

SUPPORTING INFORMATION

The Amplified Circularly Polarized Luminescence Regulated from D-A type AIE-active Chiral Emitters *via* Liquid Crystals System

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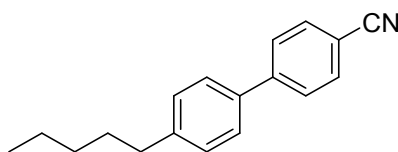
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1. Instrumentation and Materials

NMR spectra were obtained by using 400 MHz Bruker AVANCE III-400 spectrometer with 400 MHz for ^1H NMR and 100 MHz for ^{13}C NMR and reported as parts per million (ppm) from the internal standard TMS. Ultraviolet-visible (UV-*vis*) absorption spectra were measured on a Hitachi U-3900 spectrophotometer. Fluorescence spectra (FL) were recorded on a HORIBA Scientific Fluoromax-4 Spectrofluorometer. Circular dichroism (CD) spectra were recorded on a JASCO J-1500 spectropolarimeter, and the length of the sample cell was 1 cm. Circularly polarized luminescence (CPL) spectra were recorded with a JASCO CPL-300 spectrofluoropolarimeter and the excitation wavelength was 350 nm, scan speed was 200 nm/min, number of scans was 1, and slit width was 3000 μm . All starting materials were purchased from Acros, Energy, Bidepharm and used directly. Nematic liquid crystal 5CB ($n_e = 1.6975$, $n_o = 1.5350$, at 589 nm; $\epsilon_{\perp} = 7.0$, $\Delta\epsilon = 11.5$, at 1KHz, 25°C; viscosity = 82cp at 25°C; $T_m = 24^\circ\text{C}$, $T_i = 35.3^\circ\text{C}$) was purchased from Suzhou King Optonics Co. Ltd.



Scheme S1. Molecular structure of nematic liquid crystal 5CB.

2. Synthesis of *R*-/*S*-1 and *R*-/*S*-2

Intermediate 1, 2, and *R*-/*S*-NAP were prepared as previously described¹. ^1H NMR spectra are in accordance with literature values.

Synthesis of *R*-/*S*-1

The compound 1 (0.300 g, 0.785 mmol), *R*-/*S*-NAP (0.298g, 0.785 mmol), $\text{Pd}(\text{PPh}_3)_4$ (27mg, 23.5 μmol) and K_2CO_3 (0.22g, 1.57 mmol) were added to a mixed solvent of 8 mL THF and 0.8 ml H_2O . The mixture was stirred at 70 °C under N_2 atmosphere for 6h. After the reaction was finished, the mixture was poured into water and extracted with CH_2Cl_2 . The organic layer was dried with anhydrous sodium sulfate. The precipitate was removed by filtration, and filtrate was evaporated under reduced pressure. The residue was purified with silica gel column chromatography (eluent: petroleum ether/DCM, v/v, 5:1) to give 0.33 g of *R*-/*S*-1 (green solid, 75.7 %). ^1H NMR (400 MHz,

CDCl₃) δ (ppm): 8.46-8.35 (m, 3H), 7.66-7.48 (m, 4H), 7.33 (m, 2H), 7.22-7.16 (m, 6H), 7.08-7.01 (m, 10H), 6.51 (m, 1H), 1.99 (m, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm): 164.20, 148.44, 144.98, 142.74, 142.37, 140.85, 137.33, 132.49, 131.29, 131.10, 130.83, 130.54, 130.39, 130.16, 129.44, 129.06, 128.66, 128.62, 128.09, 128.01, 127.77, 127.29, 127.22, 127.00, 126.89, 126.73, 126.41, 125.88, 123.26, 121.66, 50.06, 16.28.

Synthesis of *R*-/*S*-2

The compound 2 (0.300 g, 0.654 mmol), *R*-/*S*-NAP (0.249g, 0.654 mmol), Pd(PPh₃)₄ (23mg, 19.6 μ mol) and K₂CO₃ (0.18 g, 1.31 mmol) were added to a mixture solvent of 6 mL THF and 0.6 ml H₂O. The mixture was stirred at 70 °C under N₂ atmosphere for 6h. After the reaction was finished, the mixture was poured into water and extracted with CH₂Cl₂. The organic layer was dried with anhydrous sodium sulfate. The precipitate was removed by filtration, and filtrate was evaporated under reduced pressure. The residue was purified with silica gel column chromatography (eluent: petroleum ether/DCM, v/v, 5:1) to give 0.34 g of *R*-/*S*-2 (green solid, 82.2 %). ¹H NMR (400 MHz, CDCl₃) δ 8.56 (m, 2H), 8.20 (m, 2H), 7.76 (m, 3H), 7.56 (m, 3H), 7.33 (m, 3H), 7.22-6.59 (m, 16H), 6.55 (m, 1H), 2.03 (m, 3H). ¹³C NMR (100 MHz, CDCl₃) δ (ppm): 164.33, 146.62, 144.18, 143.60, 143.42, 141.94, 140.87, 140.21, 136.67, 133.76, 132.53, 131.58, 131.42, 131.35, 130.96, 129.90, 129.25, 128.81, 128.26, 128.13, 127.86, 127.79, 127.74, 127.12, 126.95, 126.91, 126.86, 126.75, 126.73, 126.70, 126.67, 123.20, 123.04, 121.90, 50.12, 16.30.

3. Preparation of N*-LCs

The samples used to investigate the UV-*vis*, fluorescence, CD and CPL spectra were obtained in the following method.

N*-LCs-1/2: The *R*-/*S*-1/2 and nematic liquid crystal 5CB were co-dissolved in the solvent CH₂Cl₂ at a mole ratio of 1:200. Then the solution was gently heated and stirred overnight to evaporate CH₂Cl₂. After completely removing the solvent, the mixture was injected into a flat liquid crystal cell consisting of two sandwiched quartz slides with a 15 μ m spacer or a wedge cell of tan θ = 0.0183.

Other N*-LCs were prepared in the similar method at different mole ratio.

4. Photophysical data of *R*-1 and *R*-2 in different solvents

Table S1. Photophysical data of *R*-1/2 in various solvents

	Toluene	CHCl ₃	THF	DCM	Pentanol	acetone	CH ₃ CN	DMSO	5CB	
									$\epsilon_{//}$	ϵ_{\perp}
ϵ^a	2.37	4.81	7.4	9.1	15.8	20.7	37.5	47.2	7	18.5
λ_{em1}^b	442	436	427	434	446	443	439.4	445	436	
λ_{em2}^c	484	534	527	546	542	554	558	560	522	

^a The dielectric constant of different solvents (ϵ). ^b Emission maxiam of *R*-1 (λ_{em1}). ^c Emission maxiam of *R*-2 (λ_{em2}).

The solvent polarity could be represented by dielectric constant. The liquid crystal host 5CB has two different dielectric constant in the horizontal and vertical direction respectively($\epsilon_{\perp}=7.0$, $\Delta\epsilon=11.5$, at 1Khz, 25°C).

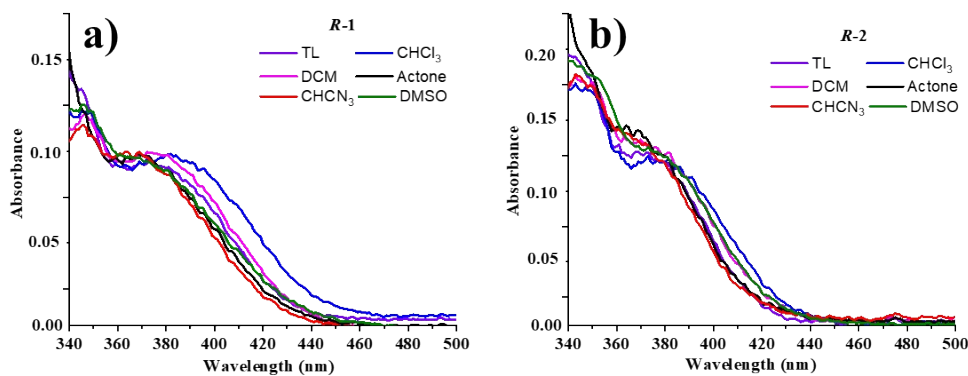


Fig. S1 UV-*vis* absorption spectra of (a) *R*-1 and (b) *R*-2 in different solvents having different polarities (1.0×10^{-5} M).

5. Fluorescence spectra of *R*-1 in THF-H₂O mixtures

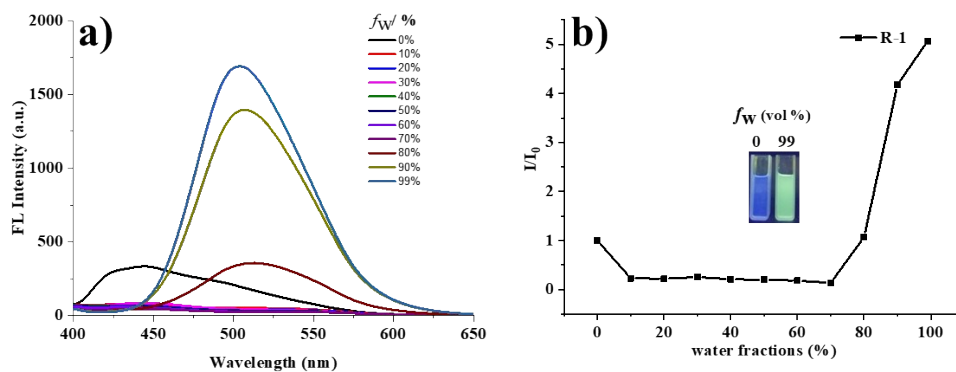


Fig. S2 (a) Fluorescence emission spectra of *R*-1 in THF and THF-H₂O mixtures with different water fractions (f_w) at a fixed concentration (1.0×10^{-5} M, $\lambda_{ex}=350$ nm); (b) Plot of (I/I_0) values versus the compositions of the aqueous mixtures. Inset images: photograph of *R*-1 in THF-H₂O mixed solvents under 365 nm lamp.

6. Optimized molecular structures of *S*-1 and *S*-2

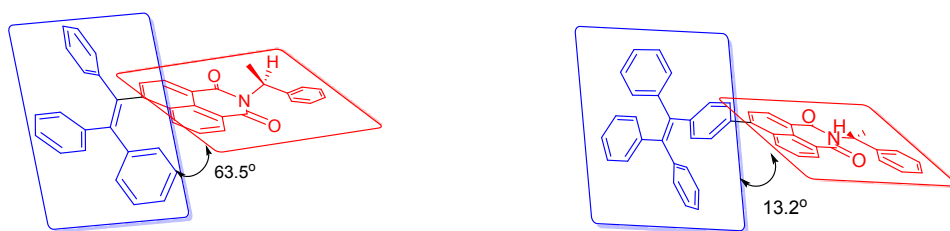


Fig. S3 Optimized molecular structures of *R*-1 (left) and *R*-2(right).

7. CD spectra of *R*-/*S*-1 and *R*-/*S*-2 in solution and suspension

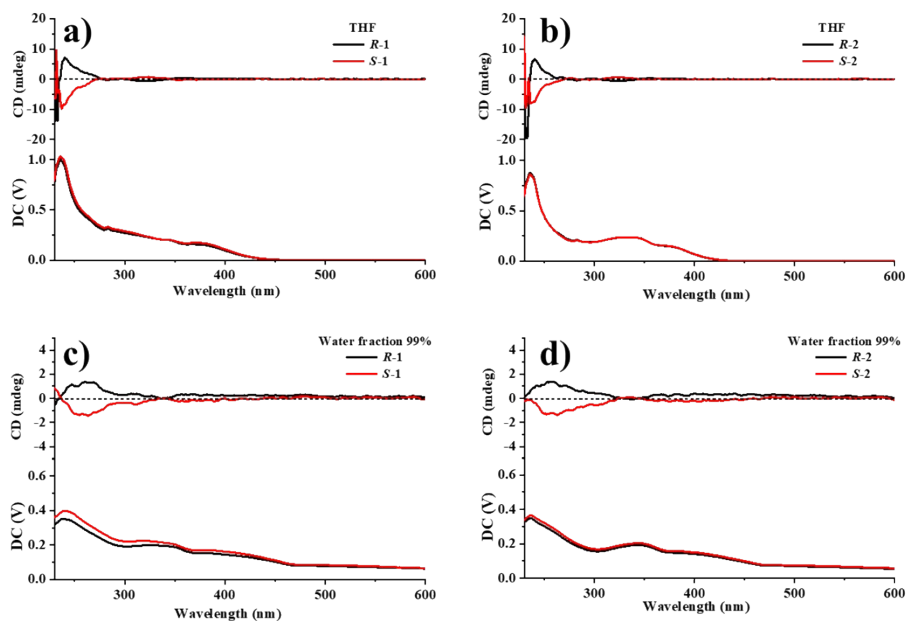


Fig. S4 CD spectra (top panel) and UV-*vis* (bottom panel) absorption spectra of the dopants. (a) *R*-/*S*-1 in THF, (b) *R*-/*S*-2 in THF, (c) *R*-/*S*-1 in the aggregates, (d) *R*-/*S*-2 in the aggregates (1.0×10^{-5} M, $\lambda_{\text{ex}}=350$ nm).

8. CPL spectra of *R*-/*S*-1 and *R*-/*S*-2 in in solution and suspension

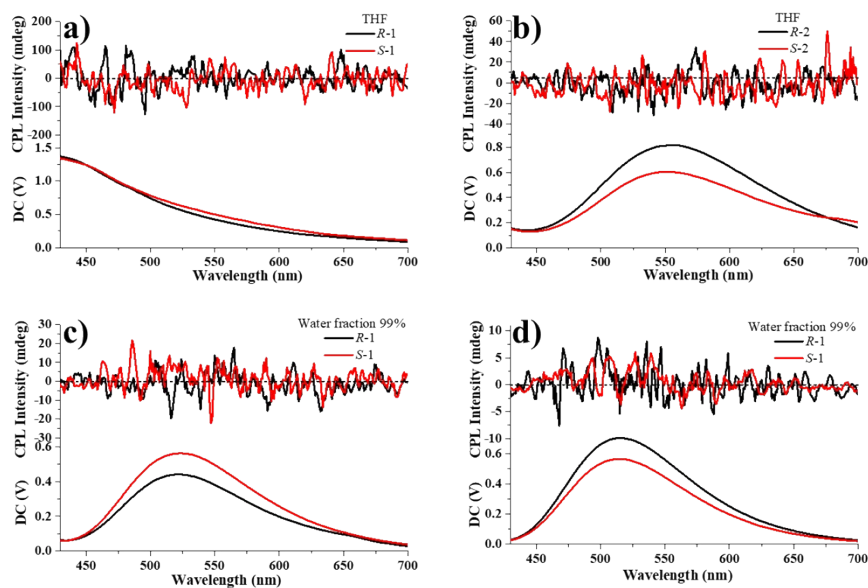


Fig. S5 CPL (top panel) and fluorescence (bottom panel) spectra of the dopants. (a) *R*-/*S*-1 in THF,

(b) *R*-/*S*-2 in THF, (c) *R*-/*S*-1 in the aggregates, (d) *R*-/*S*-2 in the aggregates (1.0×10^{-5} M, $\lambda_{\text{ex}}=350$ nm).

9. g_{lum} of N*-LCs

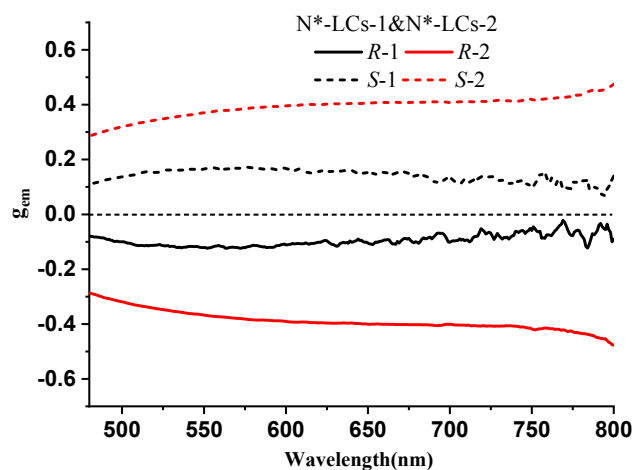


Fig. S6 g_{lum} of N*-LCs of 5CB doped with 0.5 mol% *R*-/*S*-1 and *R*-/*S*-2 in flat LC cells at 30°C. ($\lambda_{\text{ex}} = 350$ nm).

10. CPL signals of N*-LCs with different dopants concentration

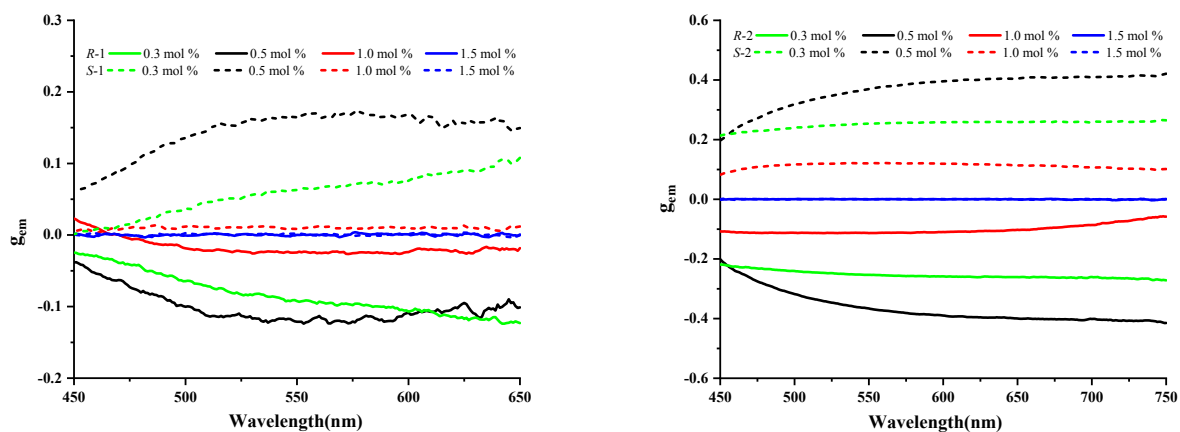


Fig. S7 CPL spectra of N*-LCs ($\lambda_{\text{ex}}=350$ nm). (a) N*-LCs of 5CB doped with 0.3, 0.5, 1.0, 1.5 mol % *R*-/*S*-1 in flat LC cells at 30°C. (b) N*-LCs of 5CB doped with 0.3, 0.5, 1.0, 1.5 mol % *R*-/*S*-2 in flat LC cells at 30°C.

11. ^1H NMR and ^{13}C NMR spectra of compounds

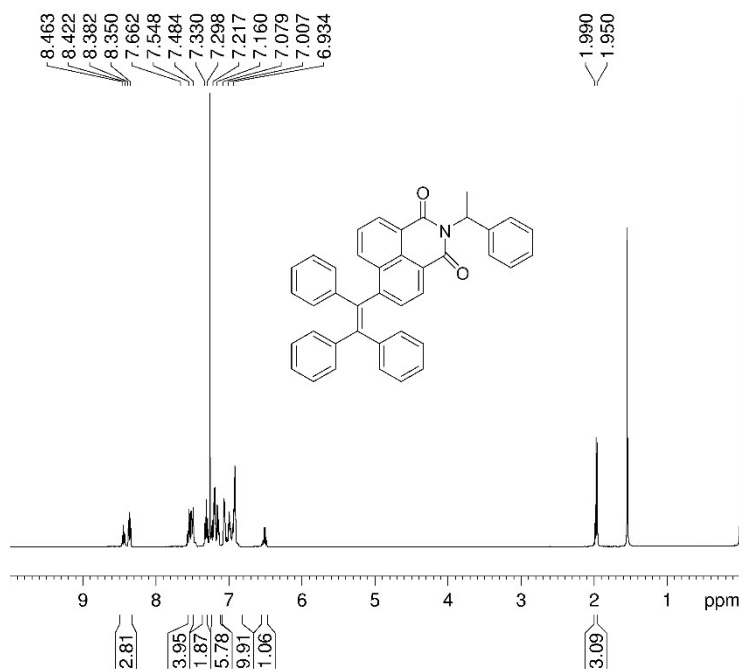


Fig. S8 ^1H NMR of *R-/S-1* (400 MHz, CDCl_3).

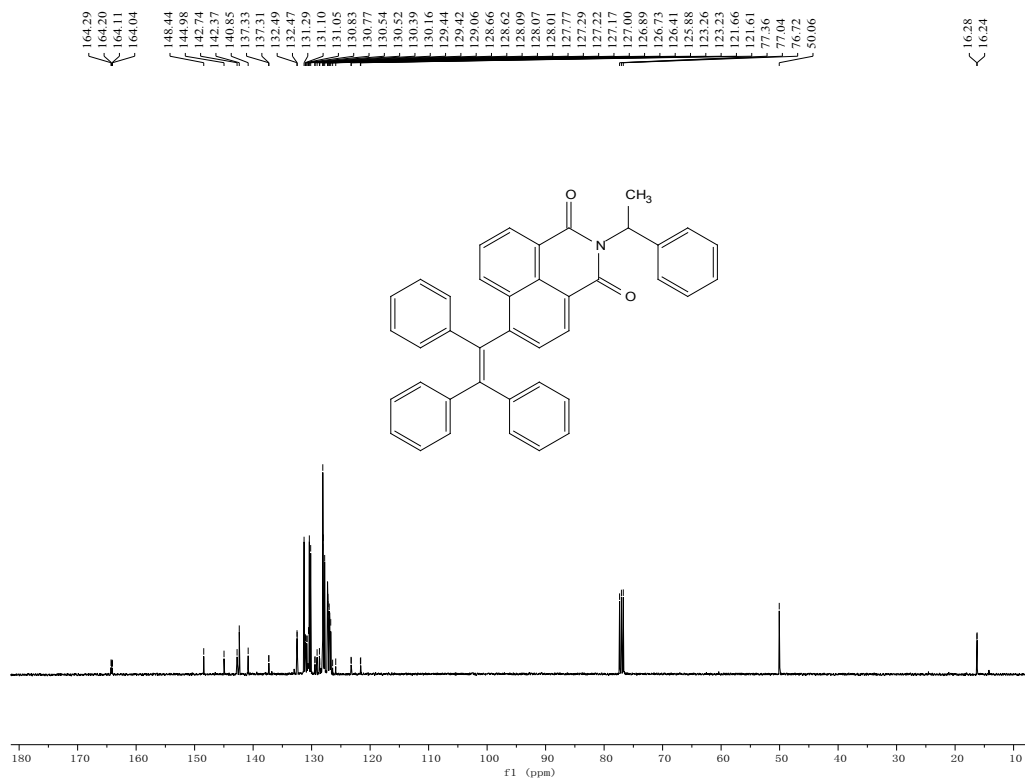


Fig. S9 ^{13}C NMR of *R-/S-1* (100 MHz, CDCl_3).

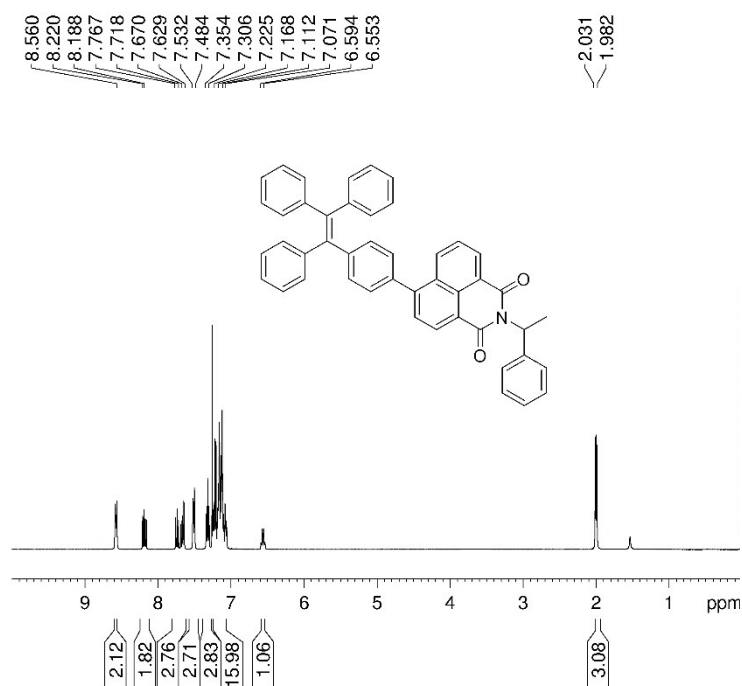


Fig. S10 ¹H NMR of *R-/S-2* (400 MHz, CDCl₃).

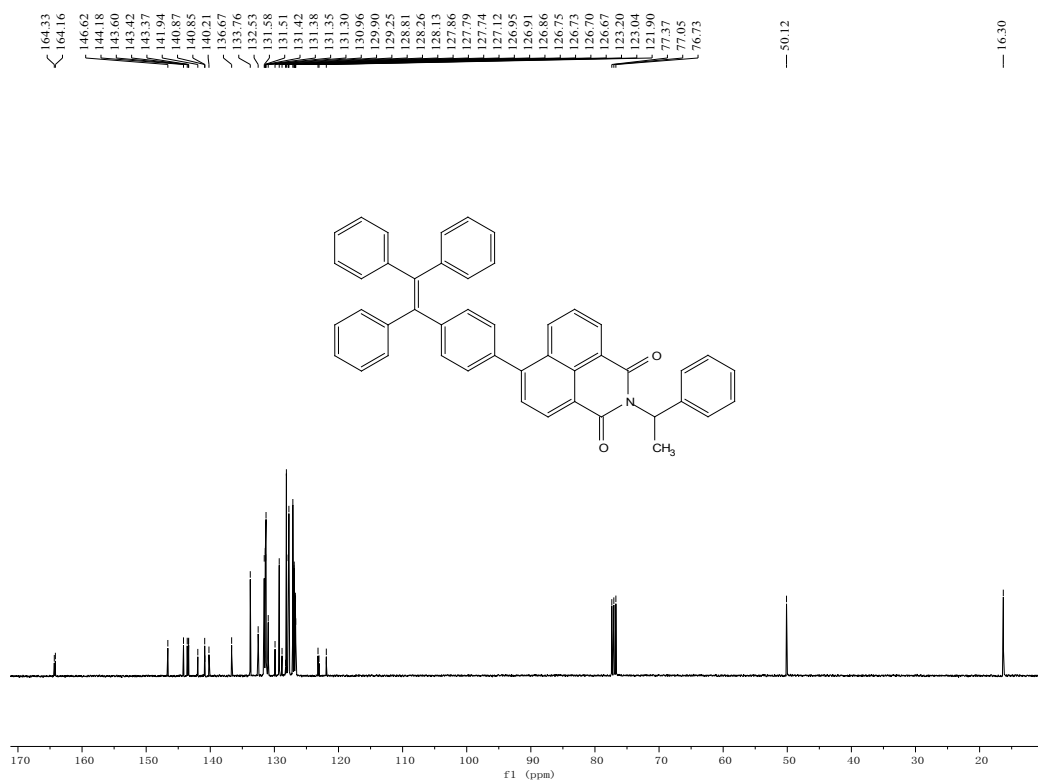


Fig. S11 ¹³C NMR of *R-/S-2* (100 MHz, CDCl₃).

12. References

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