

Supporting Information

Molecular Design and Synthetic Approach of C2,C3,C4-Modified Carbazoles: High Triplet Energy Bipolar Host Materials for Efficient Blue Phosphorescent Organic Light Emitting Diodes

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Experimental section

General methods

The chemicals and solvents purchased from commercial suppliers were used as received. All reactions were carried out under a nitrogen atmosphere. The column chromatography method was used to purify the compounds using 200-400 nm mesh silica as a stationary phase. Nuclear magnetic resonance (^1H NMR and ^{13}C NMR) spectroscopic data were collected on FT-NMR spectrometer operating at 500 MHz and the chemical shift values were correlated with the tetramethylsilane internal standard. The solutions were prepared readily at room temperature for the analytical measurements. The electronic absorption and emission spectral measurements were carried out on UV-vis spectrophotometer at room temperature. Thermal stability of the compounds were assessed using TGA under a nitrogen atmosphere at a heating rate of 10 °C/min and DSC measurements. Electrochemical analysis of the compounds were measured on CHI electrochemical analyzer with conventional three electrode configuration containing of a glassy carbon working electrode, a platinum wire auxiliary electrode and a non-aqueous Ag/AgNO₃ acetonitrile reference electrode. Fc/Fc⁺ redox couple was used as an internal standard to calibrate the peak potentials. DFT computational methods were employed according to our previous report.¹

Synthesis

The starting materials, 3-bromo-2-fluorobenzonitrile (**1**) and 3-chloro-2,6-difluorobenzonitrile (**2**), were procured from the TCI Co. chemicals.

2-Fluoro-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzonitrile (3). To the 50 ml solution of 1,4-dioxane, the components **1** (5.0 g, 25.0 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (7.0 g, 27.5 mmol), [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium(II) (0.91 g, 1.25 mmol), and potassium acetate (36.0 g, 15.0 mmol) were added and degassed for 15 min. The reaction mixture was

heated at 100 °C for 4 h. The progress of reaction was monitored by thin film chromatography (TLC) analysis. Further, the reaction mixture was washed with water and dichloromethane, and dried over anhydrous magnesium sulfate. The solvent was removed under vacuum to get the black colored residue. The crude mixture was purified on column chromatography using 1:3 ratio of dichloromethane (DCM):hexane as an eluent, which offered intermediate **2** as a colorless solid. Yield, 4.8 g (80%). ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.06-8.03 (m, 1H), 7.98-7.96 (m, 1H), 7.20-7.13 (m, 1H), 1.46 (s, 12H). MS (APCI) cal. *m/z* 247.11 and found *m/z* 248.11 [(M+H)⁺].

2-Fluoro-2'-nitro-[1,1'-biphenyl]-3-carbonitrile (5). To the 20 ml solution of tetrahydrofuran:water (3;1), the components **3** (4.5 g, 18.2 mmol), 1-bromo-2-nitrobenzene (4.4 g, 21.8 mmol), tetrakis(triphenylphosphine)palladium(0) (1.05 g, 0.91 mmol), and potassium carbonate (7.5 g, 54.6 mmol) were added and degassed for 15 min. The reaction mixture was refluxed at 80 °C for 6 h. The progress of reaction was monitored by TLC analysis. Further, the reaction mixture was washed with water and dichloromethane, and dried over anhydrous magnesium sulfate. The solvent was removed under vacuum to get the yellow colored residue. The crude mixture purified on column chromatography using 1:3 ratio of DCM:hexanes as an eluent offered intermediate **5** as a pale yellow solid. ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.16 (d, 1H, *J* = 10.0 Hz), 7.77-7.58 (m, 4H), 7.43-7.37 (m, 2H). Yield, 3.9 g (90%). MS (APCI) cal. *m/z* 242.04 and found *m/z* 243.04 [(M+H)⁺].

4-Fluoro-9H-carbazole-3-carbonitrile (7). To the mixture of **5** (3.9 g, 16.1 mmol) and triphenylphosphine (12.6 g, 48.8 mmol), *o*-dichlorobenzene was added under a nitrogen atmosphere. The reaction mixture was refluxed at 150 °C for 8 h. The progress of the reaction was monitored by TLC analysis. Further, the reaction mixture was washed with water and dichloromethane, and dried over anhydrous magnesium sulfate. The solvent was removed under vacuum to get the dark black colored residue. The crude mixture purified on column

chromatography using 1:2 ratio of DCM:hexanes as an eluent offered intermediate **7** as a pale yellow solid. ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.53 (s, 1H), 8.23 (d, *J* = 10.0 Hz, 1H), 7.58-7.50 (m, 3H), 7.39-7.36 (m, 1H), 5.29 (m, 1H). Yield, 2.5 g (75%). MS (APCI) cal. *m/z* 210.05 and found *m/z* 211.05 [(M+H)⁺].

4-Fluoro-9-phenyl-9H-carbazole-3-carbonitrile (9). A mixture of **7** (2.5 g, 11.9 mmol), copper iodide (0.22 g, 1.19 mmol), 1,10-phenanthroline (0.4 g, 2.39 mmol) and 20 ml iodobenzene was refluxed at 100 °C for 6 h. The progress of reaction was monitored by TLC analysis. Further, the reaction mixture was washed with water and dichloromethane, and dried over anhydrous magnesium sulfate. The solvent was removed under vacuum to get the black colored residue. The crude mixture purified on column chromatography using 1:2 ratio of DCM:hexanes as eluent offered intermediate **9** as a pale yellow solid. ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.29 (d, *J* = 10.0 Hz, 1H), 7.67-7.64 (m, 2H), 7.58-7.50 (m, 5H), 7.42-7.37 (m, 2H), 7.18 (d, *J* = 10.0 Hz, 1H). Yield, 3.0 g (90%). MS (APCI) *m/z* cal. *m/z* 286.09 and found 287.09 [(M+H)⁺].

9-Phenyl-9H-[4,9'-bicarbazole]-3-carbonitrile (4CzCzCN). A mixture of **9** (1.5 g, 5.2 mmol), 9H-carbazole (0.86 g, 5.2 mmol) and cesium carbonate (5.0 g, 15.6 mmol) was suspended in 10 mL of *N,N*-dimethylformamide. The reaction mixture was refluxed at 150 °C for 1 h. The progress of reaction was monitored by TLC analysis. Further, the reaction mixture was washed with water and DCM, and dried over anhydrous magnesium sulfate. The solvent was removed under vacuum to get the color less residue. The crude mixture purified on column chromatography using 1:1 ratio of DCM:hexanes as an eluent offered desired compound **4CzCzCN** as a colorless solid. Yield, 2.07 g (89%). ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.28-8.26 (m, 2H), 7.87 (d, 1H, *J* = 10.0 Hz), 7.70-7.67 (m, 2H), 7.60-7.56 (m, 4H), 7.36-7.32 (m, 6H), 7.07-7.06 (m, 2H), 6.84-6.83 (m, 1H), 6.38 (d, 1H, *J* = 10.0 Hz). ¹³C NMR (500 MHz, CDCl₃, δ ppm): 144.58, 142.09, 140.46, 136.18, 134.98, 130.90, 129.12, 127.90, 127.46,

126.46, 123.95, 123.04, 122.18, 121.57, 120.71, 117.49, 110.80, 110.08, 104.33. MS (APCI) m/z cal. m/z 433.15 and found 434.15 [(M+H)⁺]. Elemental analysis (%): calculated for C₄₆H₂₆N₆; C, 85.89; N, 9.69; H, 4.42. found: C, 85.67; N, 9.59; H, 4.39.

9-Phenyl-9H-[4,9'-bicarbazole]-3,3'-dicarbonitrile (4CzCNCzCN). The compound **4CzCNCzCN** was synthesized from **9** (1.5 g, 5.2 mmol), 9H-carbazole-3-carbonitrile (0.98 g, 5.2 mmol) and cesium carbonate (5.0 g, 15.6 mmol) using the similar procedure described above for **4CzCzCN**. Yield, 2.04 g (85%). ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.60 (s, 1H), 8.30-8.29 (m, 1H), 7.90 (d, 1H, *J* = 10.0 Hz), 7.73-7.70 (m, 2H), 7.63-7.59 (m, 5H), 7.46-7.44 (m, 2H), 7.37-7.34 (m, 2H), 7.13-7.10 (m, 2H), 6.88-6.86 (m, 1H), 6.29 (d, 1H, *J* = 10.0 Hz). ¹³C NMR (500 MHz, CDCl₃, δ ppm): 144.41, 142.23, 141.08, 136.17, 133.38, 130.70, 129.85, 129.33, 128.18, 127.56, 125.98, 124.24, 122.79, 122.58, 122.10, 121.40, 120.47, 119.70, 117.07, 111.31, 110.99, 110.54, 104.04. MS (APCI) cal. m/z 458.15 and found m/z 459.15 [(M+H)⁺]. Elemental analysis (%): calculated for C₄₆H₂₆N₆; C, 83.82; N, 12.22; H, 3.96. found: C, 83.69; N, 12.23; H, 3.98.

2,6-Difluoro-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzotrile (4). The **4** intermediate was prepared from **2** (5.0 g, 28.9 mmol), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (8.07 g, 31.8 mmol), [1,1'-bis(diphenylphosphino)ferrocene]dichloropalladium(II) (1.0 g, 1.4 mmol), and potassium acetate (8.2 g, 86.7 mmol) using the similar procedure described above for **3**. Yield, 5.7 g (70%). ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.01-7.97 (m, 1H), 7.07-7.03 (m, 1H). MS (APCI) cal. m/z 265.10 and found m/z 266.10 [(M+H)⁺].

2,4-Difluoro-2'-nitro-[1,1'-biphenyl]-3-carbonitrile (6). The intermediate **6** was prepared from **4** (5.7 g, 21.5 mmol), 1-bromo-2-nitrobenzene (4.7 g, 23.6 mmol), Tetrakis(triphenylphosphine)palladium(0) (1.1 g, 1.0 mmol), and potassium carbonate (8.9 g,

64.5 mmol) using similar procedure described above for **5**. Yield, 4.5 g (75%). ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.17 (d, 1H, *J* = 10.0 Hz), 7.78-7.75 (m, 1H), 7.68-7.65 (m, 1H), 7.60-7.55 (m, 1H), 7.41 (m, 1H), 7.19-7.16 (m, 1H). MS (APCI) cal. *m/z* 260.03 and found *m/z* 261.03 [(M+H)⁺].

2,4-Difluoro-9H-carbazole-3-carbonitrile (8). The intermediate **8** was prepared from **6** (4.5 g, 17.3 mmol) and triphenylphosphine (13.5 g, 51.9 mmol) using similar procedure described above for **7**. Yield, 3.1 g (80%). ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.51 (s, 1H), 8.17 (d, *J* = 10.0 Hz, 1H), 7.52-7.47 (m, 2H), 7.39-7.369 (m, 1H), 7.07 (d, *J* = 10.0 Hz, 1H). MS (APCI) cal. *m/z* 228.04 and found *m/z* 229.04 [(M+H)⁺].

2,4-Difluoro-9-phenyl-9H-carbazole-3-carbonitrile (10). The intermediate **10** was prepared from **8** (3.1 g, 13.5 mmol), copper iodide (0.25 g, 1.35 mmol), and 1,10-phenanthroline (5.1 g, 2.7 mmol) using similar procedure described above for **9**. Yield, 3.3 g (81%). ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.22 (d, *J* = 1.0 Hz, 1H), 7.68-7.65 (m, 2H), 7.60-7.57 (m, 1H), 7.50-7.48 (m, 3H), 7.43-7.40 (m, 1H), 7.35 (d, *J* = 10.0 Hz, 1H), 6.93 (d, *J* = 10.0 Hz, 1H). MS (APCI) cal. *m/z* 304.08 and found *m/z* 305.08 [(M+H)⁺].

9'-Phenyl-9'H-[9,2':4',9''-tercarbazole]-3'-carbonitrile (24CzCzCN). It was prepared from **10** (1.5 g, 4.9 mmol), 9H-carbazole (1.71 g, 10.2 mmol) and cesium carbonate (4.7 g, 14.7 mmol) using the similar procedure described above for **4CzCzCN**. Yield, 2.4 g (85%). ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.31 (d, 2H, *J* = 10.0 Hz), 8.17 (d, 2H, *J* = 10.0 Hz), 7.71 (s, 1H), 7.64-7.60 (m, 4H), 7.53-7.46 (m, 5H), 7.45-7.33 (m, 8H), 7.33 (d, 2H, *J* = 10.0 Hz), 6.95-6.91 (m, 1H), 6.48 (d, 1H, *J* = 10.0 Hz). ¹³C NMR (500 MHz, CDCl₃, δ ppm): 144.55, 142.71, 141.42, 140.27, 138.85, 136.34, 135.89, 130.78, 129.33, 128.45, 127.40, 126.79, 126.60, 124.14, 123.38, 122.40, 121.22, 120.90, 119.98, 114.15, 111.24, 110.55, 110.25, 109.84, 106.25. MS (APCI) cal. *m/z* 598.21 and found *m/z* 599.21 [(M+H)⁺]. Elemental analysis (%): calculated for C₄₆H₂₆N₆; C, 86.26; N, 9.36; H, 4.38. found: C, 85.98; N, 9.54; H, 4.34.

9'-Phenyl-9'H-[9,2':4',9''-tercarbazole]-3,3',3''-tricarbonitrile (24CzCNCzCN). The compound **24CzCNCzCN** was synthesized from **10** (1.5 g, 4.9 mmol), 9*H*-carbazole-3-carbonitrile (1.97 g, 10.2 mmol) and cesium carbonate (4.7 g, 14.7 mmol) using the similar procedure described above for **4CzCzCN**. Yield, 2.6 g (86%). ¹H NMR (500 MHz, CDCl₃, δ ppm): 8.59 (s, 1H), 8.46 (s, 1H), 8.30 (d, 1H, *J* = 10.0 Hz), 8.15 (d, 1H, *J* = 5.0 Hz), 7.73-7.40 (m, 14H), 7.36-7.32 (m, 2H), 7.28-7.25 (m, 2H), 6.98-6.95 (m, 1H), 6.40 (d, 1H, *J* = 5.0 Hz). ¹³C NMR (500 MHz, CDCl₃, δ ppm): 144.51, 143.06, 142.09141.81, 140.84, 137.25, 135.47, 134.89, 131.08, 130.26, 129.84, 129.64, 129.16, 128.47, 128.25, 127.42, 126.12, 125.77, 124.57, 124.31, 122.79, 122.52, 122.38, 121.68, 121.21, 120.09, 119.39, 113.51, 111.82, 110.95, 110.48, 110.12, 104.61, 104.18. MS (APCI) cal. *m/z* 648.10 and found *m/z* 649.20 [(M+H)⁺]. Elemental analysis (%): calculated for C₄₆H₂₆N₆; C, 83.62; N, 12.95; H, 4.73. found: C, 83.83; N, 12.74; H, 4.34.

Device fabrication

The blue PHOLEDs were fabricated using a device stack of indium tin oxide (ITO, 50 nm)/ PEDOT:PSS (60 nm)/di-[4-(*N,N*-ditolyl-amino) phenyl]cyclohexane (TAPC) (20 nm)/ 1,3-bis(*N*-carbazolyl)benzene (mCP) (10 nm)/emitting layer (EML) (25 nm)/ diphenyl phosphine oxide-4-(triphenylsilyl)-phenyl (TSPO1) (5 nm)/ 2,2',2''-(1,3,5-Benzinetriyl)-tris(1-phenyl-1-*H*-benzimidazole) (TPBi) (20 nm)/LiF(2 nm)/Al(200 nm). The emitting layers were formed by doping of 10 wt% CNIm in either **4CzCzCN** or **4CzCNCzCN** or **24CzCzCN** or **24CzCNCzCN** hosts. All layers of the device were deposited by vacuum thermal evaporation under a high pressure of 3.0×10^{-7} Torr. The blue devices were encapsulated with a glass lid in a nitrogen-filled glove box to protect them from oxygen, and all device performances were measured outside the glove box. Electrical characterization of the devices was done using a Keithley 2400 source meter, and optical characterization was carried out using a CS 2000 spectroradiometer.

Single carrier devices were fabricated to study the carrier transport properties. The device configuration of ITO/PEDOT:PSS/4CzCzCN or 4CzCNCzCN or 24CzCzCN or 24CzCNCzCN/TAPC/Al for hole-only device (HOD) and ITO/PEDOT:PSS/TSP01/4CzCzCN or 4CzCNCzCN or 24CzCzCN or 24CzCNCzCN /LiF/Al for electron-only device (EOD) were employed. Here, TAPC and TSP01 layers were introduced in HOD and EOD to prevent the flow of electrons and holes from the cathode and anode, respectively.

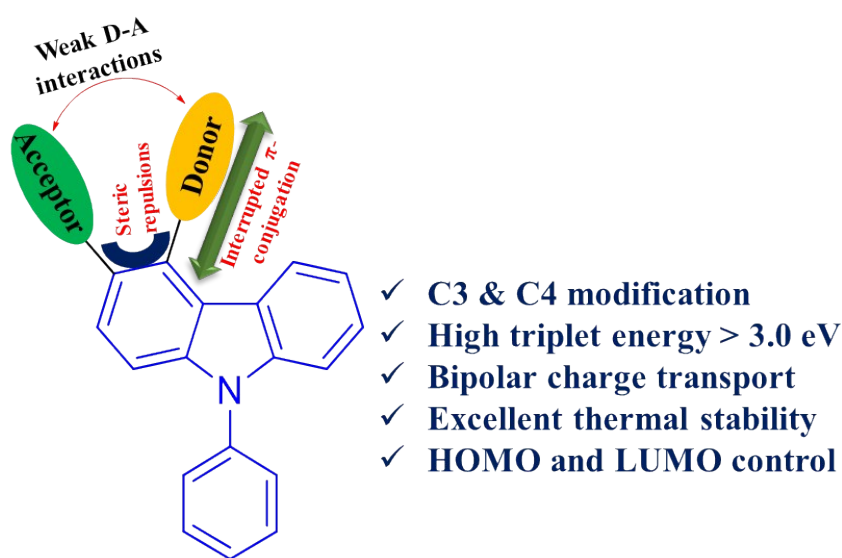


Fig. S1 Molecular design concept of the high triplet energy bipolar host materials based on carbazole core.

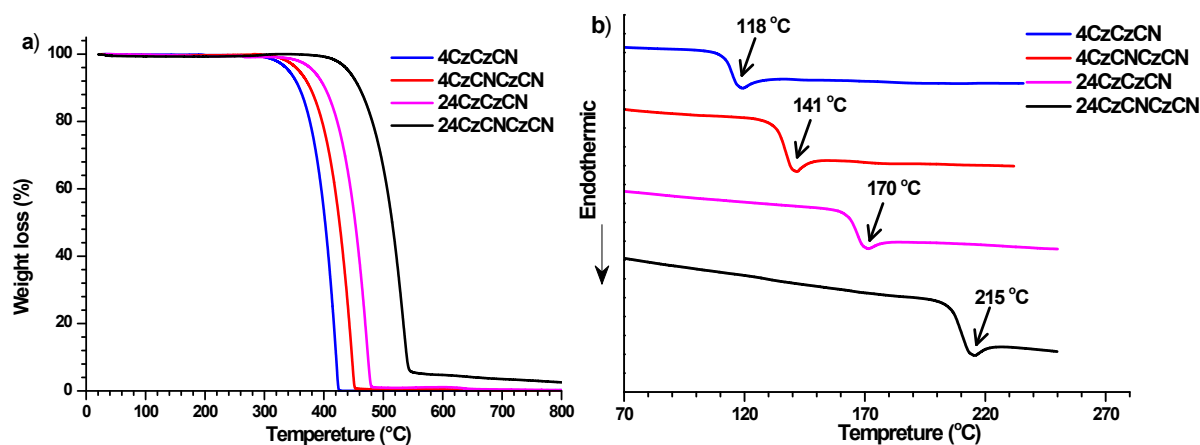


Fig. S2 a) TGA and b) DSC traces of the compounds.

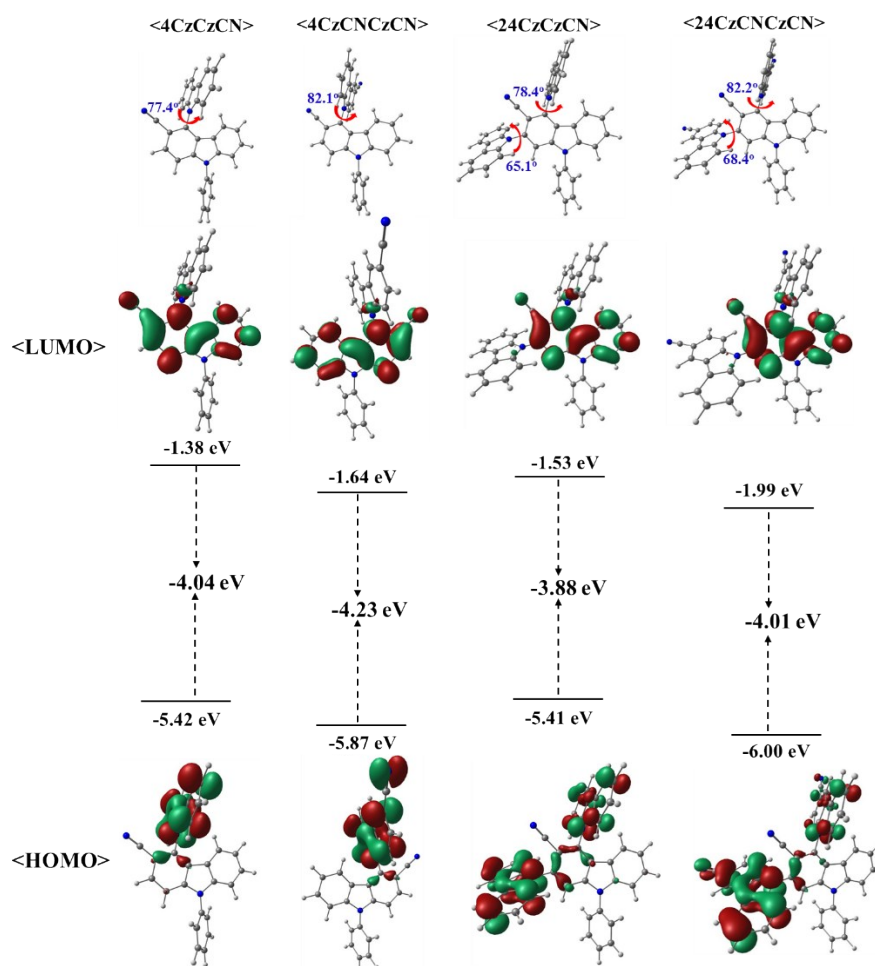


Fig. S3. Optimized geometries and FMO (HOMO/LUMO) distributions of the compounds estimated by DFT computations.

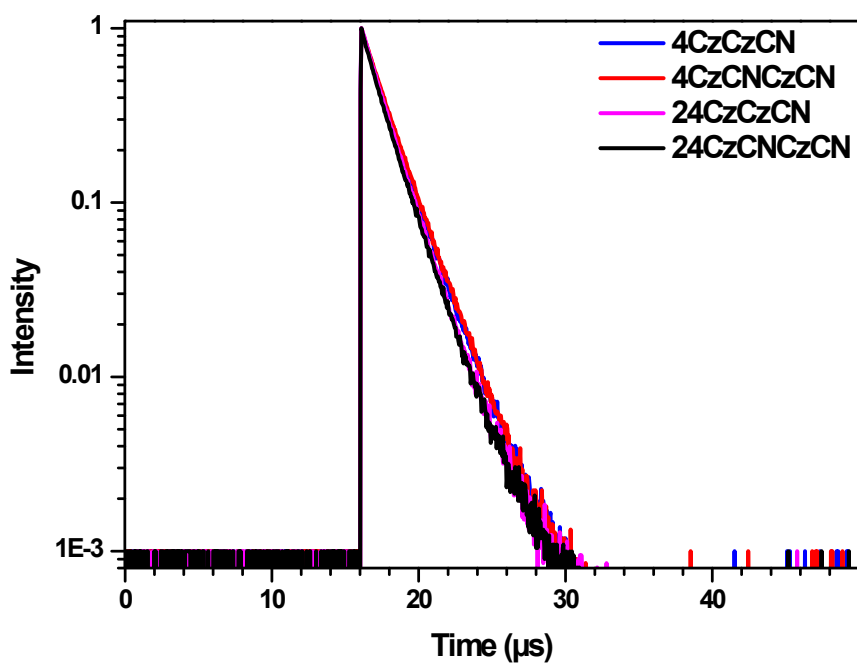


Fig. S4. Transient PL decay profiles of the 10wt% emitter doped films in hosts.

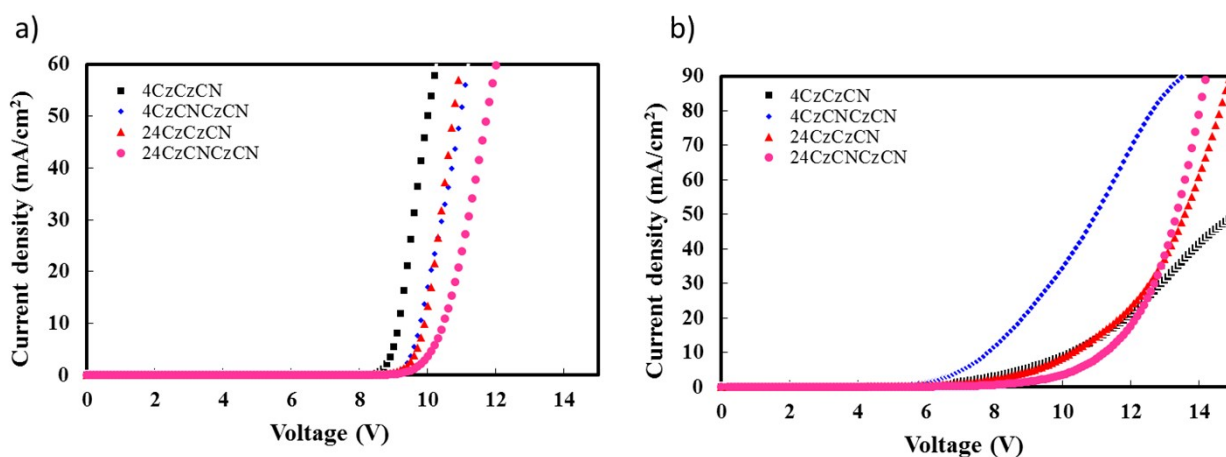


Fig. S5 *I-V* characteristics of a) hole-only and b) electron-only devices of the compounds.

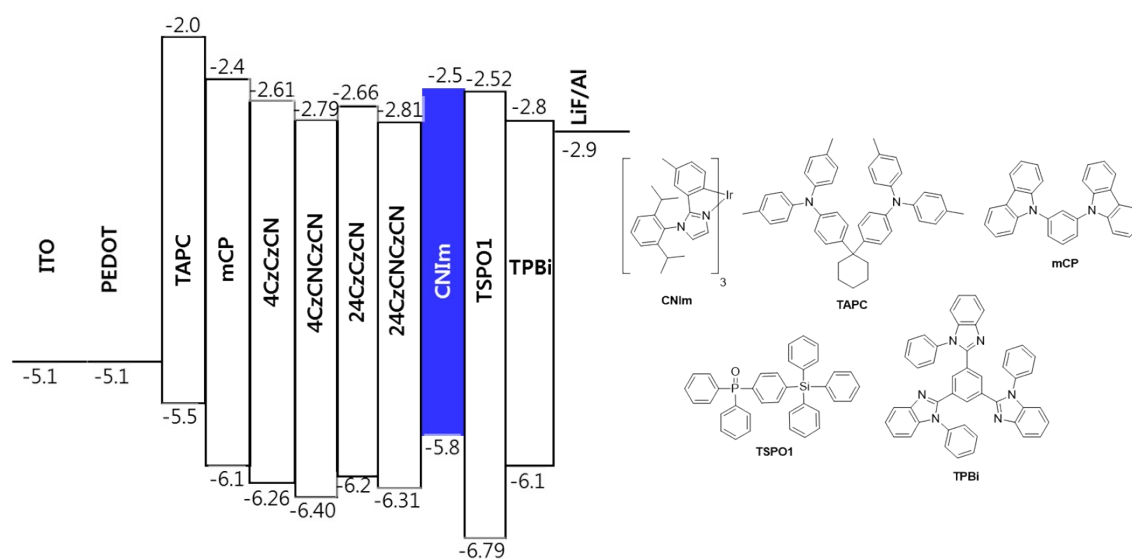


Fig. S6 The energy level alignment and materials chemical structures used for the device.

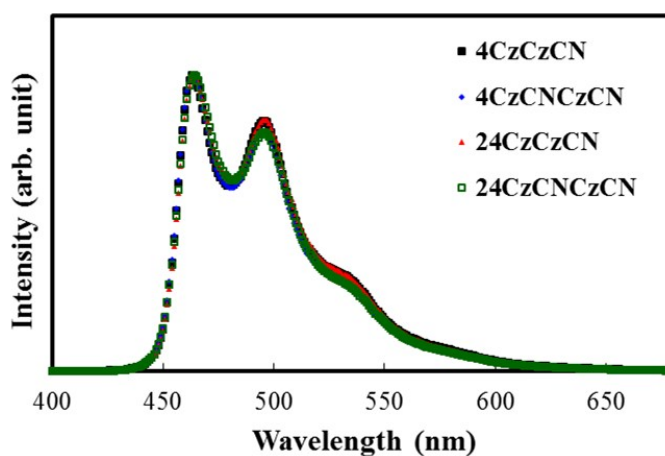


Fig. S7 EL plot of the devices.

Table S1. Photophysical, electrochemical and thermal properties of the compounds

Compound	λ_{abs} , nm (ϵ_{max} , M ⁻¹ cm ⁻¹ × 10 ³) ^a	λ_{em} (nm) ^a	E_{T} (exp./TDDFT) (eV) ^b	Φ_{PL} (%) ^c	t_{d} (μs) ^c	HOMO/LUMO (eV) ^d	E_{g} (eV) ^e	$T_{5\text{d}}$ (°C) ^f	T_{g} (°C) ^g
4CzCzCN	277 (50.0), 321 (17.2), 333 (8.2), 352 (3.9)	360 (sh), 373	3.00/3.03	90.3	1.80	-6.26/-2.61	3.65	342	118
4CzCNCzCN	281 (49.2), 322 (15.3), 333 (15.0), 352 (3.2)	359 (sh), 374	3.06/3.05	97.3	1.79	-6.40/-2.79	3.61	359	141
24CzCzCN	270 (92.5), 279 (sh), 321 (13.3), 335 (11.3), 353 (2.7)	390	2.81/2.91	83.6	1.67	-6.20/-2.66	3.54	382	170
24CzCNCzCN	255 (119.2), 282 (117.3), 335 (21.2), 356 (4.9)	370 (sh), 389	2.85/2.97	83.5	1.68	-6.31/-2.81	3.57	441	215

^aMeasured in THF solution. ^bEstimated from onset of phosphorescence spectra/TDDFT computations. ^c10wt% doped CNIm in host matrix.

^dHOMO and LUMO estimated from the cyclic voltagrams. ^eBand gap estimated from the intersection of absorption and emission spectra.

^fThermal decomposition temperature ($T_{5\text{d}}$). ^gGlass transition temperature (T_{g}).

Table S2. Summarized EL performances of the devices

Host	dopant	Voltage (V_{on}) ^a	EQE (%)		CE (cd/A)		PE (lm/W)		CIE (x, y)
			Max.	@1000 cd/m ²	Max.	@1000 cd/m ²	Max.	@1000 cd/m ²	
4CzCzCN	5wt%	4.4	23.8	17.3	46.0	33.2	31.9	14.5	0.15, 0.29
	10wt%	4.4	24.5	18.0	48.0	35.2	31.8	14.8	0.15, 0.30
4CzCNCzCN	5wt%	3.7	24.0	18.3	45.4	35.4	35.6	16.5	0.15, 0.28
	10wt%	3.6	25.3	19.4	48.1	36.8	39.3	17.9	0.15, 0.29
24CzCzCN	5wt%	4.1	19.1	15.2	38.2	30.1	24.8	13.2	0.15, 0.30
	10wt%	4.1	22.2	17.6	43.7	34.6	31.7	15.3	0.15, 0.30

24CzCNCzCN	5wt%	3.3	20.4	16.4	38.3	30.5	34.4	16.4	0.15, 0.28
	10wt%	3.2	21.4	18.1	40.8	34.5	34.4	18.0	0.15, 0.29

^aturn-on voltage (V) at 1 cd/m²

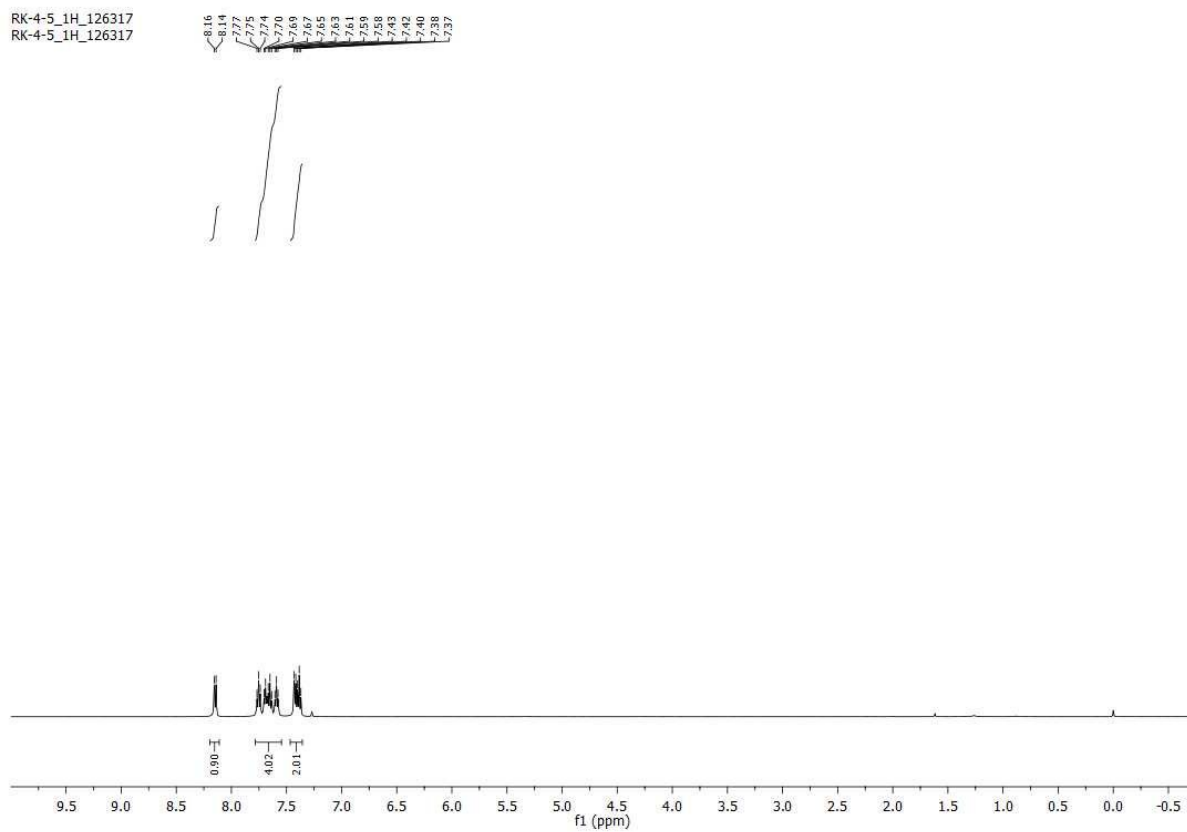


Fig. S8 ^1H NMR spectra of **5** recorded in CDCl_3

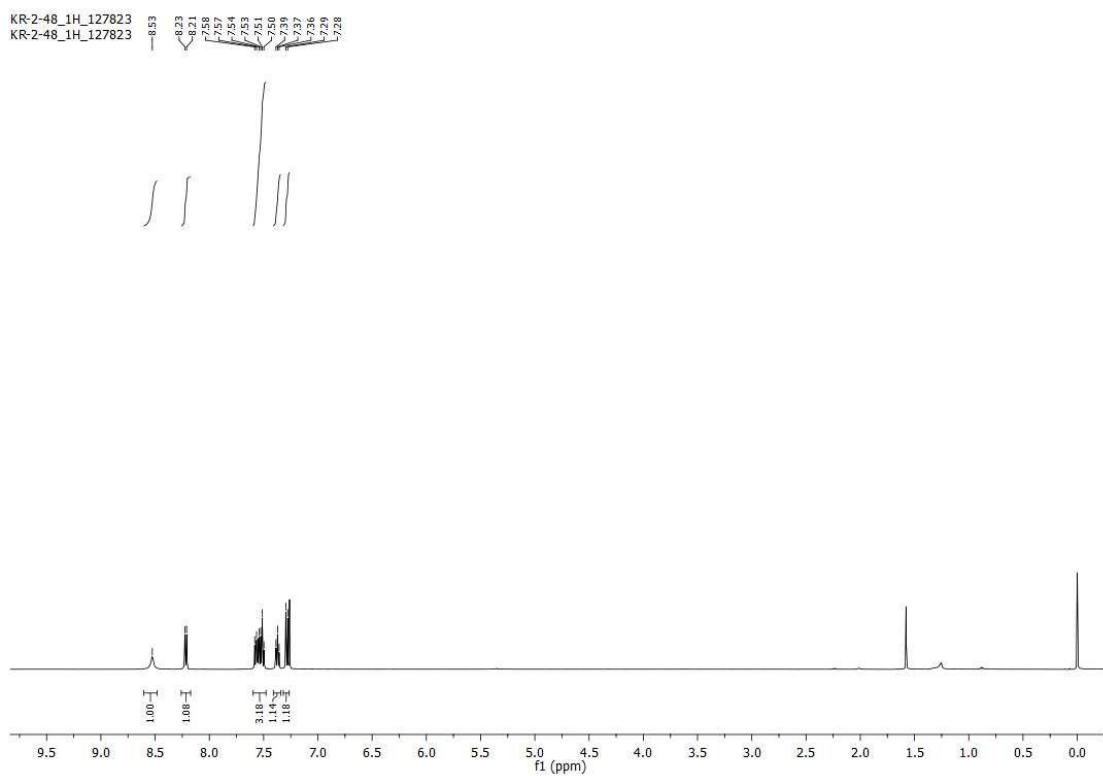


Fig. S9 ^1H NMR spectra of **7** recorded in CDCl_3

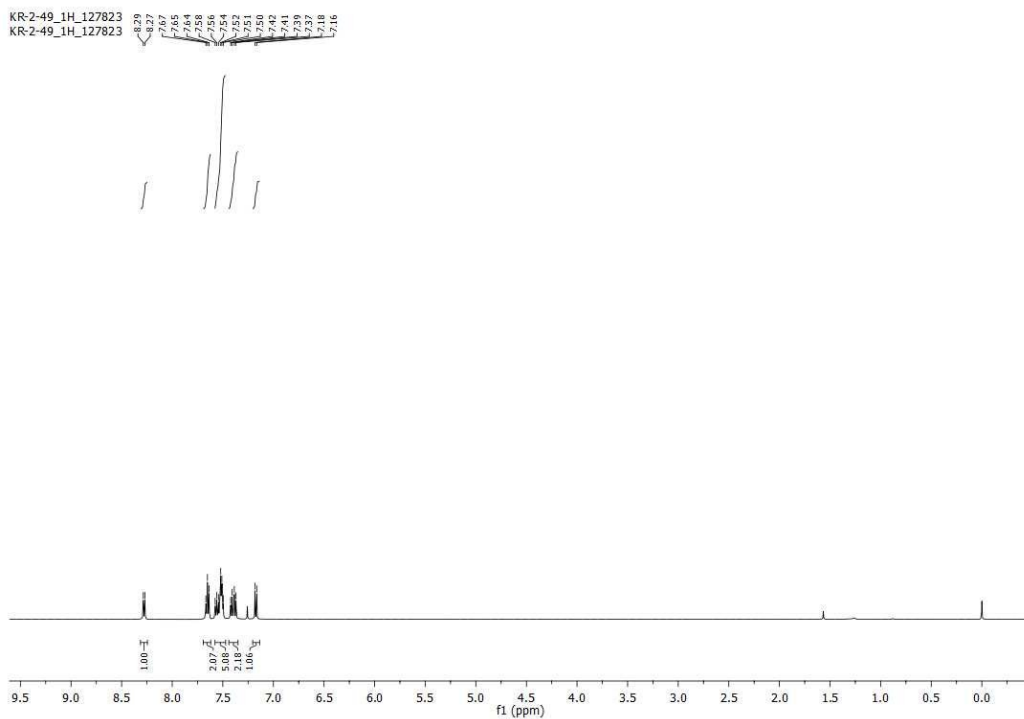


Fig. S10 ^1H NMR spectra of **9** recorded in CDCl_3

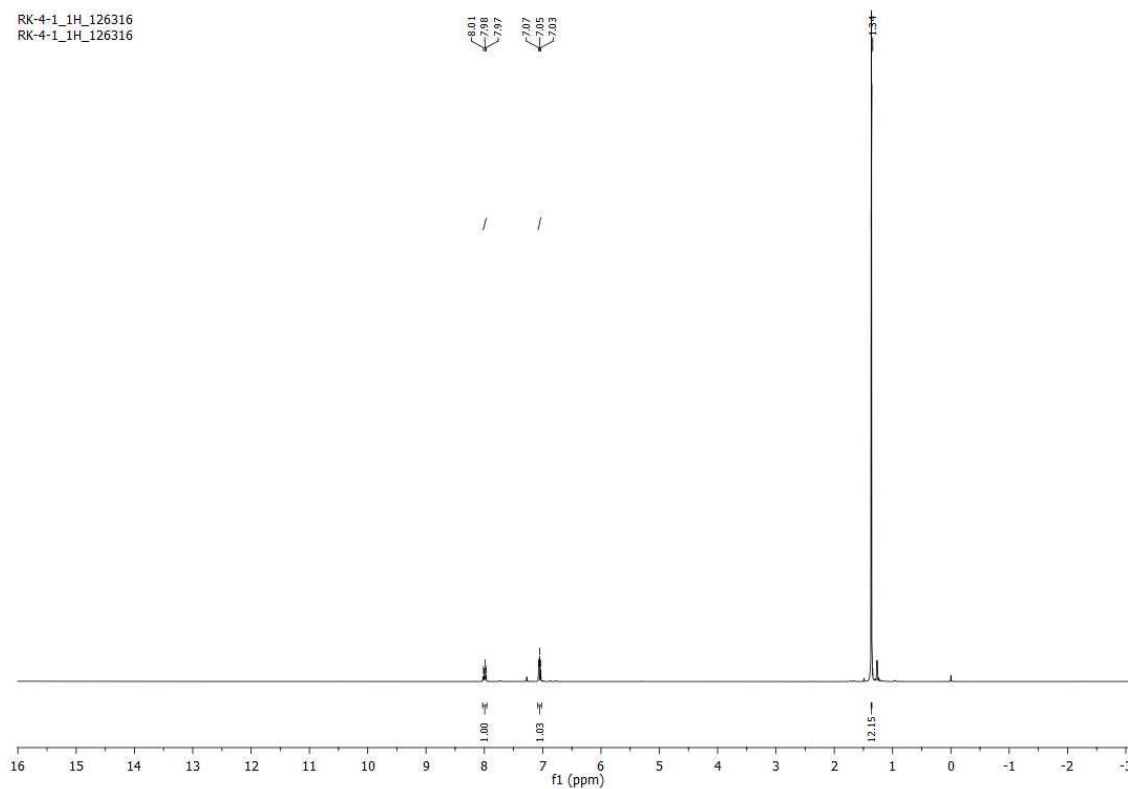


Fig. S11 ^1H NMR spectra of **4** recorded in CDCl_3

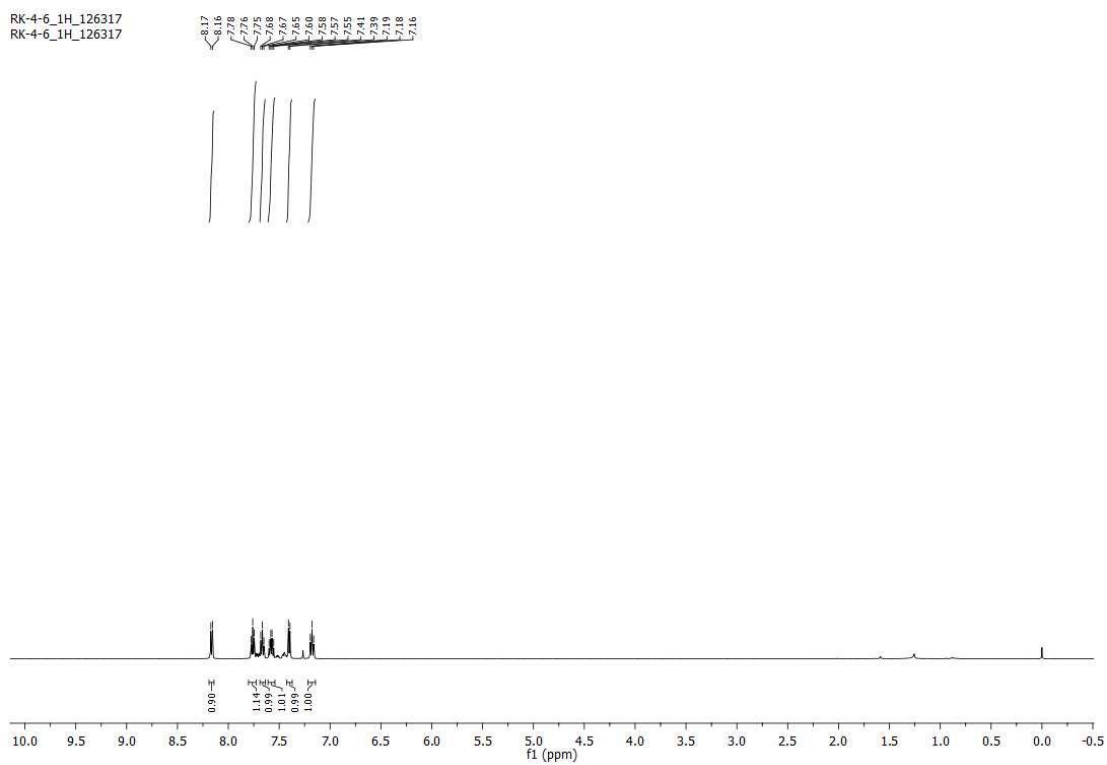


Fig. S12 ^1H NMR spectra of **6** recorded in CDCl_3

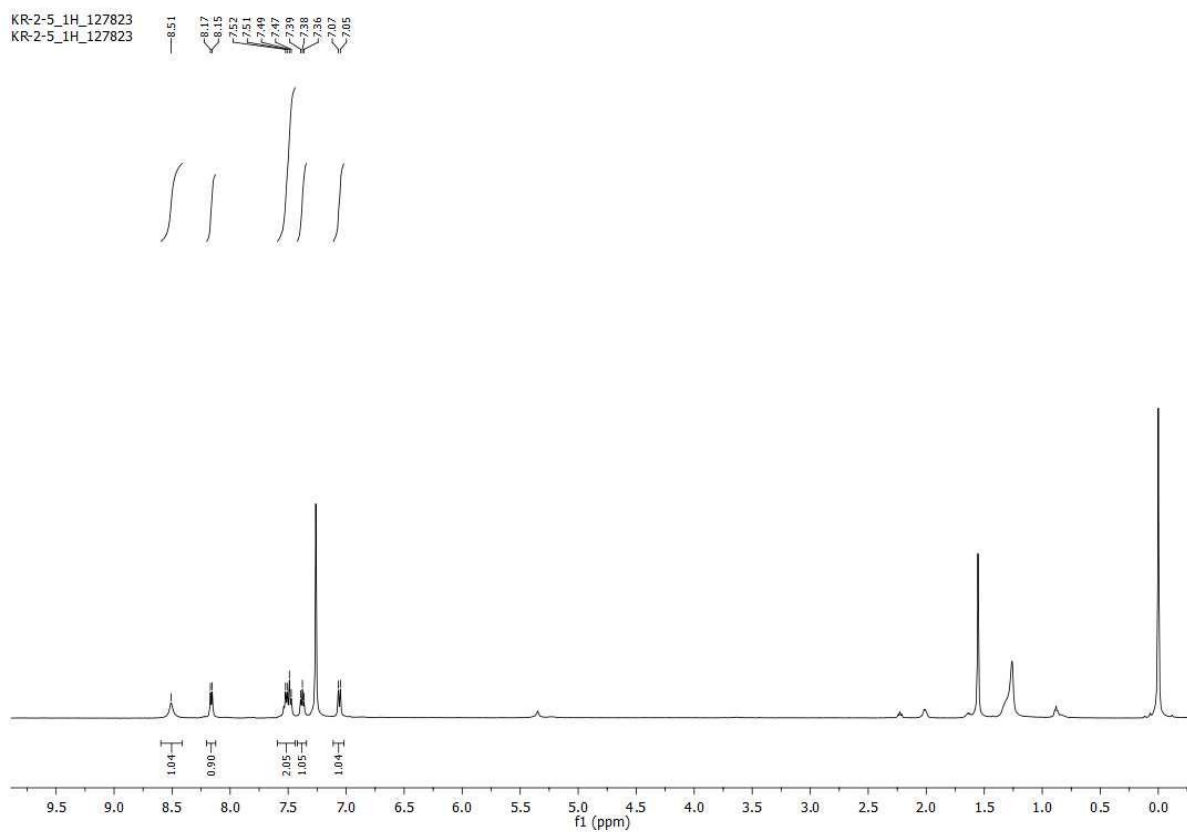


Fig. S13 ^1H NMR spectra of **8** recorded in CDCl_3

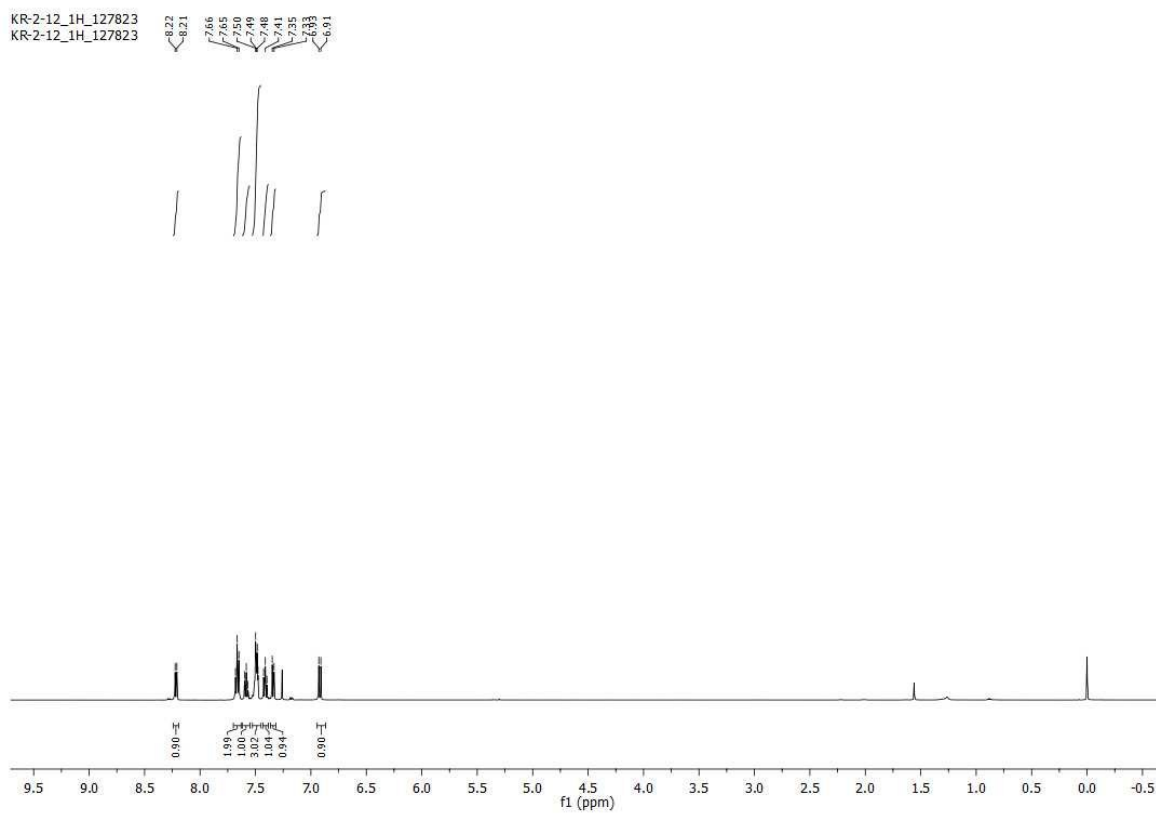


Fig. S14 ^1H NMR spectra of **10** recorded in CDCl_3

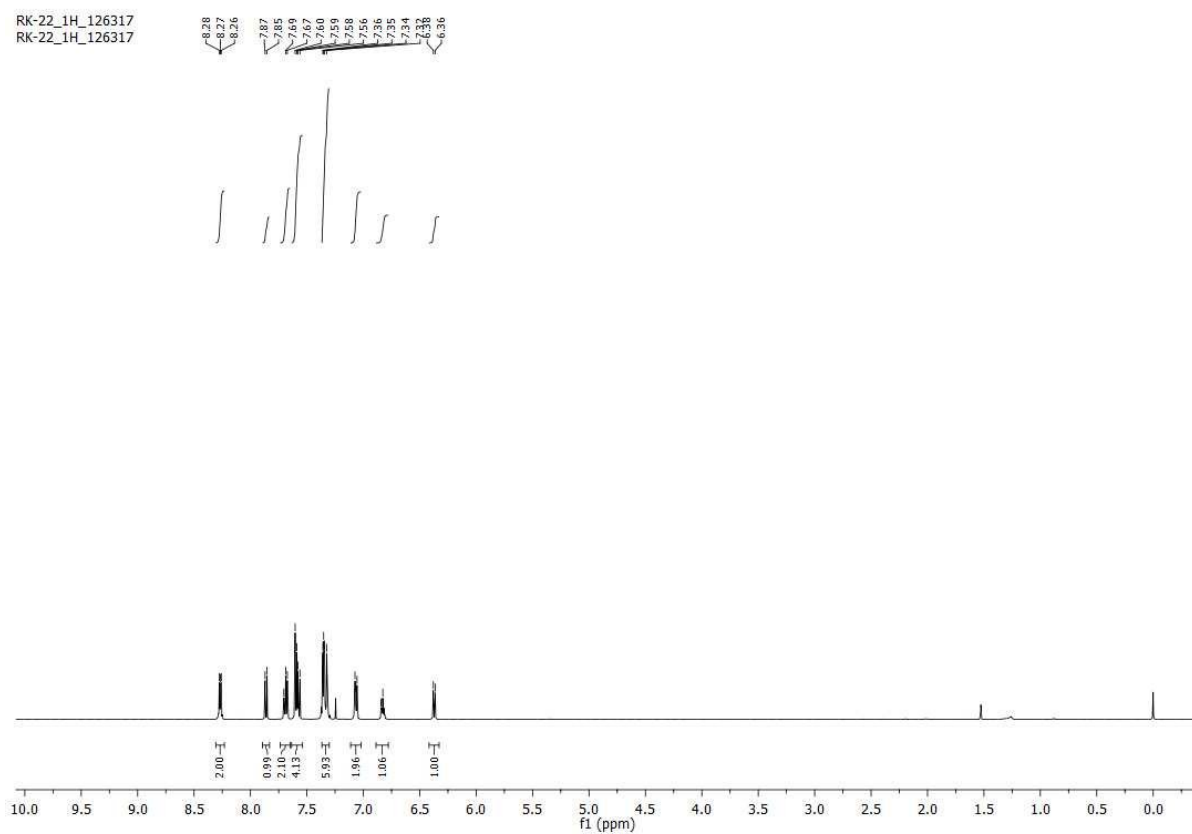


Fig. S15 ^1H NMR spectra of **4CzCzCN** recorded in CDCl_3

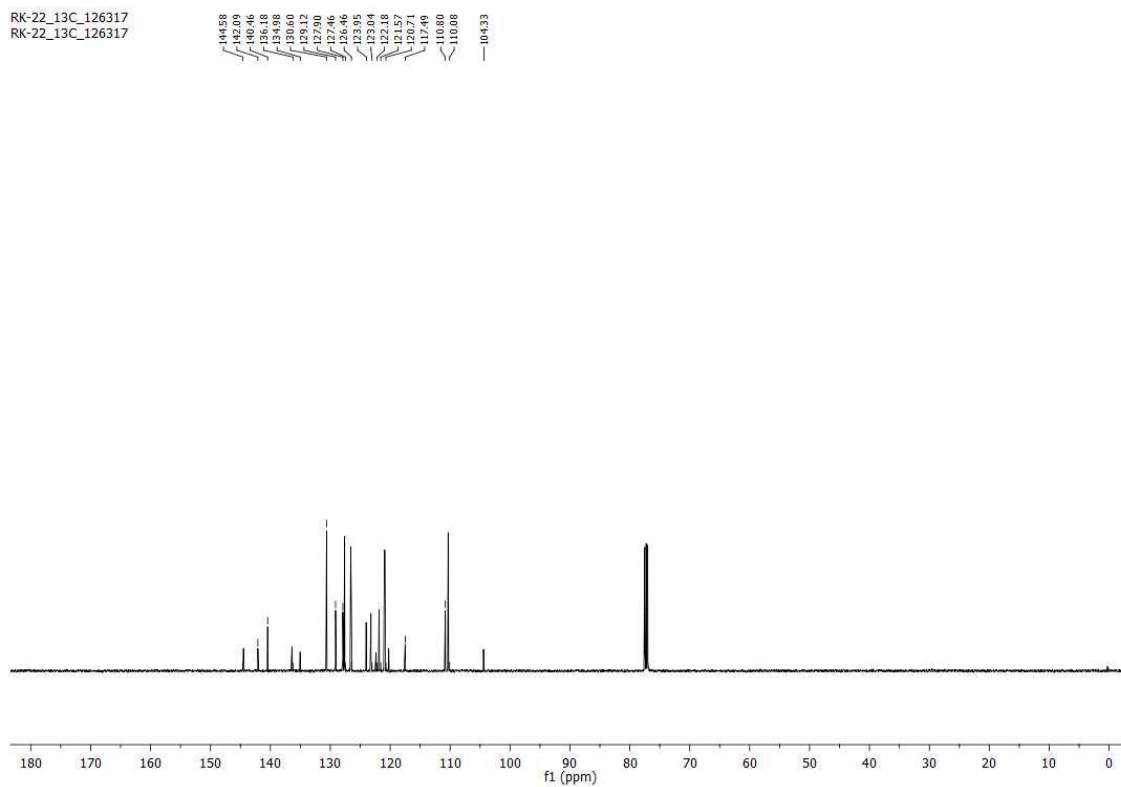


Fig. S16 ^{13}C NMR spectra of **4CzCzCN** recorded in CDCl_3

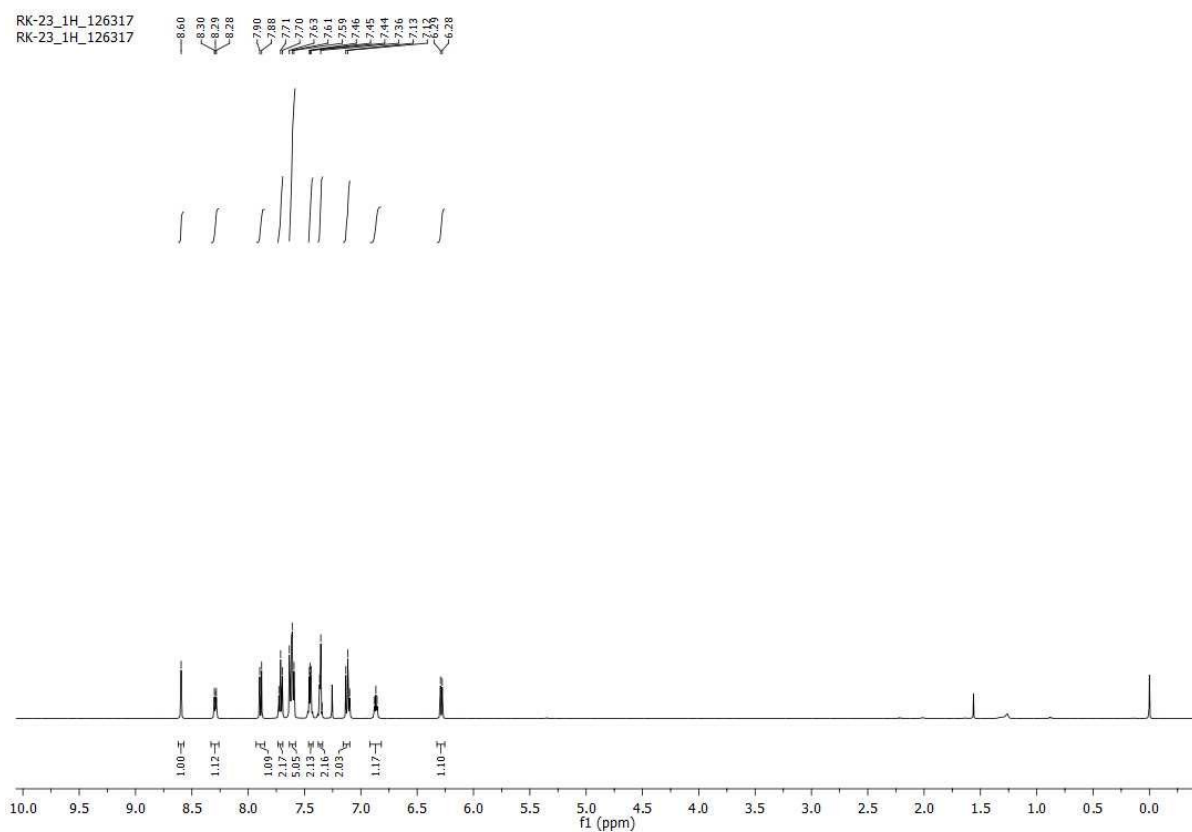


Fig. S17 ^1H NMR spectra of **4CzCNCzCN** recorded in CDCl_3

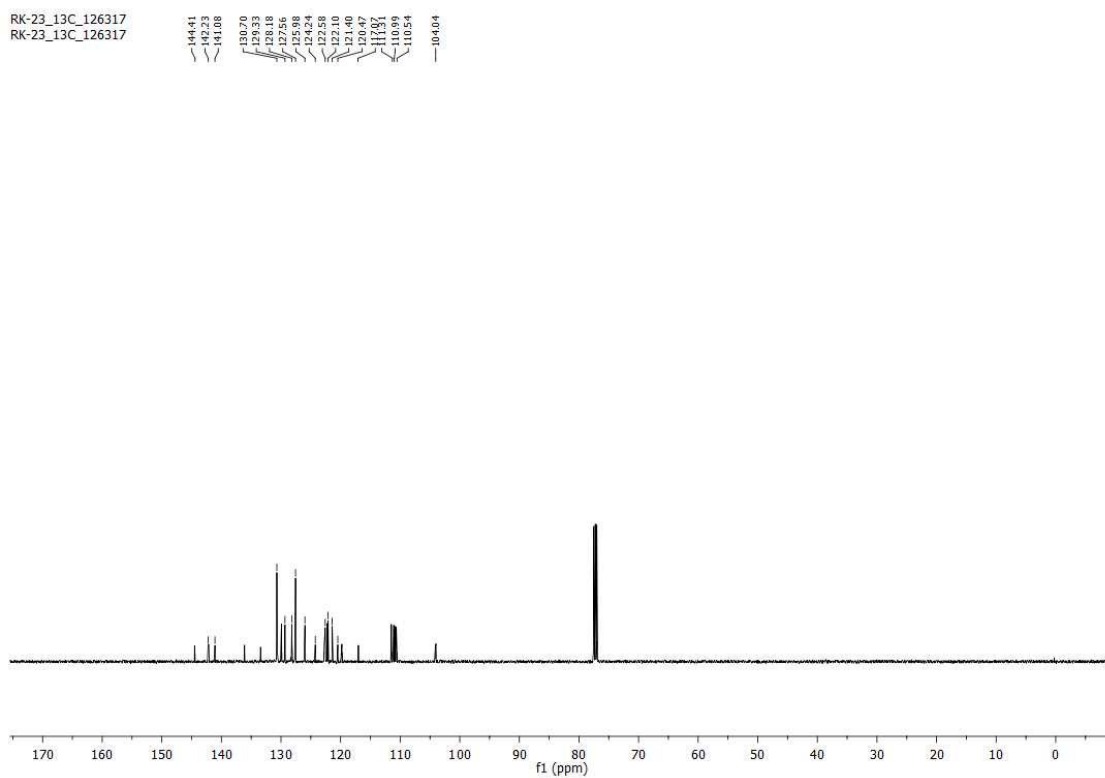


Fig. S18 ^{13}C NMR spectra of **4CzCNCzCN** recorded in CDCl_3

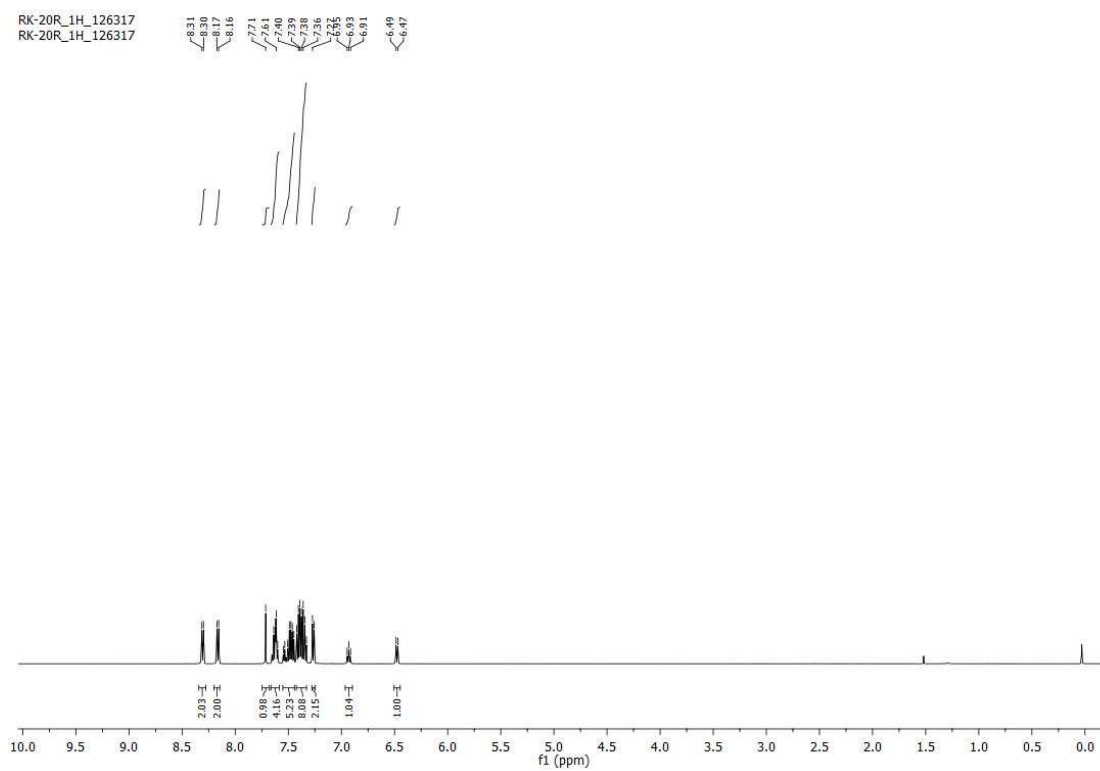


Fig. S19 ^1H NMR spectra of **24CzCzCN** recorded in CDCl_3

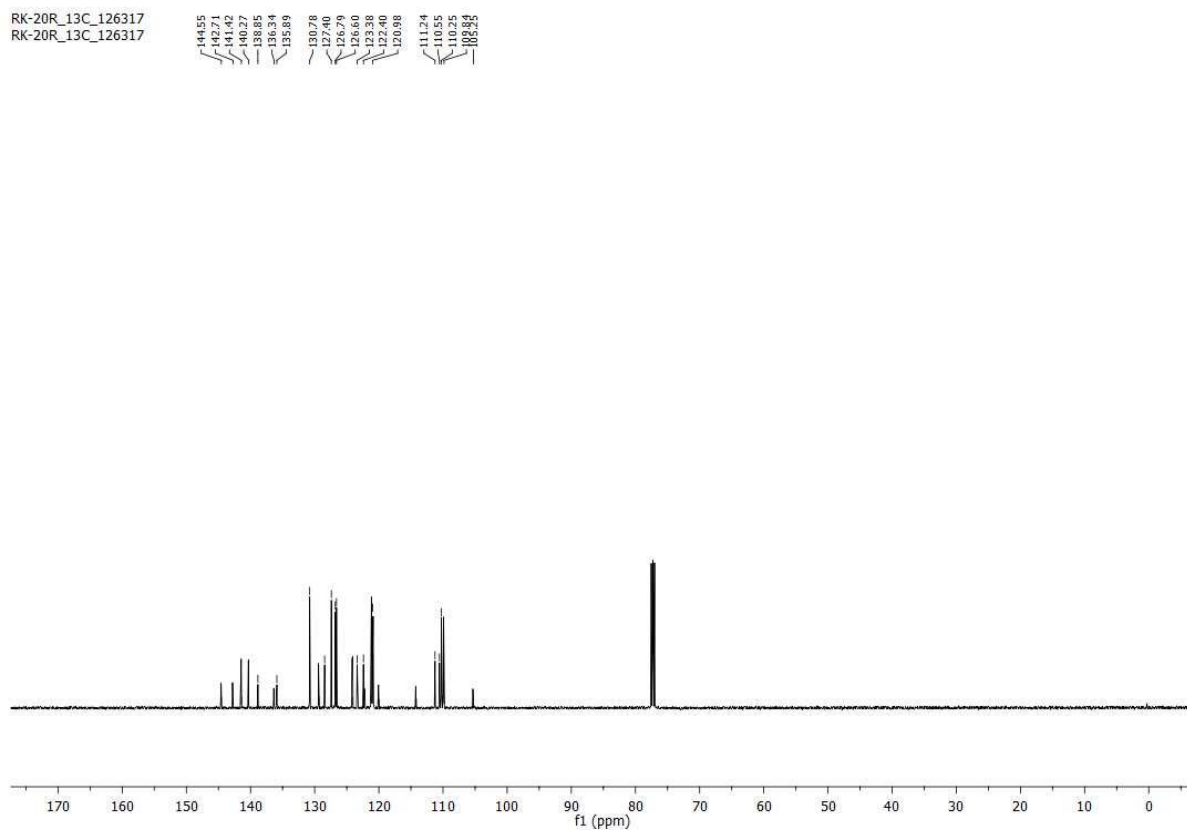


Fig. S20 ^{13}C NMR spectra of **24CzCzCN** recorded in CDCl_3

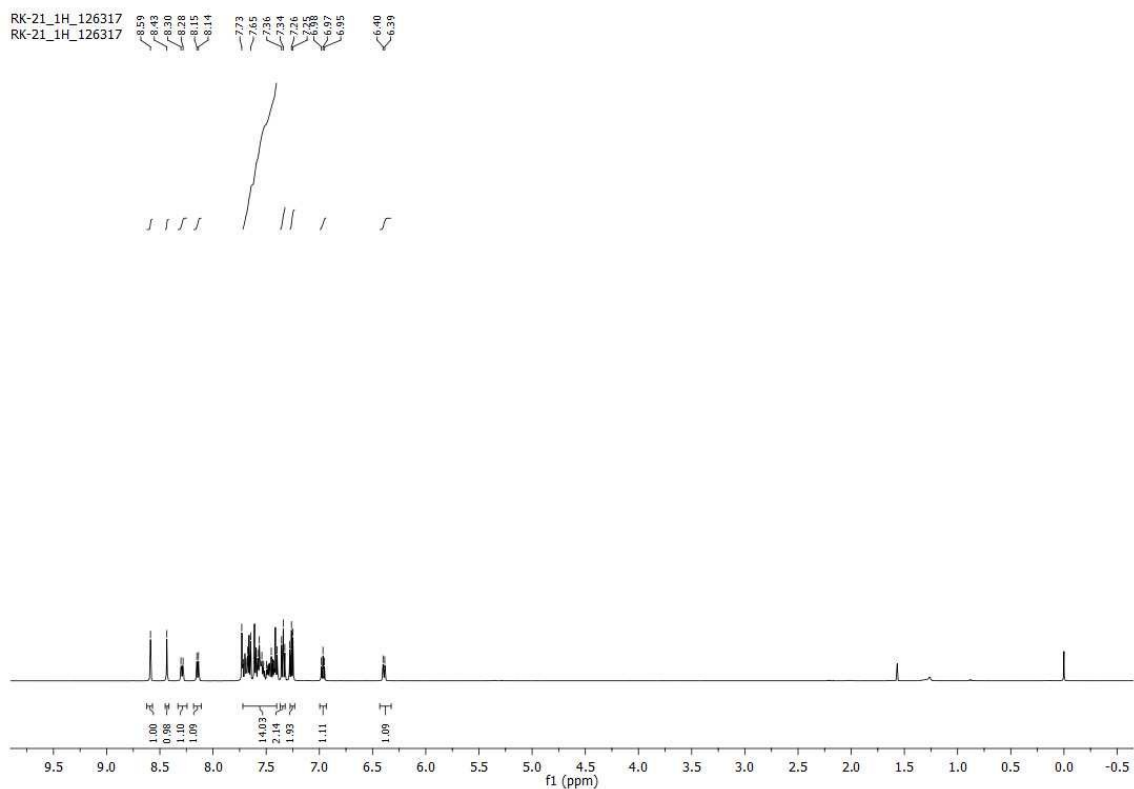


Fig. S21 ^1H NMR spectra of **24CzCzCN** recorded in CDCl_3

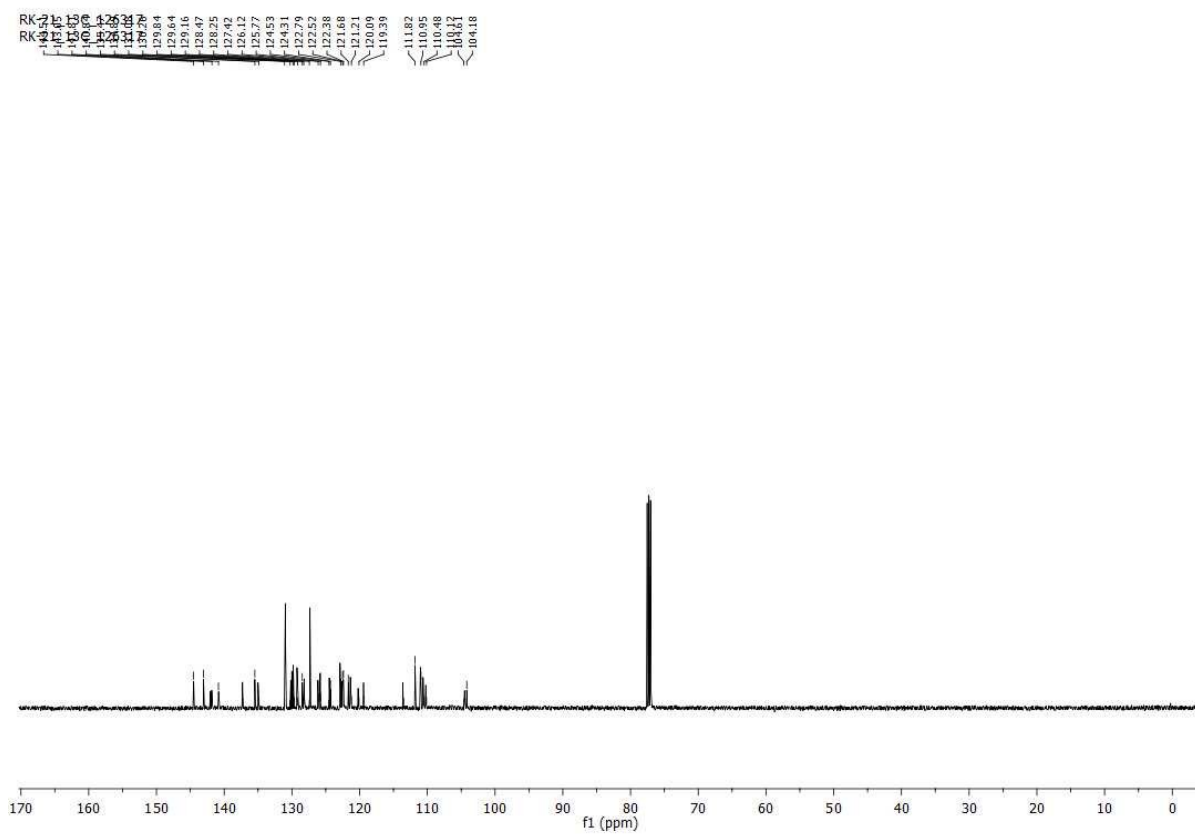


Fig. S22 ^{13}C NMR spectra of **24CzCNCzCN** recorded in CDCl_3

References

1. S. Y. Byeon, J. Kim, D. R. Lee, S. H. Han, S. R. Forrest and J. Y. Lee, *Adv. Optical Mater.* 2018, **6**, 1701340.