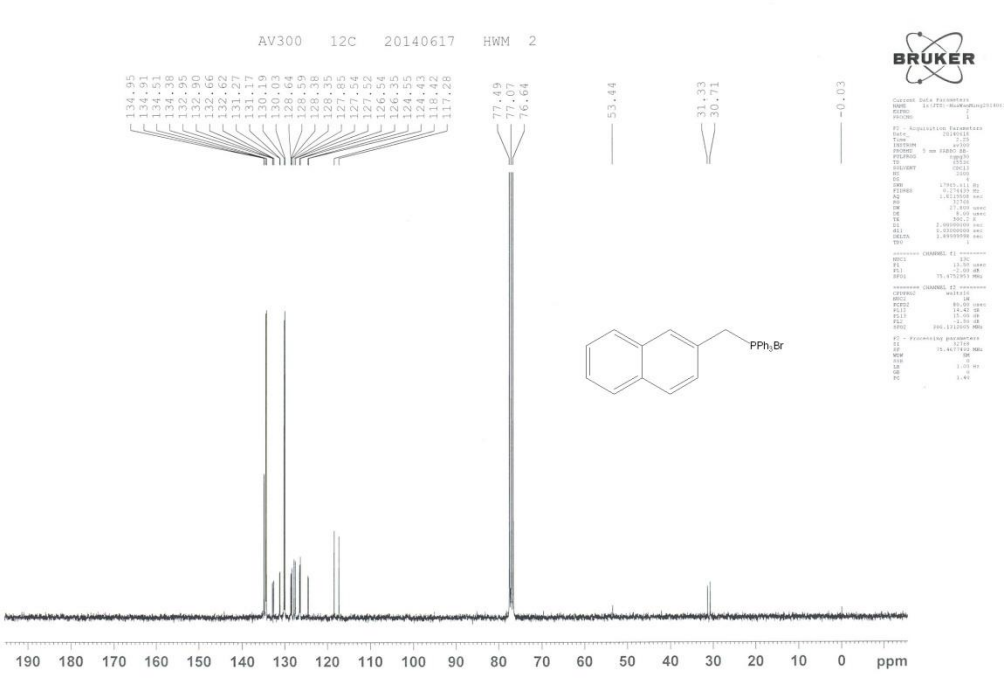

Fig. S9 [13] C NMR spectrum of compound **3**

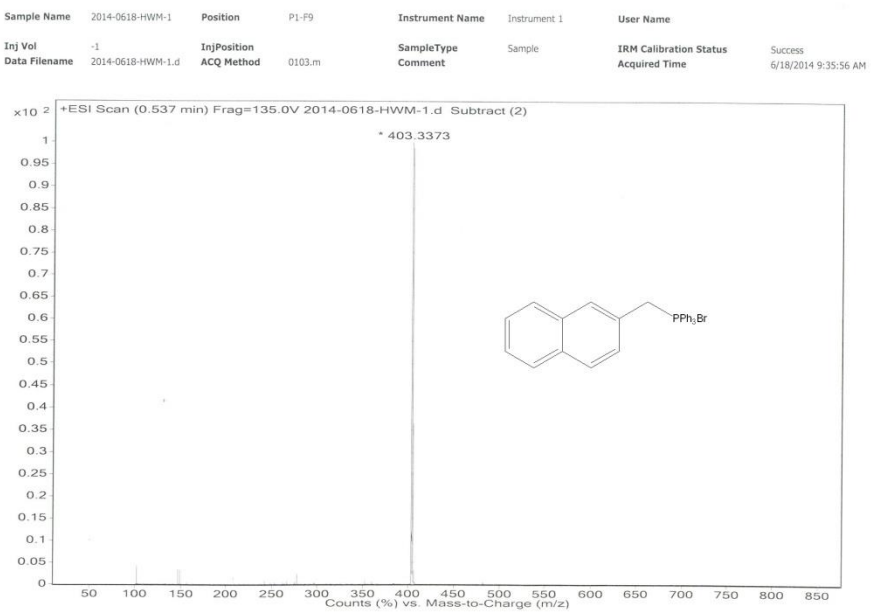

Fig. S10 HRMS spectrum of compound **3**

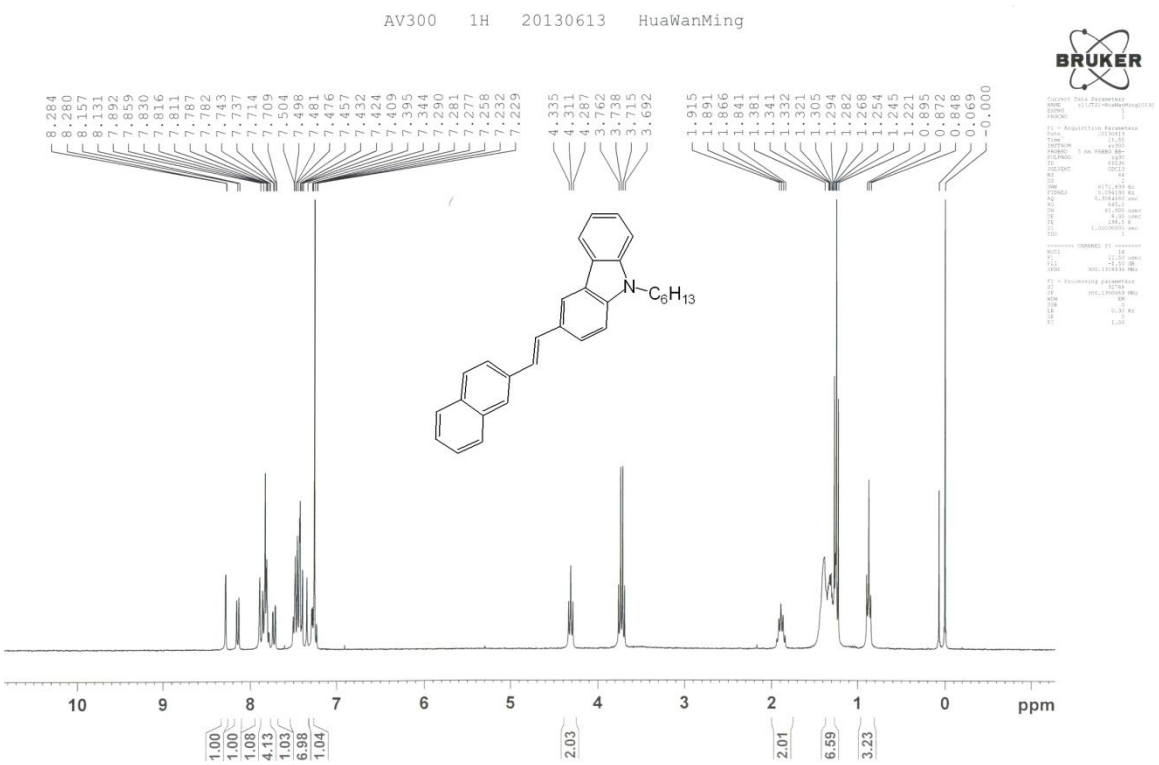

Fig. S11 ^{1}H NMR spectrum of compound **2.**

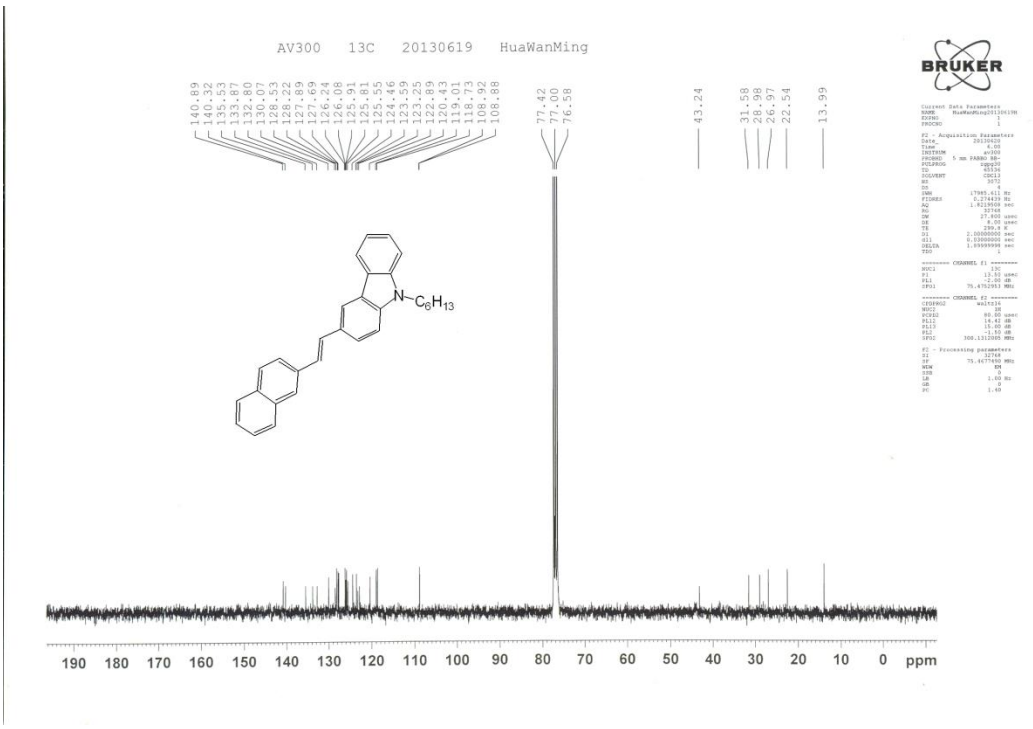

Fig. S12 ^{13}C NMR spectrum of compound **2.**

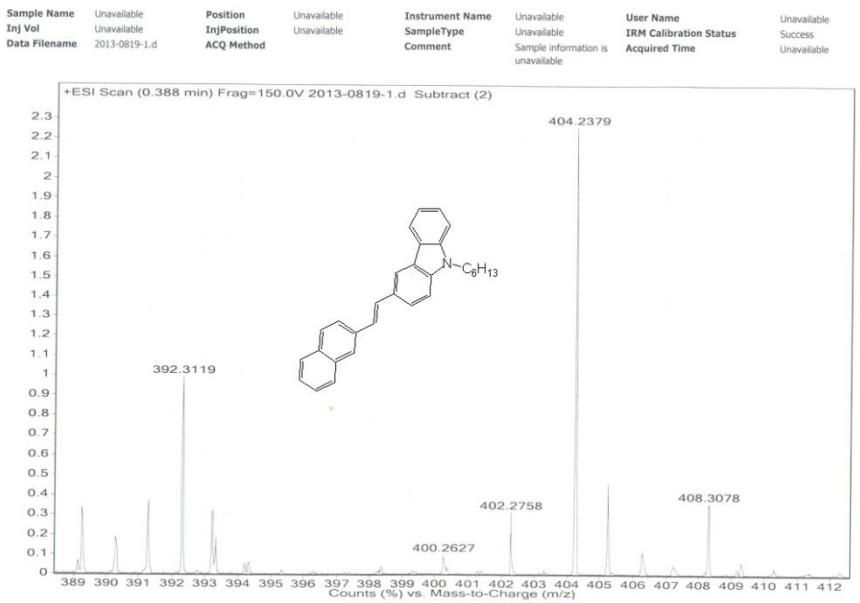

Fig. S13 HRMS spectrum of compound **2.**

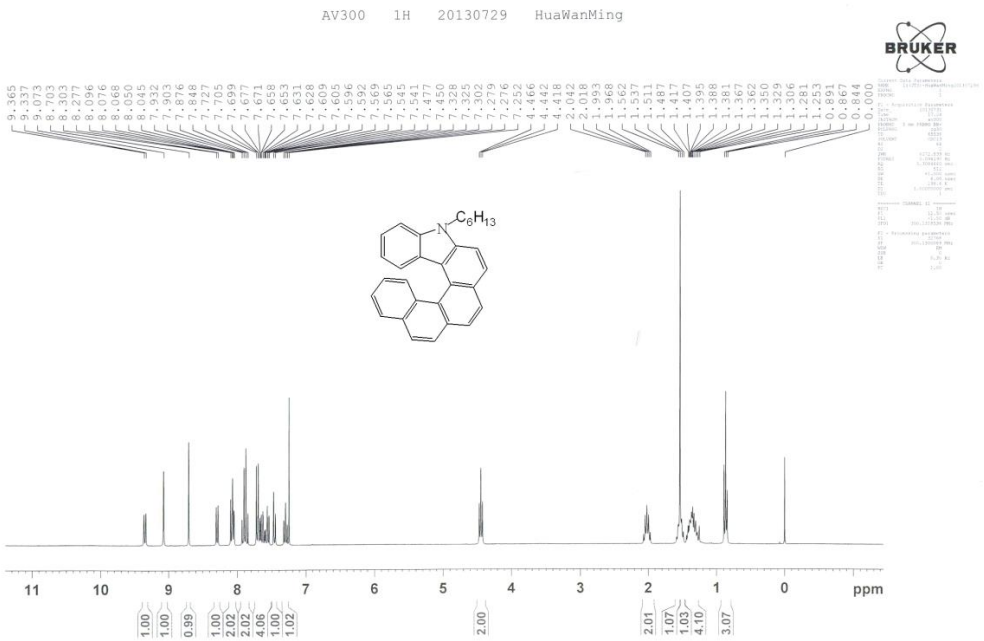

Fig. S14 ^{1}H NMR spectrum of compound **1.**

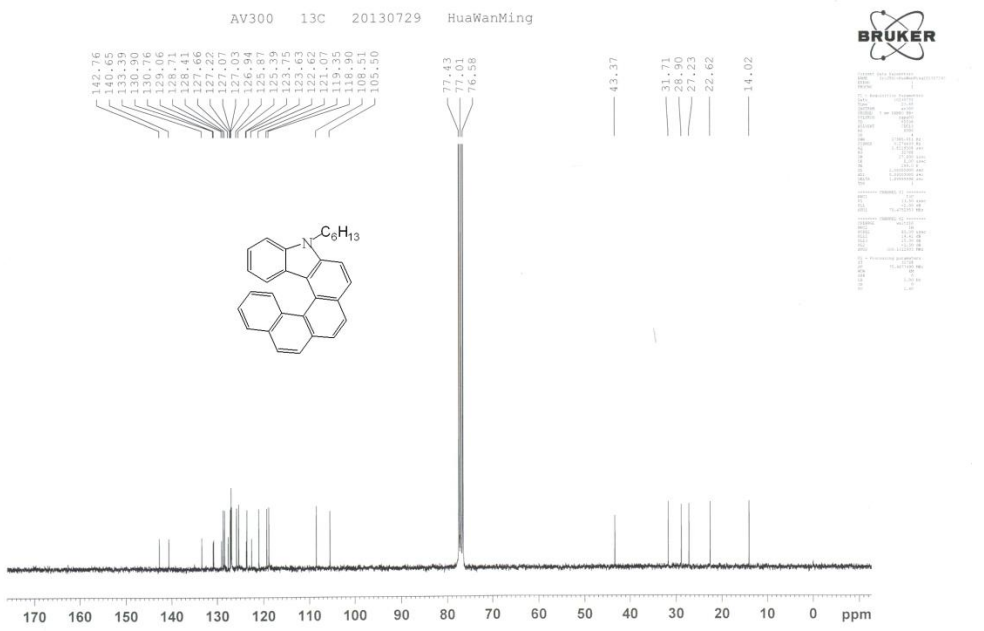

Fig. S15 ^{3}C NMR spectrum of compound **1.**

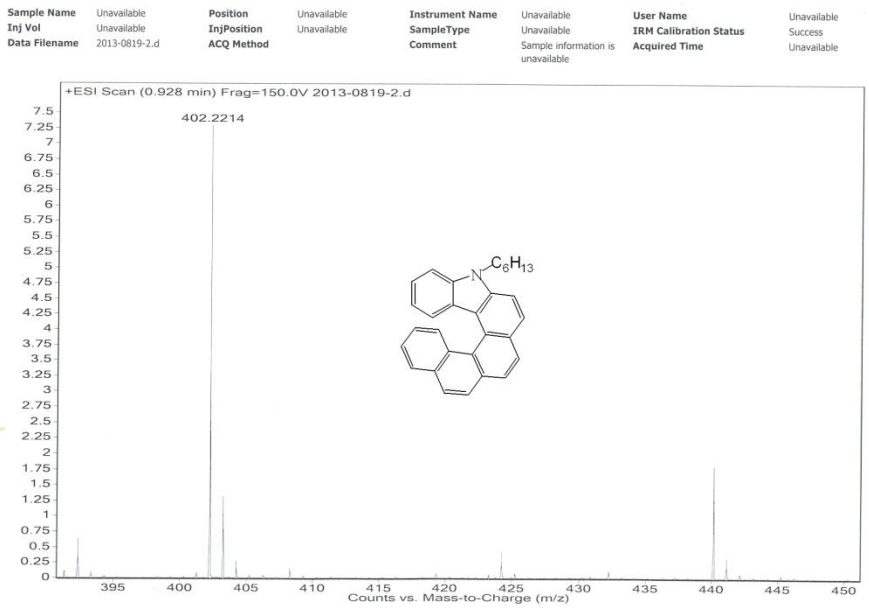

Fig. S16 HRMS spectrum of compound **1.**

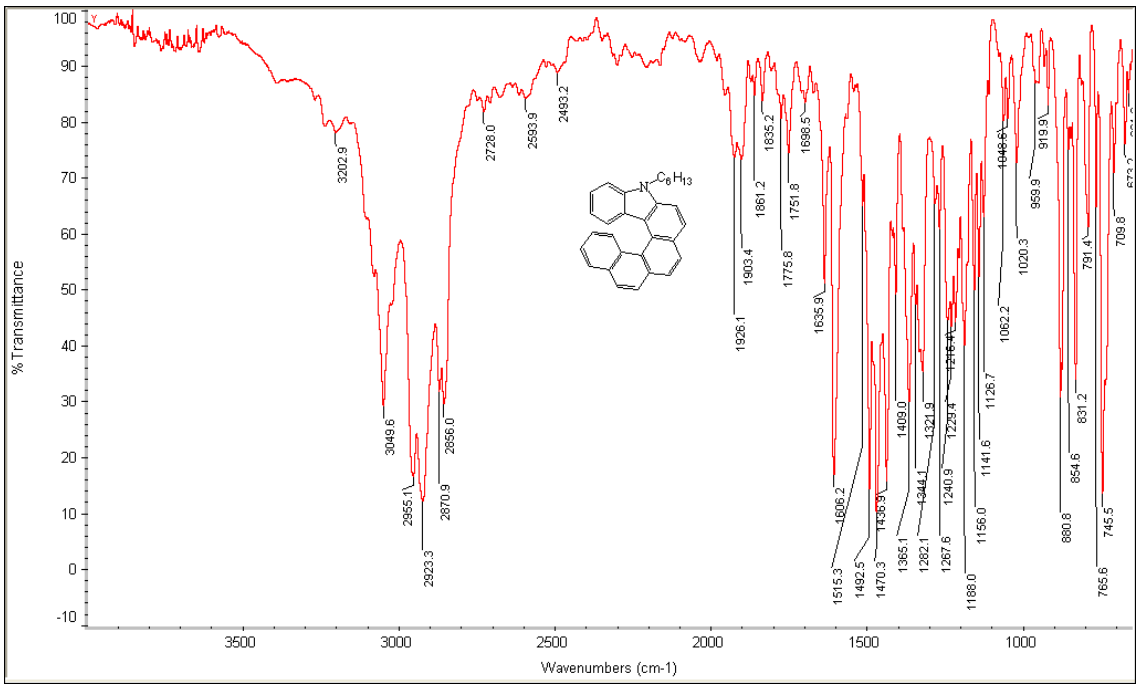

Fig. S17 FTIR spectrum of compound **1.**

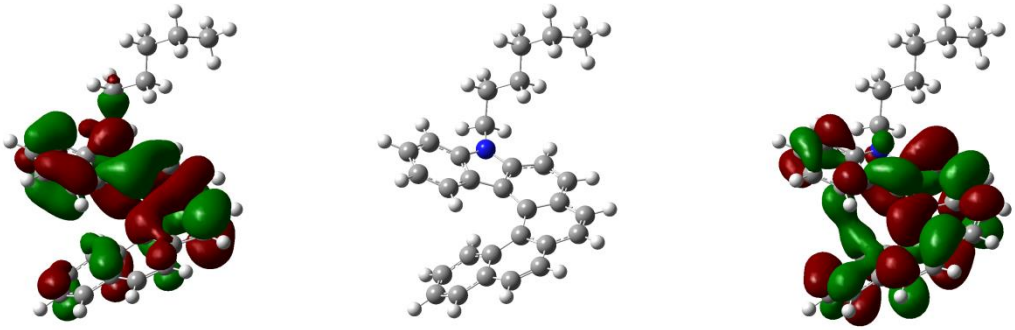

Fig. S18 View of the HOMO (left), optimized molecule shape(middle) and LUMO (right) of compound **1.**

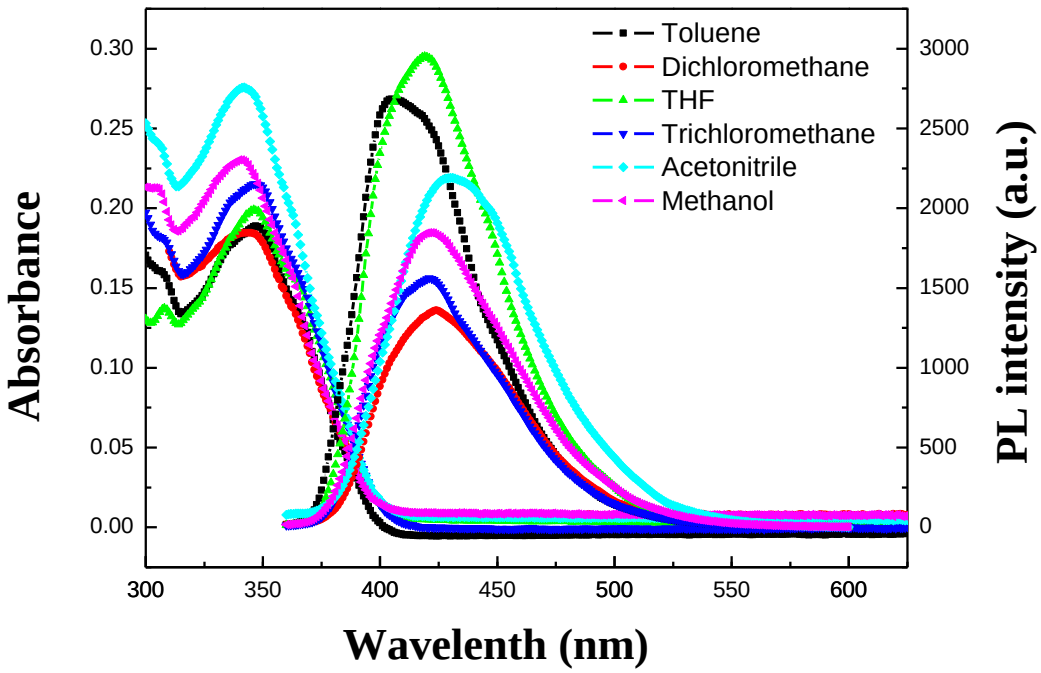

Fig. S19 UV-vis and photoluminescence spectra of compound **2.**

Table S1. PL quantum yields of compound **1** in different solvents.

solvent	λ^{a}_{max} [a](nm)	λ^{e}_{max} [b](nm)	Φ_f[c](%)
toluene	320	425	19
dichloromethane	320	428	18
THF	318	426	21
trichloromethane	320	427	17
acetonitrile	317	428	17
methanol	315	426	20

[a]: λ^{a}_{max} maximum absorption wavelength. [b]: λ^{e}_{max} maximum emission wavelength excited at 320 nm.
[c]: Φ_f PL quantum yields calculated using a quinine sulfates in 0.1mol·L^{-1} H_2SO_4.

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Table S2. PL quantum yields of compound **2** in different solvents.

solvent	λ^{a}_{max} [a](nm)	λ^{e}_{max} [b](nm)	Φ_f[c](%)
toluene	347	405	33
dichloromethane	342	424	18
THF	346	419	32
trichloromethane	346	421	18
acetonitrile	342	430	19
methanol	341	421	21

[a]: λ^{a}_{max} maximum absorption wavelength. [b]: λ^{e}_{max} maximum emission wavelength excited at 345 nm.
[c]: Φ_f PL quantum yields calculated using a quinine sulfates in 0.1mol·L^{-1} H_2SO_4.

Table S3. absorption wavelength and oscillator strength of compound **1** evaluated by the b3lyp/6-31+g(d) calculation.

Absorption [nm] (Oscillator strength)	Transition energy(eV)	Assignment(%)
390.5(0.0421)	3.17	H→L(85)
365.6(0.0402)	3.39	H-1→L(74)
		H→L+1(22)
328.0(0.3745)	3.78	H→L+1(61)
321.9(0.0375)	3.85	H-1→L+1(47)
		H-3→L(20)
315.2(0.0790)	3.93	H-2→L(62)
306.1(0.0183)	4.05	H→L+2(56)
296.7(0.1332)	4.18	H-3→L(44)
288.6(0.0567)	4.30	H-1→L+2(65)
282.9(0.0443)	4.38	H-2→L+1(64)
272.3(0.0242)	4.55	H→L+3(29)
		H→L+4(27)
267.5(0.0085)	4.64	H→L+3(55)
		H→L+4(31)
265.6(0.0192)	4.67	H-3→L+1(29)
		H-4→L(23)
		H-1→L+4(18)
260.0(0.1164)	4.77	H-3→L+1(26)
256.2(0.0509)	4.84	H-1→L+3(63)
255.0(0.0422)	4.86	H-2→L+2(65)
253.0(0.0099)	4.90	H→L+5(63)
250.1(0.0275)	4.96	H→L+5(28)

		H-1→L+4(19)
245.8(0.0180)	5.04	H→L+6(57)
245.7(0.1296)	5.05	H-3→L+2(41)
		H→L+6(18)
242.7(0.0436)	5.11	H-1→L+5(26)
		H→L+8(19)
		H→L+7(19)