Electronic Supplementary Information

Luminescent chiral triangular prisms capable of forming double helices for detecting traces of acids and anion recognition

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Experimental Procedures

Section A. General Information

All commercially available reagents were used without further purification. Anhydrous THF was prepared on a solvent drying system. All CH_2Cl_2 and $CHCl_3$, unless otherwise stated, were deacidified with potassium carbonate (K_2CO_3) for 24 h, and the remaining K_2CO_3 was removed by filtration. Thin layer chromatography (TLC) was performed on silica gel HSGF254 (Huang Hai, China). Column chromatography was carried out using 300−400 mesh silica gel (Huang Hai, China).

Nuclear Magnetic Resonance Spectroscopy (NMR): Solution NMR spectra were recorded on Bruker AVANCE NEO 500 MHz (equipped with Bruker 5 mm direct broadband BBFO RT Probe and BBO CryoProbe) with working frequencies of 500 MHz for ^1H, as well as 126 MHz for ^{13}C nuclei. $CDCl_3$ was used as the deuterated solvent. Chemical shifts are reported in ppm relative to the resonances corresponding to the residual non-deuterated solvents ($CDCl_3$: δ_H = 7.26 ppm for ^1H NMR and δ_C = 77.16 ppm for ^{13}C NMR). The resonances have been designated as follows: s (singlet), d (doublet), m (multiplet), spin coupling constant *J* (Hz). All spectra were processed with Bruker TopSpin 4.0.7 software.

High-Resolution Mass Spectrometry (HRMS): HRMS spectra were measured on a Waters Synapt-G2-Si Electrospray Ionization Time-of-Flight (ESI-TOF) mass spectrometer.

Infrared Spectroscopy (IR): IR-Spectra were recorded on a Nicolet iS50 FTIR micro spectrometer.

Melting points (Mp.): The non-corrected melting points were determined with a SGW X-4A micromelting point meter.

Single-Crystal X-Ray Crystallography: Single-crystal X-ray diffraction (SCXRD) data were collected on a Bruker D8 Venture diffractometer with PHOTON III detector in shutterless mode with an incoatec microfocus source (Mo-Diamond K_α radiation, λ = 0.71073 Å) equipped with an Oxford 800 Plus liquid nitrogen vapor cooling device.

Fluorescence Spectroscopy: Fluorescence spectra were recorded on an FS5 Fluorescence Spectrometer (Edinburgh Instruments Ltd., Livingston) using a 1-cm quartz cell in the wavelength range of 200–900 nm. Unless otherwise stated, all experiments were carried out at room temperature. All PL spectra were collected at excitation wavelength of 380 nm. The dwelling time for each curve is 0.2 s, while the measuring time is 81 s.

Photoluminescence Lifetime and Quantum Efficiency: The lifetime and photoluminescence quantum efficiency were obtained on an Edinburgh steady state and time-resolved Photoluminescence Spectrometer (FLS1000+FS5) at room temperature. The concentrations of **(*R*)-** and **(*S*)-Δ** in $CHCl_3$ are 1×10^{-5} M and 1×10^{-6} M, respectively.

UV-Vis Spectroscopy: UV-vis absorption measurements were performed on a SHIMADZU UV-2700 spectrometer making use of conventional quartz cells with 1 cm pathlength. The slit width was set to be 2 nm. All absorbance spectra were recorded at room temperature.

Circular Dichroism Spectroscopy (CD): CD spectra were collected on a Chirascan V100 spectrometer at room temperature. The concentrations of **(*R*)-** and **(*S*)-Δ** in $CHCl_3$

are 2×10^{-4} M.

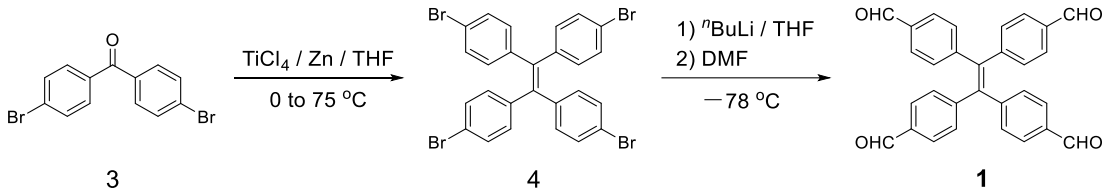
Circularly Polarized Luminescence Spectroscopy (CPL): CPL spectra were measured on a JASCO CPL-300 at room temperature. The concentration of **(*R*)-** and **(*S*)-Δ** in $CHCl_3$ is 2×10^{-4} M.

Crystal Photography: The crystal photos were taken by a BKL-AL20 Honor V10 phone and microscope under ambient conditions.

Section B. Syntheses of (*R*)- and (*S*)-Δ

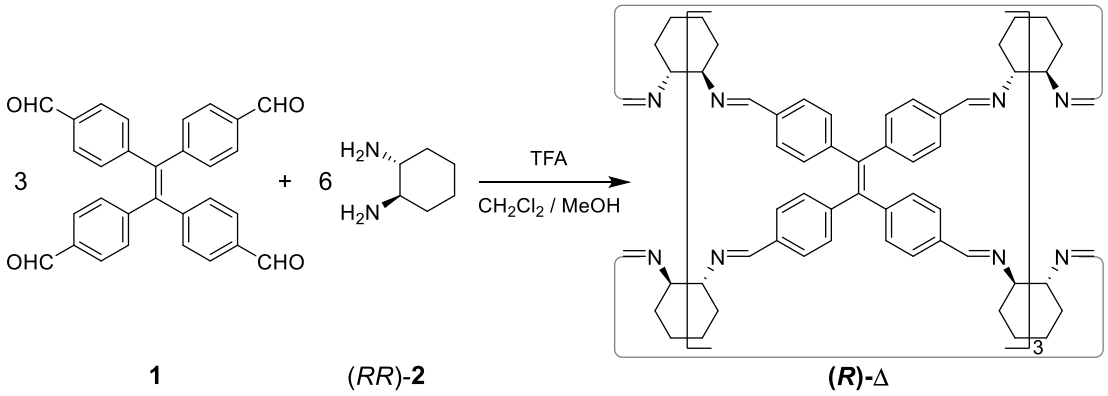
1. Synthetic Details

Scheme S1 Synthesis of Compound **1**.



Tetrakis(4-bromophenyl)ethylene (**4**) and tetrakis(4-benzaldehyde)ethylene (**1**) were synthesized according to a reported procedure [1].

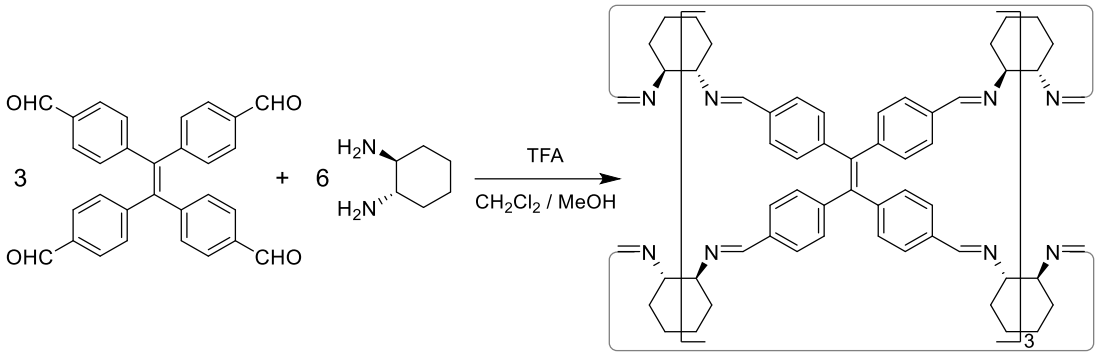
Scheme S2 Synthesis of **(*R*)-Δ**.



(*R*)-Δ. A solution of (1*R*,2*R*)-diaminocyclohexane ((*RR*)-**2**, 45.6 mg, 0.4 mmol) in a mixed anhydrous solvent of CH_2Cl_2/MeOH (1:1, 6 mL) was added to a solution of **1** (88 mg, 0.2 mmol) in anhydrous CH_2Cl_2/MeOH (1:1, 28 mL) under an N_2 atmosphere. Catalytic amounts of trifluoroacetic acid (TFA) were added to the mixture and left to stand at room temperature. After 12 days, small yellow crystals appeared. The resulting yellow crystals were collected by filtration, and then dried. The remaining solid was recrystallized from $CHCl_3$ and MeOH to afford **(*R*)-Δ** as yellow crystals (118 mg) in 88% yield. Mp. > 280 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ_H = 7.82 (s, 2H, H*7*), 7.76 (s, 2H, H*7*), 7.32 (d, *J* = 8.5 Hz, 4H, H*8*), 7.03 – 6.95 (m, 8H, H*9* and H*11*), 6.91 (d, *J* = 8.5 Hz, 4H, H*10*), 3.34 – 3.08 (m, 4H, H*1* and H*6*), 2.20 – 1.39 (m, 16H, H*2*,

H*3*, H*4*, and H*5*); ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) δ_C = 164.2, 161.7, 144.6, 144.3, 140.1, 135.4, 134.7, 131.5, 131.4, 127.3, 126.8, 73.2, 71.9, 32.5, 32.4, 24.5, 24.3; ESI-HRMS Calcd for $C_{126}H_{120}N_{12}$: *m/z* = 901.4957 $[M + 2H]^{2+}$; found: 901.4970.

Scheme S3 Synthesis of **(*S*)-Δ**.



1 (*SS*)-**2** **(*S*)-Δ**

(*S*)-Δ. The enantiomer **(*S*)-Δ** (120 mg) was obtained in 90% yield from (1*S*,2*S*)-diaminocyclohexane ((*SS*)-**2**, 45.6 mg, 0.4 mmol) and **1** (88 mg, 0.2 mmol) following the same procedure as that described above for **(*R*)-Δ**. Mp. > 280 °C. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ_H = 7.82 (s, 2H, H*7*), 7.76 (s, 2H, H*7*), 7.32 (d, *J* = 8.5 Hz, 4H, H*8*), 7.04 – 6.95 (m, 8H, H*9* and H*11*), 6.91 (d, *J* = 8.5 Hz, 4H, H*10*), 3.33 – 3.08 (m, 4H, H*1* and H*6*), 2.20 – 1.39 (m, 16H, H*2*, H*3*, H*4* and H*5*); ^{13}C NMR (126 MHz, $CDCl_3$, 298 K) δ_C = 164.2, 161.7, 144.6, 144.3, 140.1, 135.4, 134.7, 131.5, 131.4, 127.3, 126.8, 73.2, 71.9, 32.5, 32.4, 24.5, 24.3; ESI-HRMS Calcd for $C_{126}H_{120}N_{12}$: *m/z* = 901.4957 $[M + 2H]^{2+}$; found: 901.4926.

2. NMR Spectroscopy

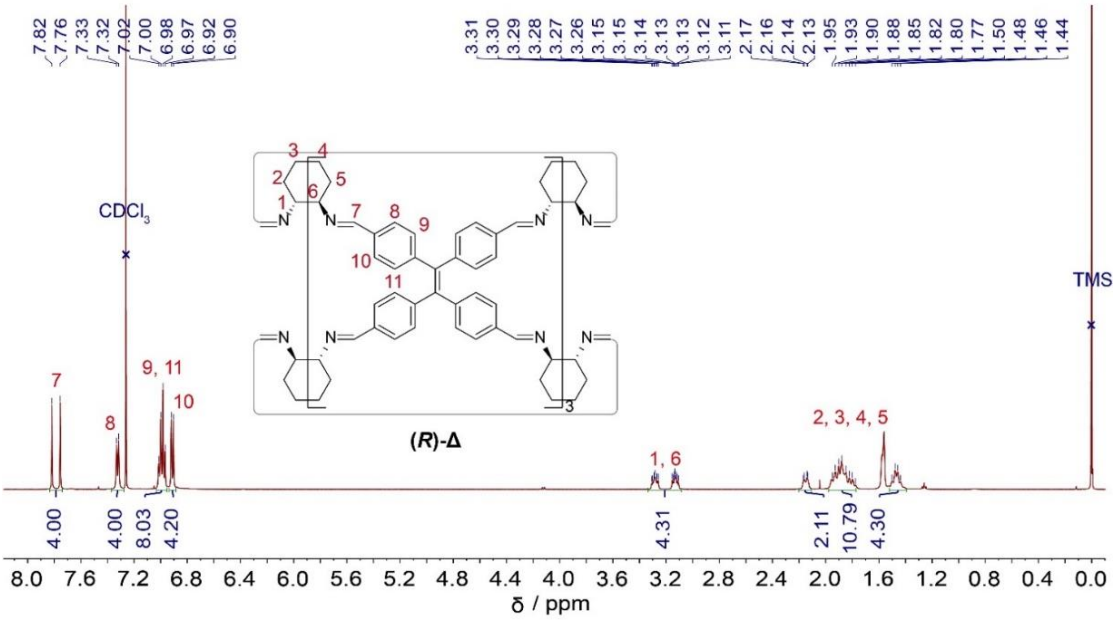


Figure S1 ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298K) of **(*R*)-Δ**.

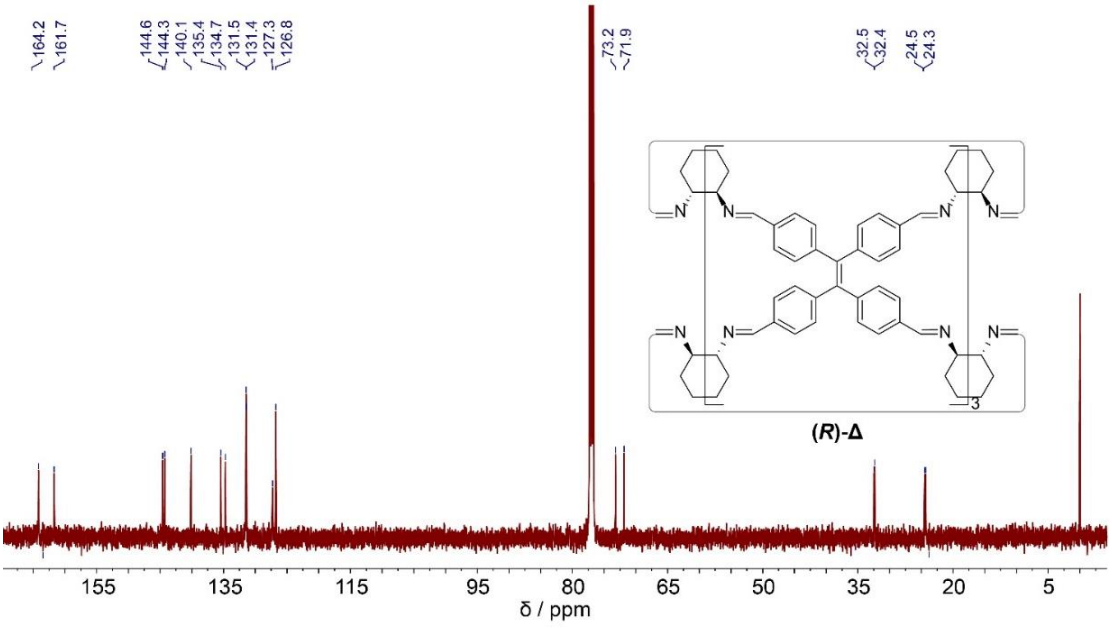


Figure S2 ^{13}C NMR spectrum (126 MHz, $CDCl_3$, 298K) of **(*R*)-Δ**.

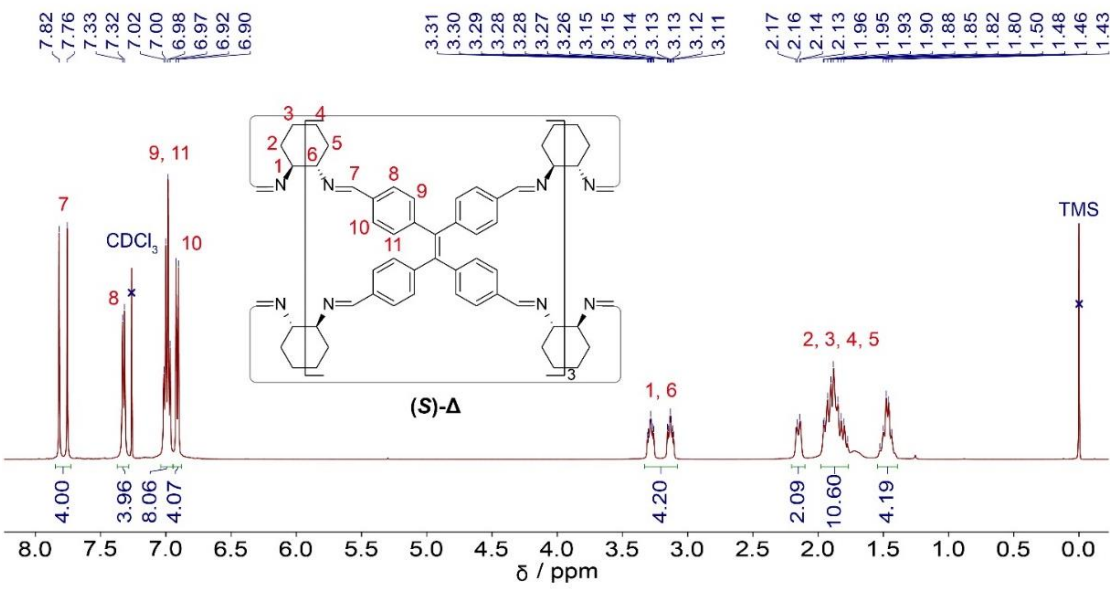


Figure S3 ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298K) of **(*S*)-Δ**.

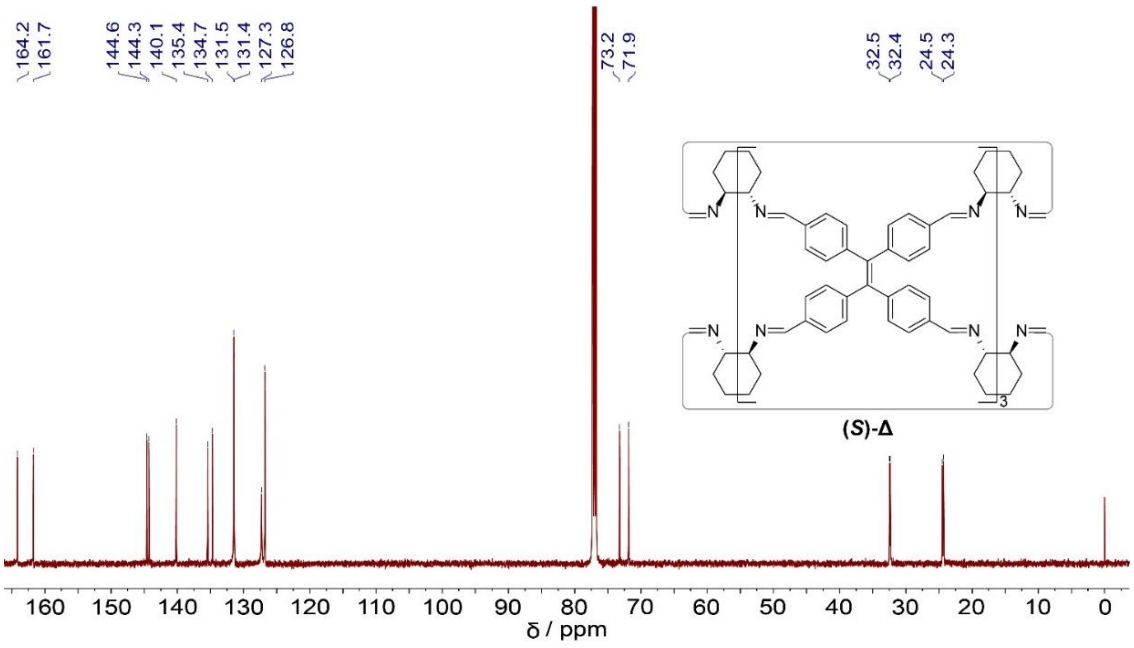


Figure S4 ^{13}C NMR spectrum (126 MHz, $CDCl_3$, 298K) of **(*S*)-Δ**.

3. High-Resolution Mass Spectrometry

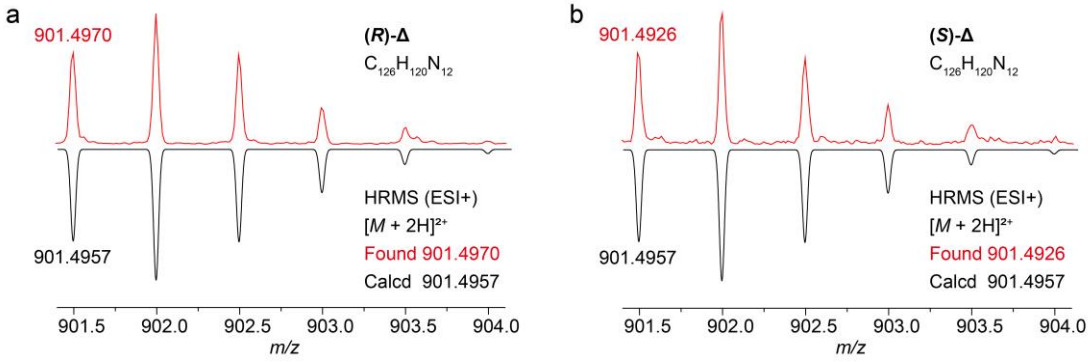


Figure S5 HRMS spectra of (a) **(*R*)-Δ** and (b) **(*S*)-Δ**. The experimentally obtained isotopic distribution patterns (red) for **(*R*)-Δ** ($[M + 2H]^{2+}$) and **(*S*)-Δ** ($[M + 2H]^{2+}$) correlate well with the calculated patterns (black), respectively.

4. Infrared Spectroscopy

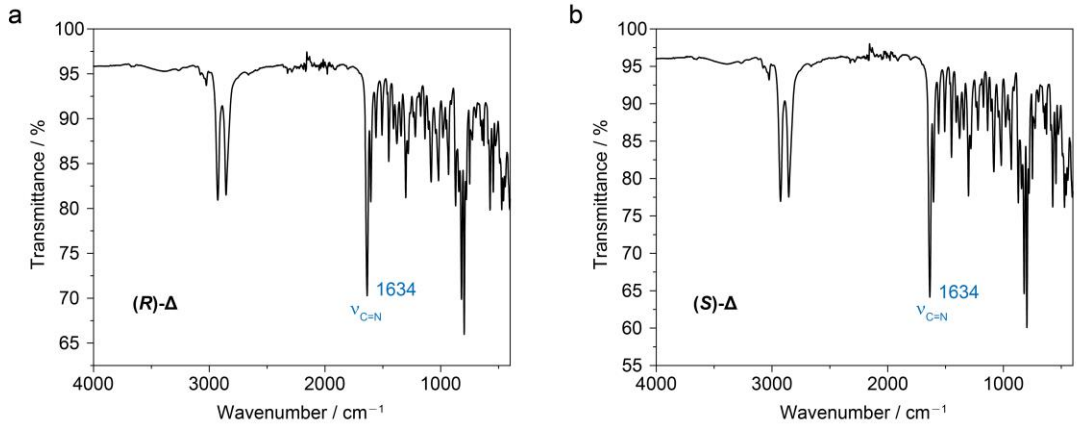


Figure S6 IR spectra of (a) **(*R*)-Δ** and (b) **(*S*)-Δ** in solid states.

Section C. Single-Crystal X-ray Crystallography of (*R*)- and (*S*)-Δ

Single crystals of (*R*)- and (*S*)-Δ

Single crystals of **(*R*)-** and **(*S*)-Δ** were obtained as regular yellow blocks by slow liquid-liquid diffusion of MeOH into a $CHCl_3$ solution at room temperature for two days.

Single-crystal-to-single-crystal transformation of (*R*)-Δ to [I_3^-⊂(*R*)-Δ]

A saturated solution of tetrabutylammonium triiodide ($TBAI_3$) in MeOH was added to crystals of **(*R*)-Δ** within mother liquor, and allowed to diffuse for one day to afford the inclusion complex **[I_3^-⊂(*R*)-Δ]** as regular purplish black block crystals.

X-Ray diffraction (XRD) measurements were performed on a Bruker D8 Venture diffractometer with PHOTON III detector in shutterless mode with an incoatec microfocus source (Mo-Diamond K_α radiation, $\lambda = 0.71073$ Å) equipped with an Oxford 800 Plus liquid nitrogen vapor cooling device. All data were collected at 100 K. The computing indexing, cell refinement and data reduction were processed using APEX3 software. Frame integration, including Lorentz-polarization corrections, and final cell-parameter calculations were processed with SAINT software. The data were corrected for absorption with SADABS program. Structures were solved using direct methods with SHELXT,[2] subsequent difference Fourier calculations and full-matrix least-squares refinement against F^2 were performed with SHELXL [2]. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were inserted in calculated positions and refined with a riding model.

Refinement Details. Refinement of F^2 against all reflections. The weighted *R*-factor

wR and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) etc., and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on all data will be even larger.

For the single-crystal X-ray structure of the inclusion complex **[I_3^-⊂(*R*)-Δ]**, the squeeze procedure in PLATON was used to remove electronic contributions from disordered solvent molecules and the $[Bu_4N]^+$ cations. Total solvent accessible volume / cell = 6413 $Å^3$, Total electron count / cell =1213.

All crystallographic data for the structures reported here have been deposited on to the Cambridge Crystallographic Data Centre (CCDC) and can be downloaded free of charge from www.ccdc.cam.ac.uk/data_request/cif. Crystallographic information and structural parameter details are summarized in **Table S1**.

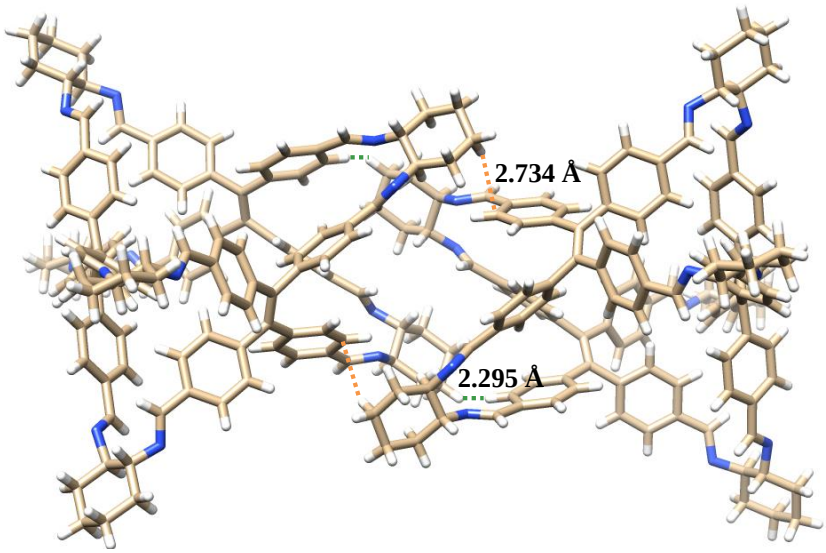


Figure S7 Non-covalent bonding interactions between two adjacent **(*R*)-Δ** in its single-crystal X-ray superstructure. Orange and green dashed lines indicate [C–H···π] and [C–H··· H–C] interactions, respectively.

Table S1 Crystal data and structure refinement for **(*R*)-Δ**, **(*S*)-Δ**, and **[I_3^-⊂(*R*)-Δ]**.

Parameter	**(*R*)-Δ**	**(*S*)-Δ**	**[I_3^-⊂(*R*)-Δ]**
Empirical formula	$C_{126}H_{120}N_{12}$	$C_{126}H_{120}N_{12}$	$C_{126}H_{120.12}I_{0.37}N_{12}$
Molecular weight	1802.33	1802.33	1849.96
T / K	100(2)	100.15	100(2)
Crystal system	cubic	cubic	cubic
Space group	*P*23	*P*23	*P*23
$a = b = c$ / Å	25.0321(16)	25.0680(9)	25.0940(2)
V / Å^3	15685(3)	15753(2)	15802(4)
Z	4	4	4
ρ_{calc} / mg mm^{-3}	0.763	0.760	0.778
μ / mm^{-1}	0.045	0.045	0.118
F(000)	3840	3840	3920
Crystal size / mm^3	0.3 × 0.2 × 0.1	0.3 × 0.2 × 0.1	0.2 × 0.2 × 0.1
2θ range for data collection / °	3.638 to 50.684	3.632 to 48.794	1.988 to 27.735
Index ranges	$-30 \le h \le 29$ $-29 \le k \le 29$ $-29 \le l \le 29$	$-29 \le h \le 29$ $-29 \le k \le 29$ $-29 \le l \le 29$	$-32 \le h \le 32$ $-32 \le k \le 27$ $-32 \le l \le 26$
Reflections collected	612717	433046	59252
Independent reflections	9486 [R(int) = 0.1726]	8656 [R(int) = 0.0695]	12252 [R(int) = 0.0609]
Data / restraints / parameters	9486 / 5 / 368	8656 / 1 / 416	12252 / 92 / 438
Goodness-of-fit on F^2	1.040	1.078	0.998
Final R indexes [I>2σ (I)]	R_1 = 0.0951 wR_2 = 0.2797	R_1 = 0.0492 wR_2 = 0.1489	R_1 = 0.0740 wR_2 = 0.2134
Final R indexes [all data]	R_1 = 0.1397 wR_2 = 0.3322	R_1 = 0.0543 wR_2 = 0.1542	R_1 = 0.0966 wR_2 = 0.2323
Largest diff. peak/hole / e Å^{-3}	0.28 / −0.26	0.19 / −0.17	0.56 / −0.27
CCDC No	2114993	2114994	2114992

Section D. Photophysical Properties of (*R*)- and (*S*)-Δ

1. UV-Vis Absorption and Steady-State Photoluminescence (PL) Spectra of (*R*)- and (*S*)-Δ

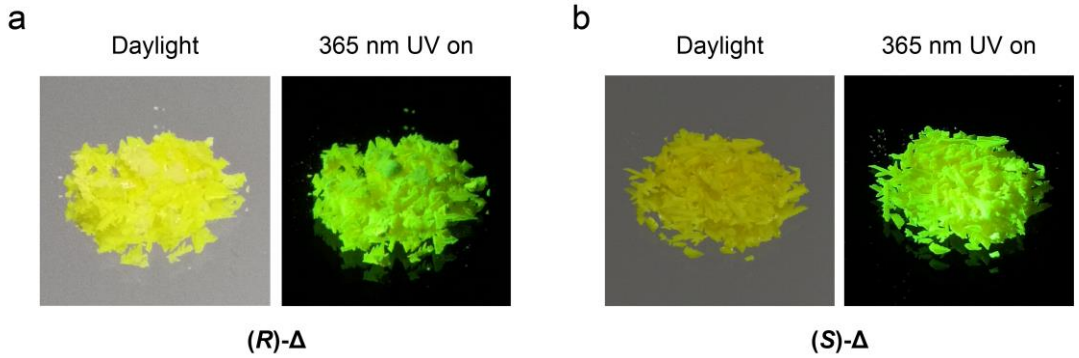


Figure S8 Colors of crystalline powders of (a) **(*R*)-Δ** and (b) **(*S*)-Δ** under daylight (left) and 365 nm UV lamp (right).

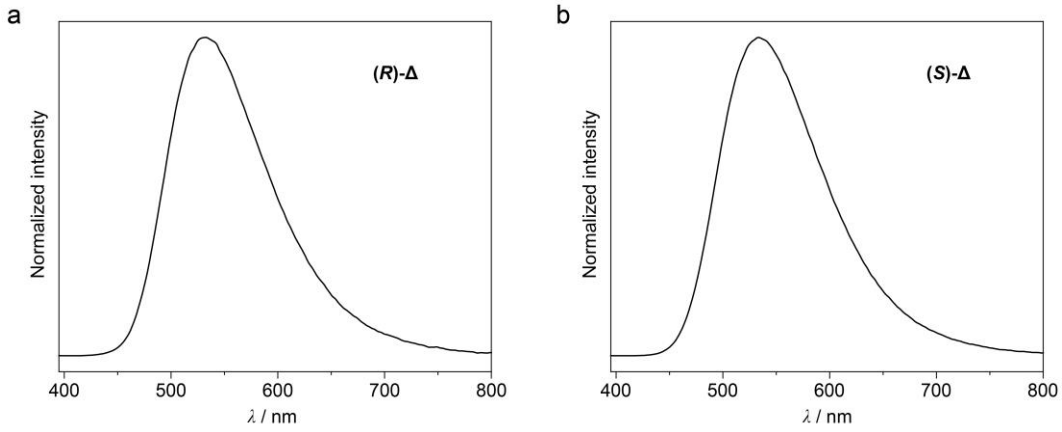


Figure S9 Steady-state PL spectra of crystals of (a) **(*R*)-Δ** and (b) **(*S*)-Δ** upon excitation at 380 nm.

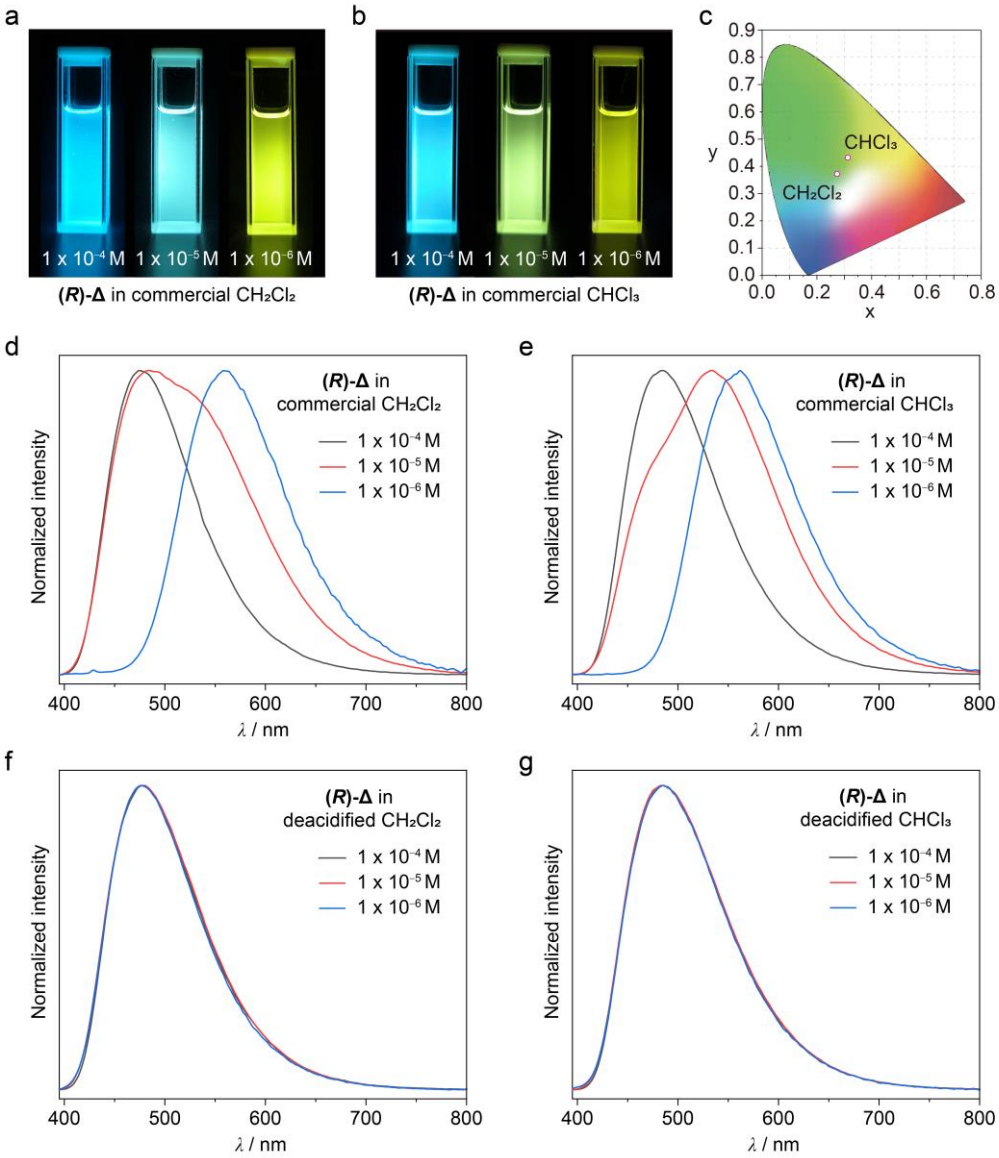


Figure S10 (a) and (b) Luminescence photographs of solutions of **(*R*)-Δ** in commercial grade (a) CH_2Cl_2 and (b) $CHCl_3$ at different concentrations upon 365 nm UV light irradiation. (c) PL colors in the CIE coordinate diagram of solutions of **(*R*)-Δ** in commercial grade CH_2Cl_2 and $CHCl_3$ (1×10^{-5} M). (d)–(g) Steady-state PL spectra of solutions of **(*R*)-Δ** in commercial grade (d) CH_2Cl_2 and (e) $CHCl_3$ as well as in deacidified (f) CH_2Cl_2 and (g) $CHCl_3$ at different concentrations upon excitation at 380 nm. Commercial grade CH_2Cl_2 and $CHCl_3$ were deacidified with K_2CO_3 for 24 h, and the remaining K_2CO_3 was removed by filtration.

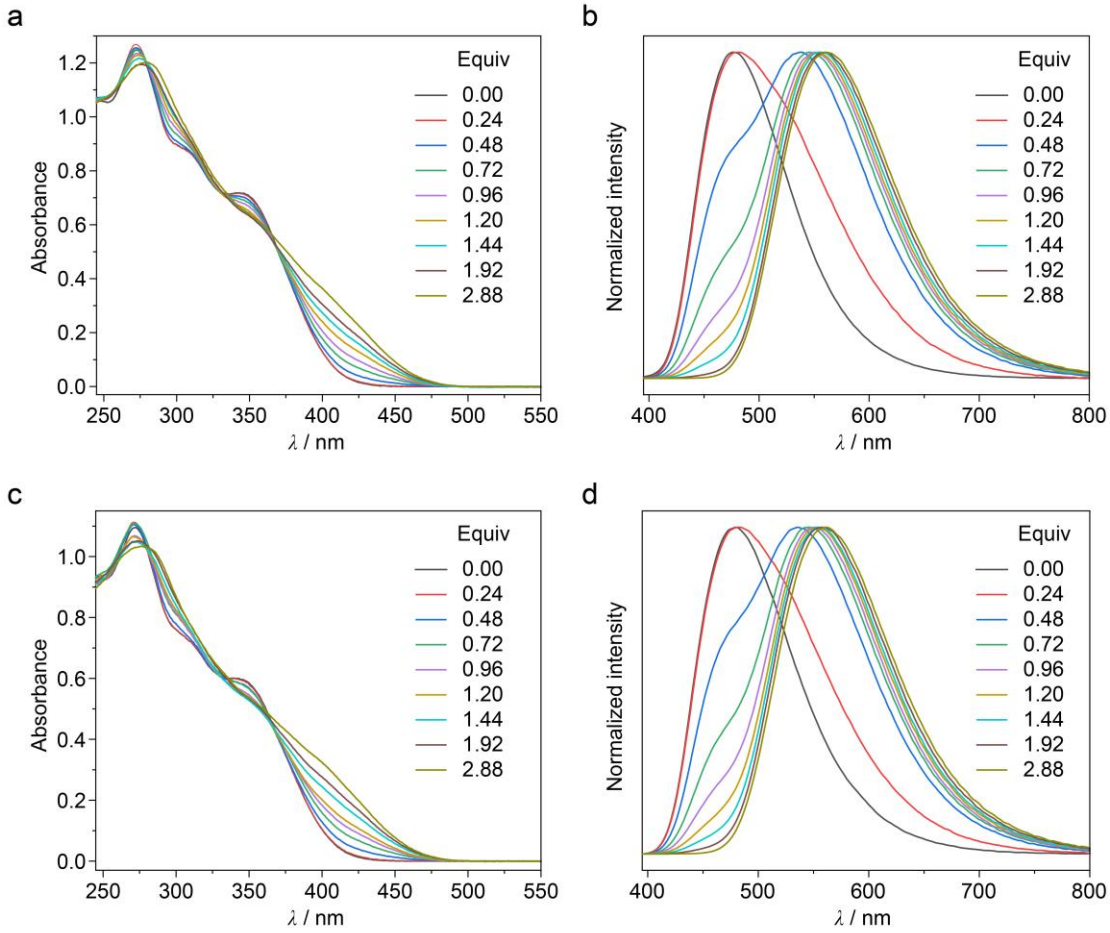


Figure S11 UV-Vis absorption spectra of solutions of (a) **(*R*)-** and (c) **(*S*)-Δ** in deacidified $CHCl_3$ upon adding different amounts of TFA ranging from 0 to 2.88 equiv relative to **(*R*)-** and **(*S*)-Δ**, respectively. Steady-state PL spectra of (b) **(*R*)-Δ** and (d) **(*S*)-Δ** in the same solutions upon excitation at 380 nm. Concentrations of **(*R*)-** and **(*S*)-Δ** are 1×10^{-5} M.

2. Photoluminescence Lifetime and Quantum Efficiency of (*R*)- and (*S*)-Δ

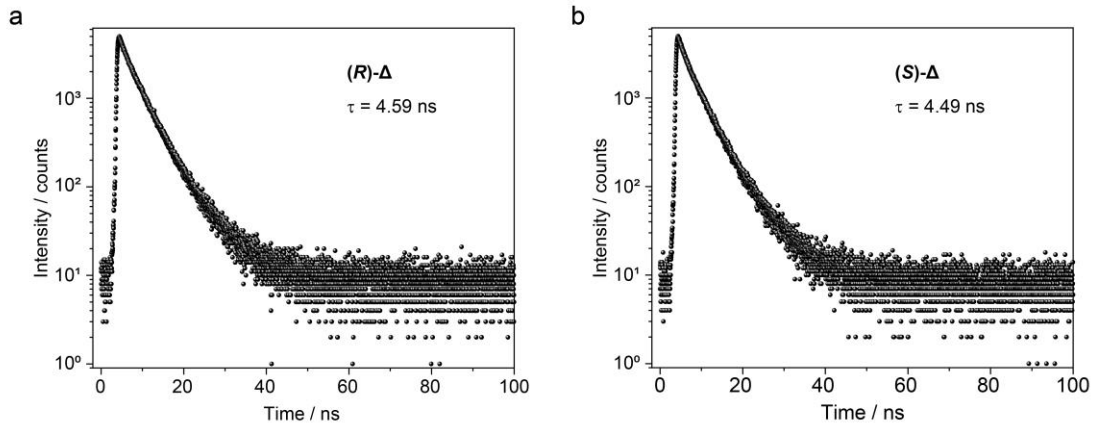


Figure S12 Lifetime decay profiles of the fluorescence emission bands of (a) **(*R*)-Δ**, and (b) **(*S*)-Δ** at 530 nm.

Table S2 Photoluminescence lifetime (τ) of crystals of **(*R*)-** and **(*S*)-Δ**. <τ> represents the average τ.

Compound	Wavelength / nm	τ_1 / ns	A_1 / %	τ_2 / ns	A_2 / %	<τ> / ns
(*R*)-Δ	530	3.10	51.44	6.16	48.56	4.59
(*S*)-Δ	530	2.79	44.89	5.89	55.11	4.49

Table S3 Photoluminescence quantum efficiency (Φ) of crystals of **(*R*)-** and **(*S*)-Δ**.

Compound	Φ / %
(*R*)-Δ	27.66
(*S*)-Δ	26.21

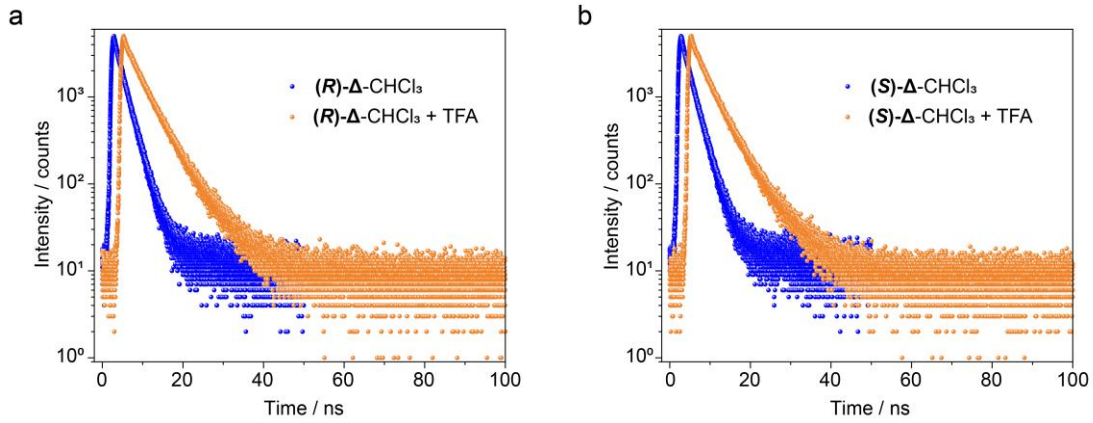


Figure S13 Lifetime decay profiles of the fluorescence emission bands of (a) **(*R*)-Δ** in deacidified $CHCl_3$ (blue curve) at 477 nm and in deacidified $CHCl_3$ containing TFA (2.88 equiv relative to **(*R*)-Δ**, orange curve) at 561 nm, and (b) **(*S*)-Δ** in deacidified $CHCl_3$ (blue curve) at 478 nm and in deacidified $CHCl_3$ containing TFA (2.88 equiv relative to **(*S*)-Δ**, orange curve) at 552 nm all at the same concentration of 1×10^{-5} M.

Table S4 Photoluminescence lifetime (τ) of **(*R*)-** and **(*S*)-Δ** in deacidified $CHCl_3$ and $CHCl_3$ containing TFA (2.88 equiv relative to **Δ**). <τ> represents the average τ.

Compound	Solvent	Wavelength	τ_1	A_1	τ_2	A_2	<τ>
		nm	ns	%	ns	%	ns
(*R*)-Δ	$CHCl_3$	477	2.30	97.30	1.81	2.70	2.29
	$CHCl_3$ + TFA	561	3.56	56.51	6.57	43.49	4.87
(*S*)-Δ	$CHCl_3$	478	2.30	96.95	9.61	3.05	2.52
	$CHCl_3$ + TFA	552	3.13	47.56	6.20	52.44	4.83

Table S5 Photoluminescence quantum efficiency (Φ) of **(*R*)-** and **(*S*)-Δ** in deacidified $CHCl_3$ and in $CHCl_3$ containing TFA (2.88 equiv relative to **Δ**).

Compound	Solvent	Φ / %
(*R*)-Δ	$CHCl_3$	25.51
	$CHCl_3$ + TFA	27.84
(*S*)-Δ	$CHCl_3$	23.44
	$CHCl_3$ + TFA	25.05

3. Time-Dependent DFT (TD-DFT) Calculation of (*R*)-Δ and the Protonated (*R*)-Δ

All density-functional theory (DFT) calculations were performed with the Gaussian 16 Rev. A.03 quantum chemistry package. Geometry optimizations and frontier molecular orbitals calculations of all compounds employed the B3LYP levels of theory under vacuum condition 6-31G(d) basis sets.

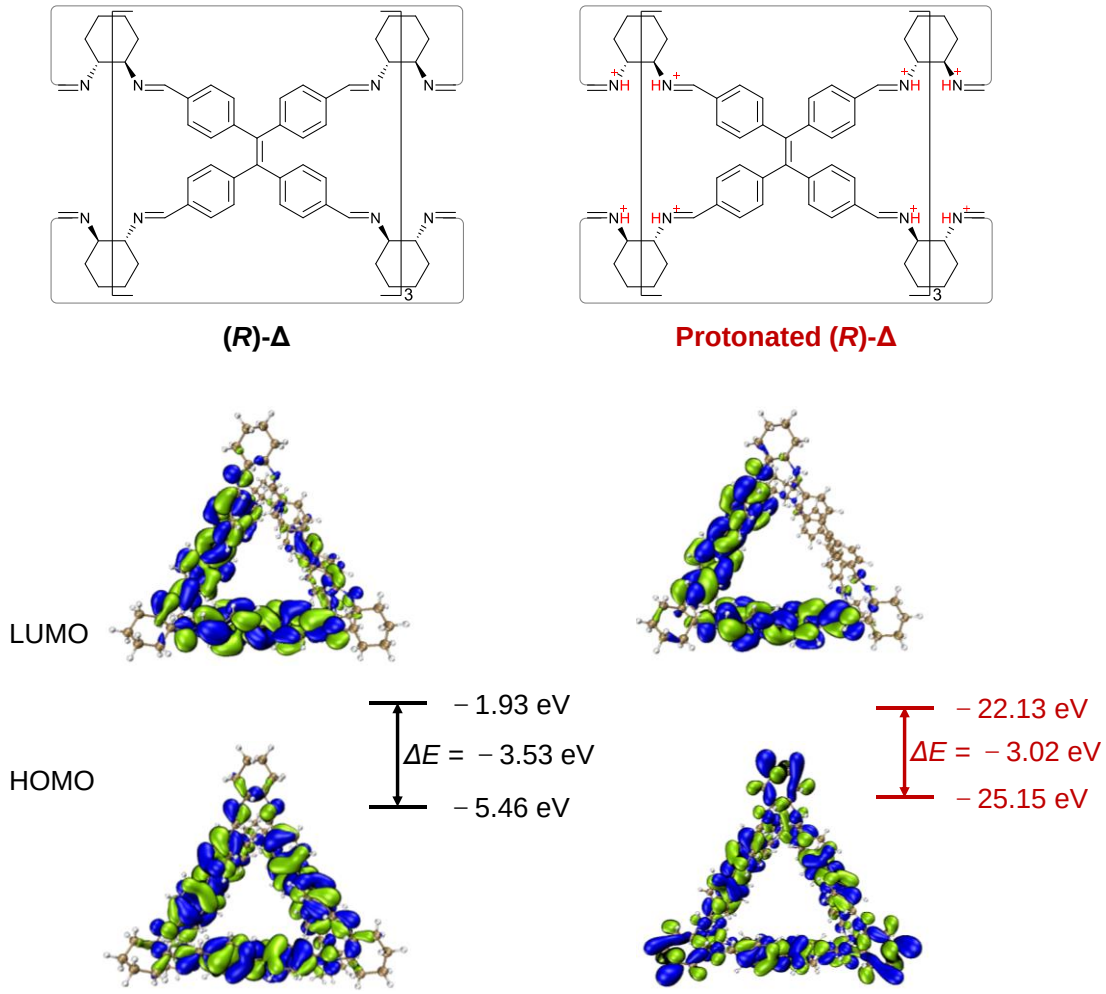


Figure S14 Structural formulas and frontier molecular orbitals (including HOMO and LUMO energy levels) of **(*R*)-Δ** and the protonated **(*R*)-Δ**.

Table S6 Cartesian coordinates of **(*R*)-Δ**.

No	atom	x	y	z	No	atom	x	y	z
1	N	7.011213	-2.524499	4.131816	130	H	-6.578802	-2.316715	3.646888
2	N	7.228529	0.39787	4.475856	131	C	-5.714855	-0.887497	2.27924
3	N	-3.61069	6.518687	-4.131038	132	H	-6.337215	-0.067243	2.626084
4	N	-0.760761	7.200095	-4.476772	133	C	-5.172338	-4.571953	2.990962
5	C	-1.373259	6.765353	2.990962	134	H	-4.751314	-5.374389	2.366429
6	H	-2.278701	6.801953	2.366429	135	C	-4.708948	4.084365	-2.85757
7	C	-0.255626	5.99087	2.421159	136	H	-5.324837	4.503088	-3.647431
8	C	1.069977	6.142173	2.857011	137	C	-5.025467	2.859807	-2.280109
9	H	1.283067	6.855767	3.646888	138	H	-5.898676	2.314371	-2.627179
10	C	1.826648	4.469989	1.246132	139	C	-3.100779	3.022945	-0.837621
11	C	7.826284	-0.555725	5.394308	140	H	-2.460814	2.609045	-0.064617
12	H	7.117821	-0.859769	6.185991	141	N	-3.840003	-6.386292	-4.131038
13	C	8.2148	-1.84075	4.596283	142	C	-3.687943	-5.834626	-2.99064
14	H	8.833663	-1.502399	3.747814	143	H	-4.547087	-5.546539	-2.366073
15	C	0.493474	4.303494	0.837155	144	C	-2.367854	-5.507715	-2.421367
16	H	0.258747	3.578294	0.064252	145	C	-5.205028	-6.617103	-4.595026
17	C	2.320383	4.197918	-1.705114	146	H	-5.898384	-6.744823	-3.746313
18	C	-0.52549	5.059552	1.408768	147	C	-7.085314	-5.669941	-6.036824
19	H	-1.553546	4.912471	1.08968	148	H	-7.823796	-5.775422	-5.230726
20	C	2.073945	5.584652	-1.670615	149	H	-7.390573	-4.796566	-6.626355
21	H	2.518196	6.183859	-0.882041	150	C	-4.146858	8.993135	6.905248
22	C	4.120066	2.516457	-1.246904	151	H	-3.575382	8.616133	7.766035
23	C	2.088833	5.392958	2.27924	152	H	-5.020368	9.515293	7.315373
24	H	3.110373	5.52181	2.626084	153	C	-3.269699	9.959245	6.098365
25	C	9.861713	-0.905283	6.905248	154	H	-2.909075	10.775839	6.736232
26	H	9.249481	-1.211695	7.766035	155	H	-3.875491	10.425067	5.307202
27	H	10.750669	-0.409881	7.315373	156	N	-1.319326	7.334138	4.131816
28	C	2.939755	3.65037	0.672145	157	C	-2.513263	8.0346	4.596283
29	C	9.072884	0.082648	6.036989	158	H	-3.115716	8.401376	3.747814
30	H	9.712519	0.466676	5.230971	159	C	-2.788484	4.252864	-1.408972
31	H	8.7573	0.953057	6.625473	160	H	-1.898769	4.788365	-1.089627
32	C	4.168337	1.173881	-0.837621	161	C	-5.222443	-7.882187	-5.468979
33	H	3.489906	0.826605	-0.064617	162	H	-4.898659	-8.734298	-4.858791
34	C	3.773507	2.961282	1.704195	163	H	-4.467617	-7.761955	-6.257851
35	C	3.133632	3.484856	-0.672996	164	C	-7.07259	-6.935129	-6.903591
36	C	5.257944	1.515626	3.636095	165	H	-8.074615	-7.113133	-7.313625
37	C	5.077331	0.288466	-1.408972	166	H	-6.404326	-6.786928	-7.764478
38	H	5.096231	-0.7498	-1.089627	167	C	-6.596263	-8.148999	-6.095224
39	C	9.026771	-2.809618	5.471756	168	H	-6.549517	-9.041235	-6.731994
40	H	9.314604	-3.67527	4.862606	169	H	-7.328103	-8.368004	-5.303797
41	H	8.365036	-3.192558	6.260429	170	C	-2.080185	9.222222	5.471756

42	C	3.859569	1.580504	3.70779	171	H	-1.474425	9.904319	4.862606
43	H	3.338573	1.045213	4.498593	172	H	-1.417682	8.840613	6.260429
44	C	10.259809	-2.14798	6.098365	173	C	3.799478	-4.588415	-1.670615
45	H	10.786688	-2.868586	6.736232	174	H	4.096281	-5.272752	-0.882041
46	H	10.966119	-1.856259	5.307202	175	C	4.376563	-3.285152	-3.63725
47	C	3.130919	2.29506	2.763439	176	C	2.111612	-3.256874	-2.764018
48	H	2.047513	2.319803	2.828584	177	H	1.090286	-2.894472	-2.828797
49	C	5.984768	0.657225	4.585945	178	C	5.361193	-2.741155	-4.586963
50	H	5.366666	0.205584	5.379459	179	H	4.944224	-2.09889	-5.380261
51	C	0.656744	5.432791	-3.63725	180	C	4.73414	-4.182082	-2.615142
52	C	5.891638	2.035886	-2.85757	181	H	5.758396	-4.538704	-2.571269
53	H	6.562207	2.3599	-3.647431	182	C	3.046623	-2.848124	-3.708495
54	C	1.76473	3.457147	-2.764018	183	H	2.75005	-2.162178	-4.498981
55	H	1.961543	2.391451	-2.828797	184	C	2.475312	-4.108469	-1.705114
56	C	-3.208963	6.111165	-2.99064	185	C	1.691435	-4.371087	0.672145
57	H	-2.5299	6.711162	-2.366073	186	C	1.451158	-4.456233	-0.672996
58	C	-0.306686	6.013507	-4.586963	187	N	6.615845	-2.941209	-4.476772
59	H	-0.65442	5.331268	-5.380261	188	N	-3.269699	-6.459025	4.475856
60	C	1.254719	6.190927	-2.615142	189	C	0.677792	-4.748594	1.704195
61	H	1.051435	7.256269	-2.571269	190	C	-1.316401	-5.311326	3.636095
62	C	5.181777	2.938621	1.669265	191	C	-0.561028	-4.132736	3.70779
63	H	5.702404	3.472457	0.880455	192	H	-0.764105	-3.413896	4.498593
64	C	-3.585895	4.804479	-2.421367	193	C	0.422121	-3.858986	2.763439
65	C	4.989399	2.922279	-2.280109	194	H	0.985252	-2.9331	2.828584
66	H	4.953642	3.951218	-2.627179	195	C	-2.42321	-5.511574	4.585945
67	C	5.910977	2.226459	2.613697	196	H	-2.505292	-4.750461	5.379459
68	H	6.995084	2.195331	2.569549	197	C	5.316059	-2.774056	2.421159
69	C	-1.367656	8.971033	-6.036824	198	C	2.9578	-3.816918	1.246132
70	H	-1.089764	9.663317	-5.230726	199	C	3.480198	-2.579108	0.837155
71	H	-0.458662	8.798707	-6.626355	200	H	2.96952	-2.013229	0.064252
72	C	-1.798225	7.638225	-5.394332	201	C	4.644446	-2.074688	1.408768
73	H	-1.985953	6.890581	-6.186103	202	H	5.031098	-1.110826	1.08968
74	C	0.943236	4.062515	-3.708495	203	C	0.119283	-4.82631	-1.246904
75	H	0.497476	3.462703	-4.498981	204	C	7.514009	-2.261804	-5.394332
76	C	-3.128066	7.816238	-4.595026	205	H	6.960395	-1.725405	-6.186103
77	H	-2.891996	8.480562	-3.746313	206	C	-4.394414	-6.499898	5.394308
78	C	-4.214953	8.463862	-5.468979	207	H	-4.303492	-5.734329	6.185991
79	H	-5.114795	8.609512	-4.858791	208	C	-4.464867	-7.898672	6.036989
80	H	-4.488242	7.750047	-6.257851	209	H	-4.452106	-8.644626	5.230971
81	C	-2.469703	9.592607	-6.903591	210	H	-3.553279	-8.060573	6.625473
82	H	-2.122846	10.549388	-7.313625	211	C	-0.045968	-5.956861	1.669265
83	H	-2.675489	8.939772	-7.764478	212	H	0.156034	-6.674655	0.880455
84	C	-3.759109	9.787031	-6.095224	213	C	-1.027319	-6.232286	2.613697
85	H	-4.55518	10.192666	-6.731994	214	H	-1.596329	-7.155586	2.569549

86	H	-3.582853	10.530325	-5.303797	215	C	4.78429	-3.997714	2.857011
87	C	-5.873423	-0.996237	-1.670615	216	H	5.295735	-4.539052	3.646888
88	H	-6.614477	-0.911108	-0.882041	217	C	3.626022	-4.505461	2.27924
89	C	-5.033307	-2.147639	-3.63725	218	H	3.226841	-5.454567	2.626084
90	C	-3.876342	-0.200273	-2.764018	219	C	6.545597	-2.193399	2.990962
91	H	-3.051829	0.503021	-2.828797	220	H	7.030015	-1.427564	2.366429
92	C	-5.054507	-3.272352	-4.586963	221	C	-1.18269	-6.120251	-2.85757
93	H	-4.289804	-3.232379	-5.380261	222	H	-1.23737	-6.862988	-3.647431
94	C	-5.988859	-2.008845	-2.615142	223	C	0.036068	-5.782086	-2.280109
95	H	-6.809831	-2.717565	-2.571269	224	H	0.945034	-6.265589	-2.627179
96	C	-3.989859	-1.214391	-3.708495	225	C	-1.067557	-4.196826	-0.837621
97	H	-3.247527	-1.300524	-4.498981	226	H	-1.029092	-3.43565	-0.064617
98	C	-4.795695	-0.089449	-1.705114	227	N	7.450693	-0.132394	-4.131038
99	C	-4.63119	0.720718	0.672145	228	C	6.896906	-0.276539	-2.99064
100	C	-4.58479	0.971377	-0.672996	229	H	7.076987	-1.164623	-2.366073
101	N	-5.855084	-4.258886	-4.476772	230	C	5.953749	0.703236	-2.421367
102	N	-3.95883	6.061155	4.475856	231	C	8.333093	-1.199134	-4.595026
103	C	-4.451299	1.787312	1.704195	232	H	8.79038	-1.735739	-3.746313
104	C	-3.941543	3.7957	3.636095	233	C	8.45297	-3.301092	-6.036824
105	C	-3.298541	2.552232	3.70779	234	H	8.91356	-3.887895	-5.230726
106	H	-2.574468	2.368683	4.498593	235	H	7.849235	-4.002141	-6.626355
107	C	-3.55304	1.563926	2.763439	236	C	-5.714854	-8.087852	6.905248
108	H	-3.032765	0.613297	2.828584	237	H	-5.674099	-7.404438	7.766035
109	C	-3.561558	4.854349	4.585945	238	H	-5.730302	-9.105413	7.315373
110	H	-2.861374	4.544877	5.379459	239	C	-6.99011	-7.811265	6.098365
111	C	-5.060433	-3.216814	2.421159	240	H	-7.877613	-7.907253	6.736232
112	C	-4.784448	-0.653071	1.246132	241	H	-7.090627	-8.568808	5.307202
113	C	-3.973672	-1.724385	0.837155	242	N	-5.691887	-4.809639	4.131816
114	H	-3.228267	-1.565066	0.064252	243	C	-5.701536	-6.19385	4.596283
115	C	-4.118955	-2.984864	1.408768	244	H	-5.717948	-6.898977	3.747814
116	H	-3.477552	-3.801646	1.08968	245	C	-2.288846	-4.54133	-1.408972
117	C	-4.239348	2.309853	-1.246904	246	H	-3.197461	-4.038565	-1.089627
118	C	-5.715784	-5.376421	-5.394332	247	C	9.437396	-0.581674	-5.468979
119	H	-4.974442	-5.165177	-6.186103	248	H	10.013453	0.124786	-4.858791
120	C	-3.43187	7.055623	5.394308	249	H	8.955859	0.011908	-6.257851
121	H	-2.814329	6.594098	6.185991	250	C	9.542293	-2.657478	-6.903591
122	C	-4.608017	7.816024	6.036989	251	H	10.197461	-3.436256	-7.313625
123	H	-5.260413	8.17795	5.230971	252	H	9.079814	-2.152845	-7.764478
124	H	-5.204022	7.107516	6.625473	253	C	10.355372	-1.638031	-6.095224
125	C	-5.135809	3.01824	1.669265	254	H	11.104698	-1.151431	-6.731994
126	H	-5.858438	3.202199	0.880455	255	H	10.910955	-2.162321	-5.303797
127	C	-4.883659	4.005827	2.613697	256	C	-6.946586	-6.412604	5.471756
128	H	-5.398755	4.960255	2.569549	257	H	-7.840179	-6.229049	4.862606
129	N	7.011213	-2.524499	4.131816	258	H	-6.947354	-5.648055	6.260429

Table S7 Cartesian coordinates of the protonated **(*R*)-Δ**.

No	atom	x	y	z	No	atom	x	y	z
1	N	4.929833	5.793461	4.349148	136	H	-6.249859	-4.118984	-3.887764
2	N	2.184039	7.288267	4.395499	137	C	-4.725674	-4.456904	-2.422524
3	N	-7.481622	-1.372295	-4.349128	138	H	-4.55898	-5.467405	-2.784282
4	N	-7.403824	1.75324	-4.395442	139	C	-4.268981	-2.658069	-0.881694
5	C	-6.966755	1.448855	3.158483	140	H	-3.710969	-2.237785	-0.052135
6	H	-7.325036	0.683566	2.470977	141	N	4.929253	-5.793127	-4.349128
7	C	-5.973126	2.369363	2.610615	142	C	4.737475	-5.308863	-3.158379
8	C	-5.692151	3.677814	3.066007	143	H	4.253811	-6.001878	-2.470992
9	H	-6.250322	4.119678	3.887693	144	C	5.037977	-3.988206	-2.610347
10	C	-3.988387	3.970837	1.317692	145	C	4.698298	-7.229926	-4.784551
11	C	3.286728	7.472633	5.406108	146	H	4.807501	-7.836536	-3.878402
12	H	3.09849	6.742984	6.200864	147	C	3.178212	-8.91624	-5.96671
13	C	4.698721	7.230302	4.784118	148	H	3.228372	-9.62705	-5.12837
14	H	4.80732	7.836559	3.877658	149	H	2.195022	-9.027963	-6.435809
15	C	-4.268846	2.658189	0.882274	150	C	-10.148504	-0.889765	6.968049
16	H	-3.71062	2.237729	0.052951	151	H	-9.559063	-0.679968	7.869414
17	C	-3.671176	4.292585	-1.68177	152	H	-10.990243	-1.511413	7.289763
18	C	-5.251934	1.891447	1.491815	153	C	-10.651019	0.407954	6.334082
19	H	-5.448657	0.888526	1.11965	154	H	-11.189919	1.012888	7.070094
20	C	-5.072951	4.485994	-1.644512	155	H	-11.36585	0.196865	5.528687
21	H	-5.506971	5.169165	-0.921211	156	N	-7.4822	1.37263	4.349148
22	C	-1.444465	5.439371	-1.317328	157	C	-8.610986	0.45406	4.784118
23	C	-4.725866	4.457302	2.422672	158	H	-9.19032	0.244982	3.877658
24	H	-4.559278	5.467883	2.784257	159	C	-5.251934	-1.891204	-1.491292
25	C	4.303693	9.233745	6.968049	160	H	-5.448709	-0.888351	-1.118975
26	H	4.190662	8.618375	7.869414	161	C	5.817879	-7.583621	-5.794952
27	H	4.186199	10.273536	7.289763	162	H	6.786826	-7.450847	-5.301142
28	C	-2.874281	4.777536	0.683292	163	H	5.769347	-6.874959	-6.635583
29	C	3.178165	8.916209	5.966541	164	C	4.303425	-9.232691	-6.968915
30	H	3.227363	9.626938	5.128062	165	H	4.186318	-10.272358	-7.291174
31	H	2.195139	9.027325	6.436137	166	H	4.189615	-8.616865	-7.869876
32	C	-0.167464	5.02608	-0.881694	167	C	5.678776	-9.018579	-6.335578
33	H	-0.082494	4.332686	-0.052135	168	H	6.471818	-9.182138	-7.072059

34	C	-1.881777	5.32568	1.682161	169	H	5.854196	-9.743394	-5.530541
35	C	-2.700185	4.878032	-0.68287	170	C	-9.478062	1.246507	5.793889
36	C	0.138554	6.152156	3.520561	171	H	-9.84785	2.151693	5.299691
37	C	0.988136	5.49391	-1.491292	172	H	-8.840724	1.5594	6.634803
38	H	1.95502	5.162896	-1.118975	173	C	6.42146	2.150307	-1.644512
39	C	5.818538	7.584989	5.793889	174	H	7.230113	2.184594	-0.921211
40	H	6.787346	7.452642	5.299691	175	C	5.258876	3.195849	-3.52023
41	H	5.770842	6.876591	6.634803	176	C	4.597928	0.988903	-2.719714
42	C	-0.465105	4.87809	3.62068	177	H	3.946708	0.126878	-2.818009
43	H	-0.152527	4.193199	4.404323	178	C	4.901076	4.271938	-4.433586
44	C	5.678808	9.020076	6.334082	179	H	4.219799	4.005162	-5.240811
45	H	6.472146	9.18431	7.070094	180	C	6.276431	3.214515	-2.535054
46	H	5.853415	9.744683	5.528687	181	H	6.987933	4.034834	-2.477579
47	C	-1.442872	4.476648	2.72047	182	C	4.456854	2.036346	-3.619991
48	H	-1.864224	3.481878	2.819102	183	H	3.707138	1.964851	-4.403373
49	C	1.249475	6.38024	4.433762	184	C	5.553075	1.033039	-1.68177
50	H	1.359053	5.656891	5.241026	185	C	5.574608	0.100433	0.683292
51	C	-5.397124	2.956395	-3.52023	186	C	5.574592	-0.100587	-0.68287
52	C	-0.338715	6.767918	-3.065889	187	N	5.220262	5.535279	-4.395442
53	H	-0.442215	7.472029	-3.887764	188	N	5.219805	-5.535567	4.395499
54	C	-3.155379	3.487471	-2.719714	189	C	5.553063	-1.033173	1.682161
55	H	-2.083234	3.354511	-2.818009	190	C	5.258646	-3.196069	3.520561
56	C	-6.966348	-1.448342	-3.158379	191	C	4.457102	-2.036252	3.62068
57	H	-7.324684	-0.682969	-2.470992	192	H	3.70768	-1.964507	4.404323
58	C	-6.150144	2.108487	-4.433586	193	C	4.598327	-0.98876	2.72047
59	H	-5.578472	1.651872	-5.240811	194	H	3.947507	-0.126474	2.819102
60	C	-5.922067	3.828291	-2.535054	195	C	4.900713	-4.272197	4.433762
61	H	-6.988235	4.034311	-2.477579	196	H	4.219485	-4.00542	5.241026
62	C	-1.347867	6.636152	1.644538	197	C	5.038492	3.988197	2.610615
63	H	-1.722184	7.353527	0.920995	198	C	5.433039	1.468626	1.317692
64	C	-5.972876	-2.368913	-2.610347	199	C	4.436482	2.367834	0.882274
65	C	-1.496955	6.321006	-2.422524	200	H	3.793241	2.094627	0.052951
66	H	-2.455421	6.681895	-2.784282	201	C	4.264008	3.602584	1.491815
67	C	-0.353673	7.042556	2.535026	202	H	3.493815	4.274413	1.11965
68	H	0.00132	8.06876	2.47728	203	C	5.432866	-1.468742	-1.317328

69	C	-9.310796	1.705707	-5.96671	204	C	4.8284	6.582244	-5.406167
70	H	-9.951456	2.017672	-5.12837	205	H	4.290864	6.054081	-6.200872
71	H	-8.915957	2.613036	-6.435809	206	C	4.828126	-6.582707	5.406108
72	C	-8.114591	0.890395	-5.406167	207	H	4.29035	-6.054863	6.200864
73	H	-7.38842	0.688956	-6.200872	208	C	6.132581	-7.210476	5.966541
74	C	-3.991954	2.841576	-3.619991	209	H	6.723492	-7.608448	5.128062
75	H	-3.55518	2.228051	-4.403373	210	H	6.720323	-6.414708	6.436137
76	C	-8.610448	-0.453883	-4.784551	211	C	6.42101	-2.150789	1.644538
77	H	-9.19039	-0.24515	-3.878402	212	H	7.229434	-2.185308	0.920995
78	C	-9.476548	-1.246621	-5.794952	213	C	6.275869	-3.214988	2.535026
79	H	-9.846036	-2.15214	-5.301142	214	H	6.987091	-4.035523	2.47728
80	H	-8.838563	-1.558922	-6.635583	215	C	6.031156	3.090641	3.066007
81	C	-10.147457	0.88947	-6.968915	216	H	6.692907	3.353099	3.887693
82	H	-10.989282	1.510721	-7.291174	217	C	6.22307	1.864069	2.422672
83	H	-9.557232	0.680119	-7.869876	218	H	7.014964	1.214509	2.784257
84	C	-10.649706	-0.408675	-6.335578	219	C	4.738123	5.308959	3.158483
85	H	-11.187874	-1.01369	-7.072059	220	H	4.254504	6.001884	2.470977
86	H	-11.365124	-0.198185	-5.530541	221	C	6.030546	-3.090623	-3.065889
87	C	-1.34851	-6.636301	-1.644512	222	H	6.692074	-3.353045	-3.887764
88	H	-1.723143	-7.353759	-0.921211	223	C	6.222629	-1.864101	-2.422524
89	C	0.138249	-6.152245	-3.52023	224	H	7.014401	-1.21449	-2.784282
90	C	-1.442549	-4.476374	-2.719714	225	C	4.436445	-2.368012	-0.881694
91	H	-1.863474	-3.481389	-2.818009	226	H	3.793463	-2.094901	-0.052135
92	C	1.249069	-6.380425	-4.433586	227	N	2.552369	7.165422	-4.349128
93	H	1.358673	-5.657034	-5.240811	228	C	2.228873	6.757205	-3.158379
94	C	-0.354364	-7.042806	-2.535054	229	H	3.070873	6.684847	-2.470992
95	H	0.000302	-8.069145	-2.477579	230	C	0.934899	6.357119	-2.610347
96	C	-0.4649	-4.877921	-3.619991	231	C	3.91215	7.683809	-4.784551
97	H	-0.151959	-4.192902	-4.403373	232	H	4.382888	8.081686	-3.878402
98	C	-1.881899	-5.325624	-1.68177	233	C	6.132584	7.210532	-5.96671
99	C	-2.700326	-4.877968	0.683292	234	H	6.723083	7.609377	-5.12837
100	C	-2.874407	-4.777445	-0.68287	235	H	6.720934	6.414927	-6.435809
101	N	2.183561	-7.288519	-4.395442	236	C	5.844811	-8.34398	6.968049
102	N	-7.403844	-1.752701	4.395499	237	H	5.368401	-7.938407	7.869414
103	C	-3.671285	-4.292507	1.682161	238	H	6.804044	-8.762123	7.289763

104	C	-5.3972	-2.956087	3.520561	239	C	4.972211	-9.42803	6.334082
105	C	-3.991997	-2.841838	3.62068	240	H	4.717773	-10.197198	7.070094
106	H	-3.555153	-2.228692	4.404323	241	H	5.512435	-9.941547	5.528687
107	C	-3.155455	-3.487888	2.72047	242	N	2.552368	-7.166091	4.349148
108	H	-2.083283	-3.355404	2.819102	243	C	3.912265	-7.684363	4.784118
109	C	-6.150188	-2.108043	4.433762	244	H	4.382999	-8.081541	3.877658
110	H	-5.578538	-1.651471	5.241026	245	C	4.263798	-3.602706	-1.491292
111	C	0.934634	-6.357561	2.610615	246	H	3.493689	-4.274545	-1.118975
112	C	-1.444653	-5.439463	1.317692	247	C	3.658669	8.830242	-5.794952
113	C	-0.167637	-5.026024	0.882274	248	H	3.05921	9.602987	-5.301142
114	H	-0.08262	-4.332356	0.052951	249	H	3.069215	8.433881	-6.635583
115	C	0.987926	-5.494032	1.491815	250	C	5.844033	8.343221	-6.968915
116	H	1.954842	-5.162939	1.11965	251	H	6.802964	8.761637	-7.291174
117	C	-3.988401	-3.970629	-1.317328	252	H	5.367617	7.936746	-7.869876
118	C	3.28619	-7.472639	-5.406167	253	C	4.97093	9.427254	-6.335578
119	H	3.097556	-6.743038	-6.200872	254	H	4.716056	10.195828	-7.072059
120	C	-8.114854	-0.889927	5.406108	255	H	5.510929	9.941579	-5.530541
121	H	-7.38884	-0.688121	6.200864	256	C	3.659524	-8.831496	5.793889
122	C	-9.310746	-1.705733	5.966541	257	H	3.060504	-9.604335	5.299691
123	H	-9.950855	-2.01849	5.128062	258	H	3.069882	-8.435991	6.634803
124	H	-8.915462	-2.612616	6.436137	259	H	2.108247	8.04721	3.713825
125	C	-5.073143	-4.485363	1.644538	260	H	5.382243	5.211355	5.05994
126	H	-5.507249	-5.168219	0.920995	261	H	5.381894	-5.21091	-5.059683
127	C	-5.922196	-3.827568	2.535026	262	H	2.107741	-8.047488	-3.713799
128	H	-6.988411	-4.033237	2.47728	263	H	5.914964	-5.849401	3.713825
129	C	-0.339005	-6.768455	3.066007	264	H	1.822044	-7.266837	5.05994
130	H	-0.442585	-7.472777	3.887693	265	H	-8.023212	-2.197809	3.713825
131	C	-1.497204	-6.321371	2.422672	266	H	-7.204287	2.055482	5.05994
132	H	-2.455687	-6.682392	2.784257	267	H	1.821833	7.266312	-5.059683
133	C	2.228632	-6.757815	3.158483	268	H	5.915458	5.849101	-3.713799
134	H	3.070532	-6.685450	2.470977	269	H	-7.203727	-2.055402	-5.059683
135	C	-5.691831	-3.677295	-3.065889	270	H	-8.0232	2.198386	-3.713799

4. Determination of Trace Acid in $CDCl_3$ Using (*R*)-Δ

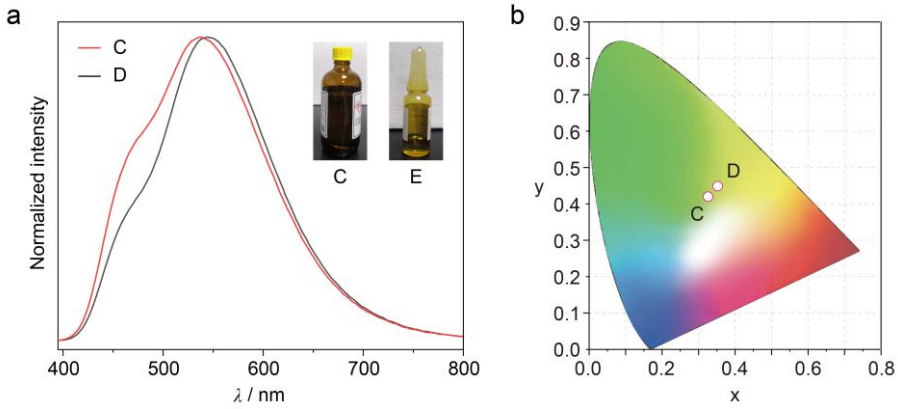


Figure S15 a Steady-state photoluminescence spectra of **(*R*)-Δ** in $CDCl_3$ (C) and $CDCl_3$ without silver foil stabilizer diluted 100 times with deacidified $CHCl_3$ (D) at the same concentration of 1×10^{-5} M upon excitation at 380 nm. Insets are photographs of commercial grade $CDCl_3$ (C) with and (E) without silver foil stabilizer. **b** CIE coordinate diagram of **(*R*)-Δ** in C and D.

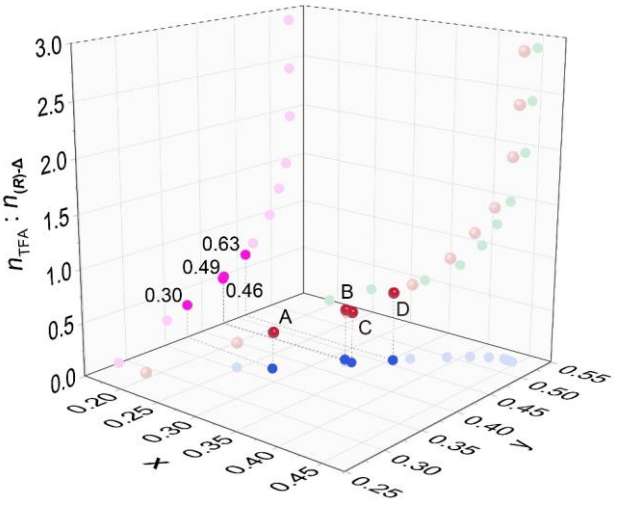


Figure S16 The fitting function based on the PL emission of **(*R*)-Δ** upon changing the amount of TFA from 0.00 to 2.88 equiv. Highlighted dots A–D represent commercial grade CH_2Cl_2 (A), $CHCl_3$ (B), $CDCl_3$ with silver foil stabilizer (C), and $CDCl_3$ without silver foil stabilizer diluted 100 times with deacidified $CHCl_3$ (D) in the fitting function, respectively.

5. Measurement of Limit of Detection of (*R*)-Δ for Trace Acid

TFA (0.3 μL) was added to the deacidified $CHCl_3$ (500 mL) and mixed completely to make a quantitatively acidified solvent. **(*R*)-Δ** (0.72 mg, 3.99×10^{-7} mol) was dissolved in 4 mL of this quantitatively acidified $CHCl_3$ to prepare a solution at concentration of 1×10^{-4} M. A solution of concentration 1×10^{-5} M was prepared by diluting it 10 times with acidified $CHCl_3$. Then 1.5 mL, 300 μL, 150 μL, and 30 μL of this **(*R*)-Δ** solution were taken and diluted to 3 mL with the deacidified $CHCl_3$ to provide four solution samples of **(*R*)-Δ** at concentrations of 5×10^{-6} M, 1×10^{-6} M, 5×10^{-7} M, and 1×10^{-7} M and with the same n_{TFA}:$n_{(R)\text{-}\Delta}$ ratio of 0.72. Their UV-Vis spectra were recorded as follows.

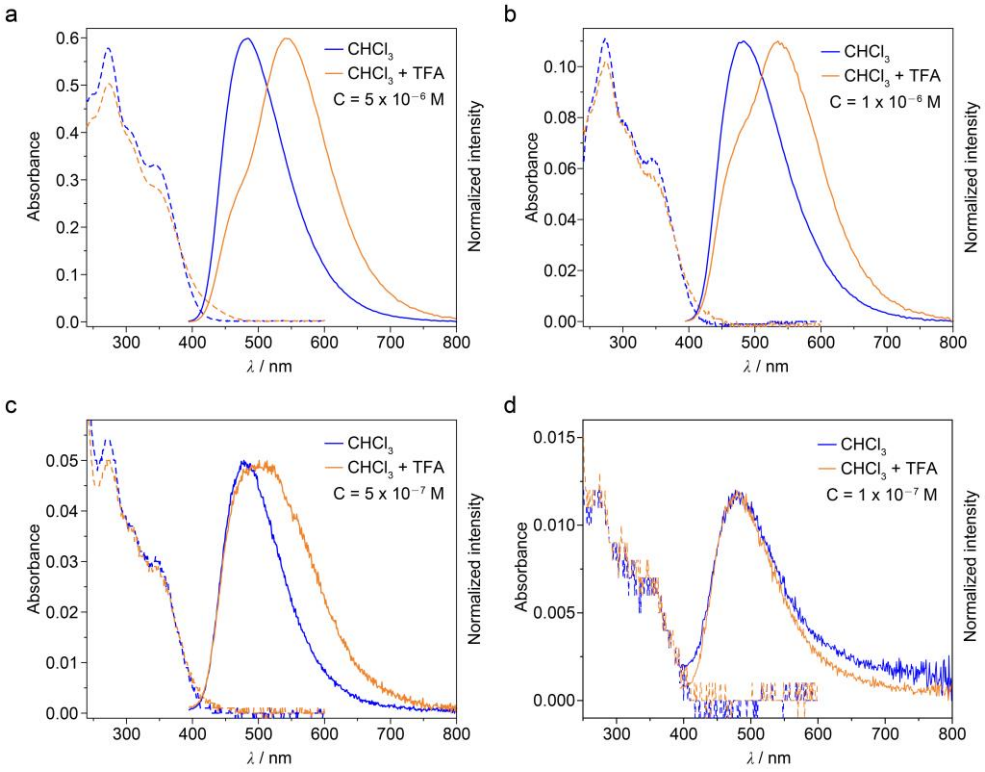


Figure S17 UV-Vis absorption (dash lines) and steady-state PL (solid lines) spectra of solutions of **(*R*)-Δ** in deacidified $CHCl_3$ (blue lines) and $CHCl_3$ acidified with TFA (0.81 equiv relative to **(*R*)-Δ**, orange lines) at concentrations of (a) 5×10^{-6} M, (b) 1×10^{-6} M, (c) 5×10^{-7} M, and (d) 1×10^{-7} M.

Section E. X-Ray Crystallography of Adduct [I_3^-⊂(*R*)-Δ]

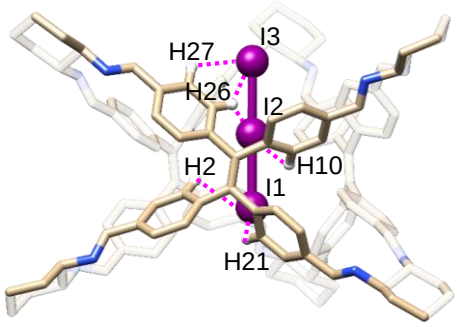


Figure S18 Superstructure of of adduct **[I_3^-⊂(*R*)-Δ]** demonstrating the encapsulation of the linear I_3^- anion (ball-stick model) in the cavity of **(*R*)-Δ** (stick model) by up to 18 [C–H···I] hydrogen bonding interactions. On account of the three-fold symmetry of this adduct, only the non-repeated 6 of 18 [C–H···I] interactions have been exhibited. All hydrogen atoms except those engaged in [C–H···I] interactions are omitted for clarity. C, tan; N, blue; H, white; I, purple.

Table S8 Hydrogen-bonding geometries in the adduct **[I_3^-⊂(*R*)-Δ]**.

No	[C–H···I]	$d_{[C–H]}$ / Å	$d_{[H···I]}$ / Å	$d_{[C···I]}$ / Å	∠C–H···I / °
1	[C27–H27···I3]	0.950	3.6179	4.2228	123.99
2	[C26–H26···I3]	0.950	3.4323	4.1367	132.78
3	[C26–H26···I2]	0.950	3.2665	3.9077	126.56
4	[C10–H10···I2]	0.950	3.5776	4.1283	119.47
5	[C2–H2···I1]	0.950	3.418	4.0068	122.29
6	[C21–H21···I1]	0.950	3.2181	3.8794	128.29

Black bold numbers and magenta dashed lines indicate [C–H···I] hydrogen bonding interactions. Except for *meso*-H, all hydrogen atoms are omitted for the sake of clarity. C, light brown; H, white; N, blue; I, purple.

References

1 J. Xue, W. Bai, H. Duan, J. Nie, B. Du, J. Sun and B. Z. Tang, *Macromolecules*, 2018, **51**, 5762−5772.

2 G. M. Sheldrick, *Acta. Crystallogr. A*, 2008, **64**, 112–122.