Supporting Information

Sign control of circularly polarized luminescence of chiral Schiff-base Zn(II) complexes through coordination geometry changes

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1. Instrumentation and Materials

Instruments

Melting points were measured by a ATM-01 melting temperature measurement device (AS ONE Corporation). IR spectra were acquired with a JASCO FT/IR4100ST spectrometer. High-resolution mass spectrometry was recorded on Bruker micrOTOF II spectrometer. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III 500 spectrometers, TMS as internal standard. Elemental analyses were performed on a J-SCIENCE MICRO CORDER JM10. UV–vis absorption spectra were obtained on a SHIMADZU UV-1900i spectrophotometer. CD spectra were recorded on JASCO J-720 and J-820 spectropolarimeter. Emission spectra were obtained on a JASCO FP-6500 spectrometer. CPL spectra were obtained at room temperature using a JASCO CPL-300 spectrofluoropolarimeter. Optical rotation was measured on a JASCO DIP-370 digital polarimeter.

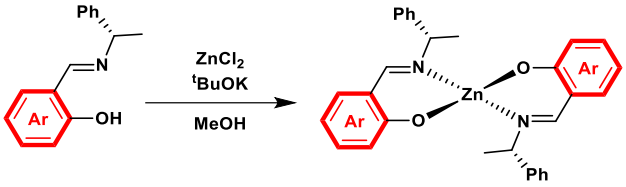
Materials and Sample Preparation

(*R*)- and (*S*)-1-phenylethylamine (Sigma Aldrich), 1-hydroxy-2-naphthaldehyde (TCI), Zinc Chloride (Kanto Chemical) and potassium *tert*-butoxide (Kanto Chemical) were obtained from commercial sources and were used without further purification. 4-Hydroxy-3-phenanthrenecarboxaldehyde was prepared by according publish procedure.[S1] The imine ligands were prepared by condensation of the corresponding aldehyde with (*R*)- and (*S*)-1-phenylethylamine in boiling ethanol. The solid-state samples were prepared according to the standard procedure for obtaining glassy KBr matrices.[S2]

2. Synthetic Procedures and Characterization

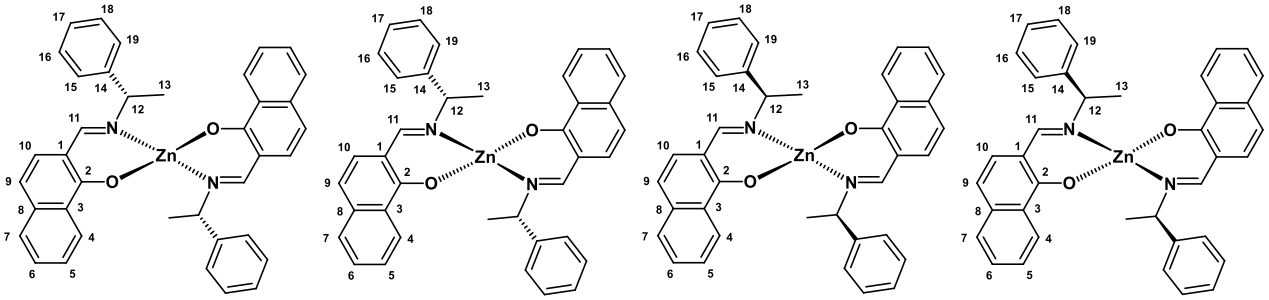
General procedure for zinc complexes

A solution of corresponding chiral ligands (2 equiv.) in MeOH was added potassium *tert*-butoxide (2 equiv.) and $ZnCl_2$ (1 equiv.). The mixture was stirred at room temperature for overnight and yellow precipitate was formed. The residue was filtered, then recrystallized from CH_2Cl_2/EtOH resulting zinc complexes **1** and **2** as yellow crystals.



Scheme. S1 Synthesis of chiral Schiff-base Zn(II) complexes studied in this work.

(*S*,*S*)/(*R*,*R*)-1: Yellow crystals (62%); m.p. 199–201 °C; IR (KBr): 1596 cm^{-1} (N=C); HRMS (APCI+): m/z $[M+H]^+$ calcd for $C_{38}H_{33}N_2O_2Zn$: 613.1828; found: 613.1827; Anal. calcd for $C_{38}H_{32}N_2O_2Zn$: C, 74.33; H, 5.25; N, 4.56. Found: C, 74.45; H, 5.17; N, 4.57. (*S*,*S*)-**1**: $[\alpha]_D^{25}$ = +246 (c 0.001, $CHCl_3$), (*R*,*R*)-**1**: $[\alpha]_D^{25}$ = –244 (c 0.001, $CHCl_3$).



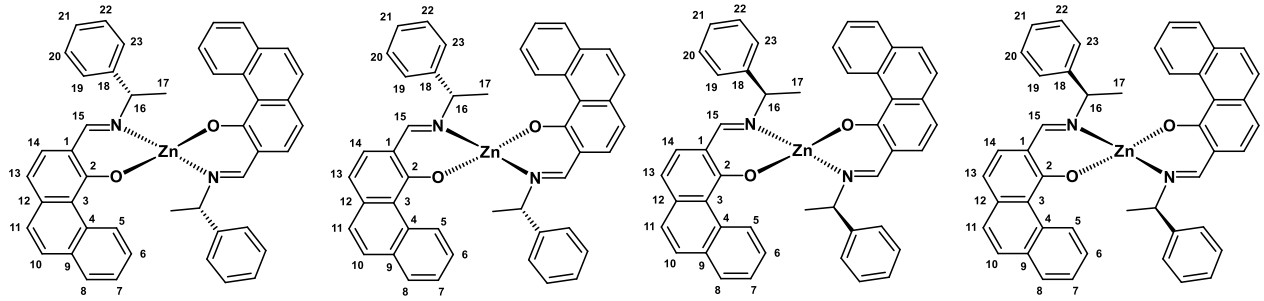
Λ-(*S*,*S*)-**1**: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.62 (d, J = 8.2 Hz, 2H, H^4), 8.07 (br, 2H, H^{11}), 7.68 (d, J = 8.2 Hz, 2H, H^7), 7.54–7.50 (m, 2H, H^6), 7.40–7.37 (m, 2H, H^5), 7.07–7.05 (m, 4H, $H^{10,17}$), 7.01 (d, J = 8.5 Hz, 2H, H^9), 6.93–6.90 (m, 4H, $H^{16,18}$), 6.79 (d, J = 7.3 Hz, 4H, $H^{15,19}$), 4.25 (q, J = 6.6 Hz, 2H, H^{12}), 1.51 (d, J = 6.6 Hz, 6H, H^{13}); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 170.02, 167.93, 140.52, 137.38, 131.07, 130.56, 129.00, 128.45, 127.69, 127.44, 126.83, 126.27, 124.32, 113.92, 111.04, 69.21, 22.05.

Δ-(*S*,*S*)-**1**: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.55 (d, J = 8.2 Hz, 2H, H^4), 8.31 (br, 2H, H^{11}), 7.63 (d, J = 7.9 Hz, 2H, H^7), 7.54–7.50 (m, 2H, H^6), 7.40–7.37 (m, 6H, $H^{5,15,19}$), 7.20–7.17 (m, 4H, $H^{16,18}$), 7.14–7.11 (m, 2H, H^{17}), 7.07–7.05 (m, 2H, H^{10}), 6.96 (d, J = 8.8 Hz, 2H, H^9), 4.63 (q, J = 6.6 Hz, 2H, H^{12}), 1.55 (d, J = 6.6 Hz, 6H, H^{13}); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 170.29, 170.02, 143.21, 137.44, 131.04, 130.43, 129.22, 128.71, 127.58, 127.44, 126.77, 126.50, 124.32, 114.11, 110.75, 68.10, 22.69.

Δ-(*R*,*R*)-**1**: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.62 (d, J = 8.2 Hz, 2H, H^4), 8.08 (br, 2H, H^{11}), 7.68 (d, J = 8.2 Hz, 2H, H^7), 7.54–7.50 (m, 2H, H^6), 7.40–7.37 (m, 2H, H^5), 7.07–7.05 (m, 4H, $H^{10,17}$), 7.01 (d, J = 8.5 Hz, 2H, H^9), 6.93–6.90 (m, 4H, $H^{16,18}$), 6.80 (d, J = 7.3 Hz, 4H, $H^{15,19}$), 4.25 (q, J = 6.6 Hz, 2H, H^{12}), 1.52 (d, J = 6.6 Hz, 6H, H^{13}).

Λ-(*R*,*R*)-**1**: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 8.55 (d, J = 8.2 Hz, 2H, H^{4}), 8.31 (br, 2H, H^{11}), 7.63 (d, J = 7.9 Hz, 2H, H^{7}), 7.54–7.50 (m, 2H, H^{6}), 7.40–7.37 (m, 6H, $H^{5,15,19}$), 7.20–7.17 (m, 4H, $H^{16,18}$), 7.14–7.11 (m, 2H, H^{17}), 7.07–7.05 (m, 2H, H^{10}), 6.96 (d, J = 8.8 Hz, 2H, H^{9}), 4.64 (q, J = 6.6 Hz, 2H, H^{12}), 1.55 (d, J = 6.6 Hz, 6H, H^{13}).

(*S*,*S*)/(*R*,*R*)-2: Yellow crystals (83%); m.p. 237–239 °C; IR (KBr): 1612, 1581 cm^{-1} (N=C); HRMS (APCI+): m/z $[M+H]^+$ calcd for $C_{46}H_{37}N_2O_2Zn$: 713.2141; found: 713.2127; Anal. calcd for $C_{46}H_{36}N_2O_2Zn$: C, 77.36; H, 5.08; N, 3.92. Found: C, 77.30; H, 4.98; N, 3.83. (*S*,*S*)-**2**: $[\alpha]_D^{25}$ = +273 (c 0.001, $CHCl_3$) (*R*,*R*)-**1**: $[\alpha]_D^{25}$ = –273 (c 0.001, $CHCl_3$).



Λ-(*S*,*S*)-**2**: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 10.56 (d, J = 8.9 Hz, 2H, H^{5}), 8.19 (br, 2H, H^{15}), 7.89–7.82 (m, 4H, $H^{8,10}$), 7.68 (d, J = 8.5 Hz, 2H, H^{11}), 7.61–7.50 (m, 4H, $H^{6,7}$), 7.26 (d, J = 8.5 Hz, 2H, H^{14}), 7.18 (d, J = 8.5 Hz, 2H, H^{13}), 7.06–7.02 (m, 2H, H^{21}), 6.90–6.86 (m, 4H, $H^{20,22}$), 6.82–6.79 (m, 4H, $H^{19,23}$), 4.30 (q, J = 6.7 Hz, 2H, H^{16}), 1.48 (d, J = 6.7 Hz, 6H, H^{17}); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 172.58, 168.88, 140.24, 138.52, 133.01, 133.00, 132.27, 130.83, 129.06, 128.44, 128.02, 127.50, 127.16, 126.92, 126.80, 125.25, 123.88, 115.46, 115.18, 69.52, 22.11.

Δ-(*S*,*S*)-**2**: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 10.44 (d, J = 8.5 Hz, 2H, H^{5}), 8.42 (br, 2H, H^{15}), 7.89–7.82 (m, 4H, $H^{8,10}$), 7.63 (d, J = 8.9 Hz, 2H, H^{11}), 7.61–7.50 (m, 4H, $H^{6,7}$), 7.33–7.31 (m, 4H, $H^{19,23}$), 7.25 (d, J = 8.2 Hz, 2H, H^{14}), 7.12 (d, J = 8.2 Hz, 2H, H^{13}), 6.93–6.86 (m, 6H, $H^{20,21,22}$), 4.66 (q, J = 6.5 Hz, 2H, H^{16}), 1.58 (d, J = 6.5 Hz, 6H, H^{17}); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 172.71, 171.19, 143.04, 138.65, 133.14, 132.90, 132.28, 131.06, 129.19, 128.72, 127.96, 172.81, 127.34, 126.97, 126.48, 125.25, 123.99, 115.33, 115.09, 68.22, 22.64.

Δ-(*R*,*R*)-**2**: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 10.56 (d, J = 8.9 Hz, 2H, H^{5}), 8.20 (br, 2H, H^{15}), 7.89–7.82 (m, 4H, $H^{8,10}$), 7.68 (d, J = 8.5 Hz, 2H, H^{11}), 7.61–7.50 (m, 4H, $H^{6,7}$), 7.26 (d, J = 8.5 Hz, 2H, H^{14}), 7.17 (d, J = 8.5 Hz, 2H, H^{13}), 7.06–7.02 (m, 2H, H^{21}), 6.90–6.86 (m, 4H, $H^{20,22}$), 6.82–6.79 (m, 4H, $H^{19,23}$), 4.31 (q, J = 6.7 Hz, 2H, H^{16}), 1.48 (d, J = 6.7 Hz, 6H, H^{17}).

Λ-(*R*,*R*)-**2**: ^{1}H NMR ($CDCl_3$, 500 MHz) δ 10.44 (d, J = 8.5 Hz, 2H, H^{5}), 8.43 (br, 2H, H^{15}), 7.89–7.82 (m, 4H, $H^{8,10}$), 7.63 (d, J = 8.9 Hz, 2H, H^{11}), 7.61–7.50 (m, 4H, $H^{6,7}$), 7.33–7.31 (m, 4H, $H^{19,23}$), 7.25 (d, J = 8.2 Hz, 2H, H^{14}), 7.12 (d, J = 8.2 Hz, 2H, H^{13}), 6.93–6.86 (m, 6H, $H^{20,21,22}$), 4.67 (q, J = 6.5 Hz, 2H, H^{16}), 1.58 (d, J = 6.5 Hz, 6H, H^{17}).

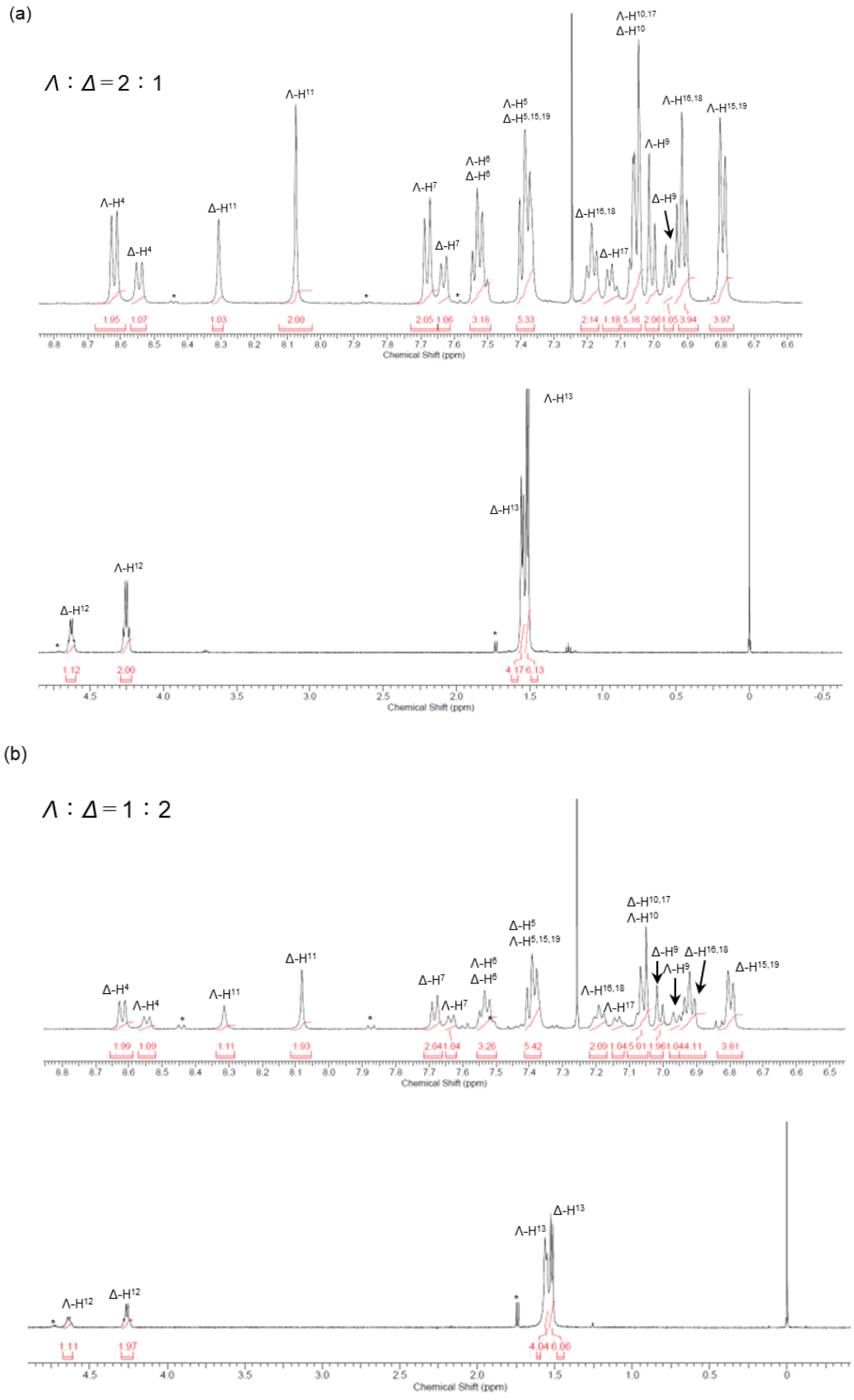


Fig. S1 ^{1}H NMR spectra of (a) (*S*,*S*)-**1** and (b) (*R*,*R*)-**1** in $CDCl_3$ (500 MHz, 298 K). Asterisked peaks correspond to the free ligand in the sample.

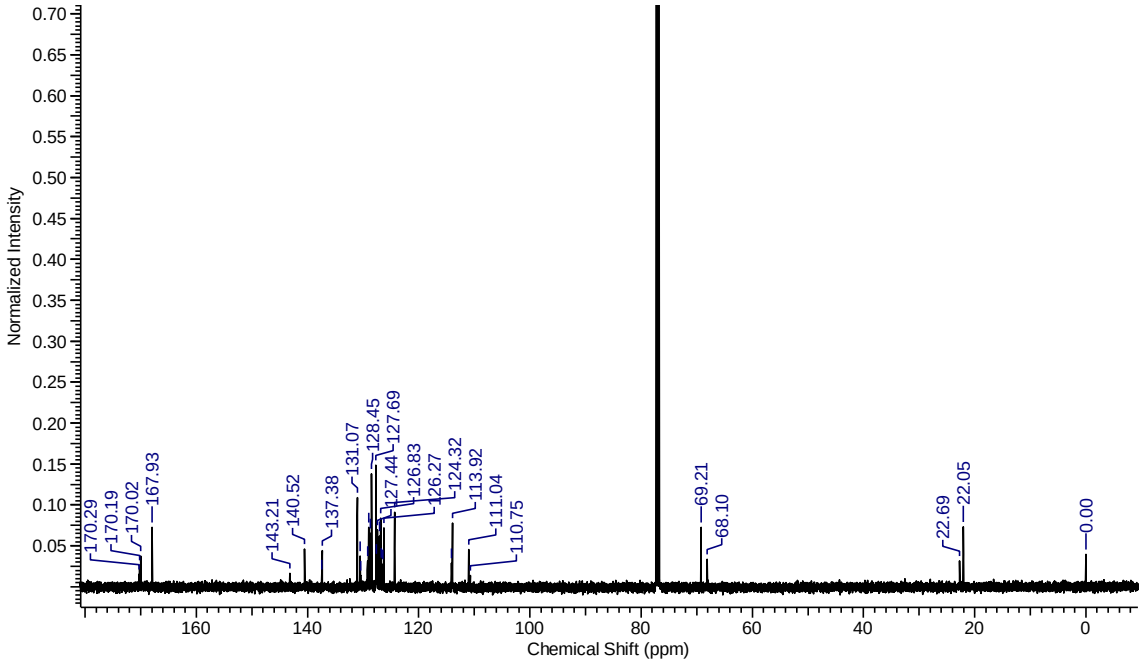


Fig. S2 ^{13}C NMR spectrum of (*S*,*S*)-**1** in $CDCl_3$ (125 MHz, 298 K).

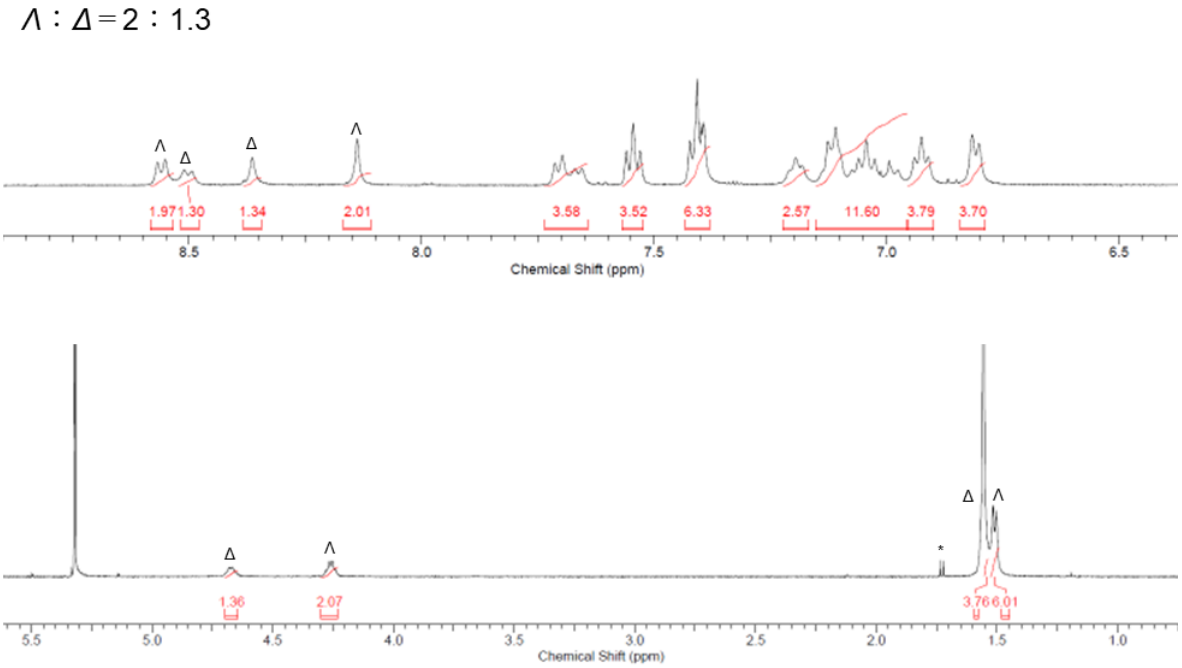


Fig. S3 ^{1}H NMR spectrum of (*S*,*S*)-**1** in CD_2Cl_2 (500 MHz, 298 K).

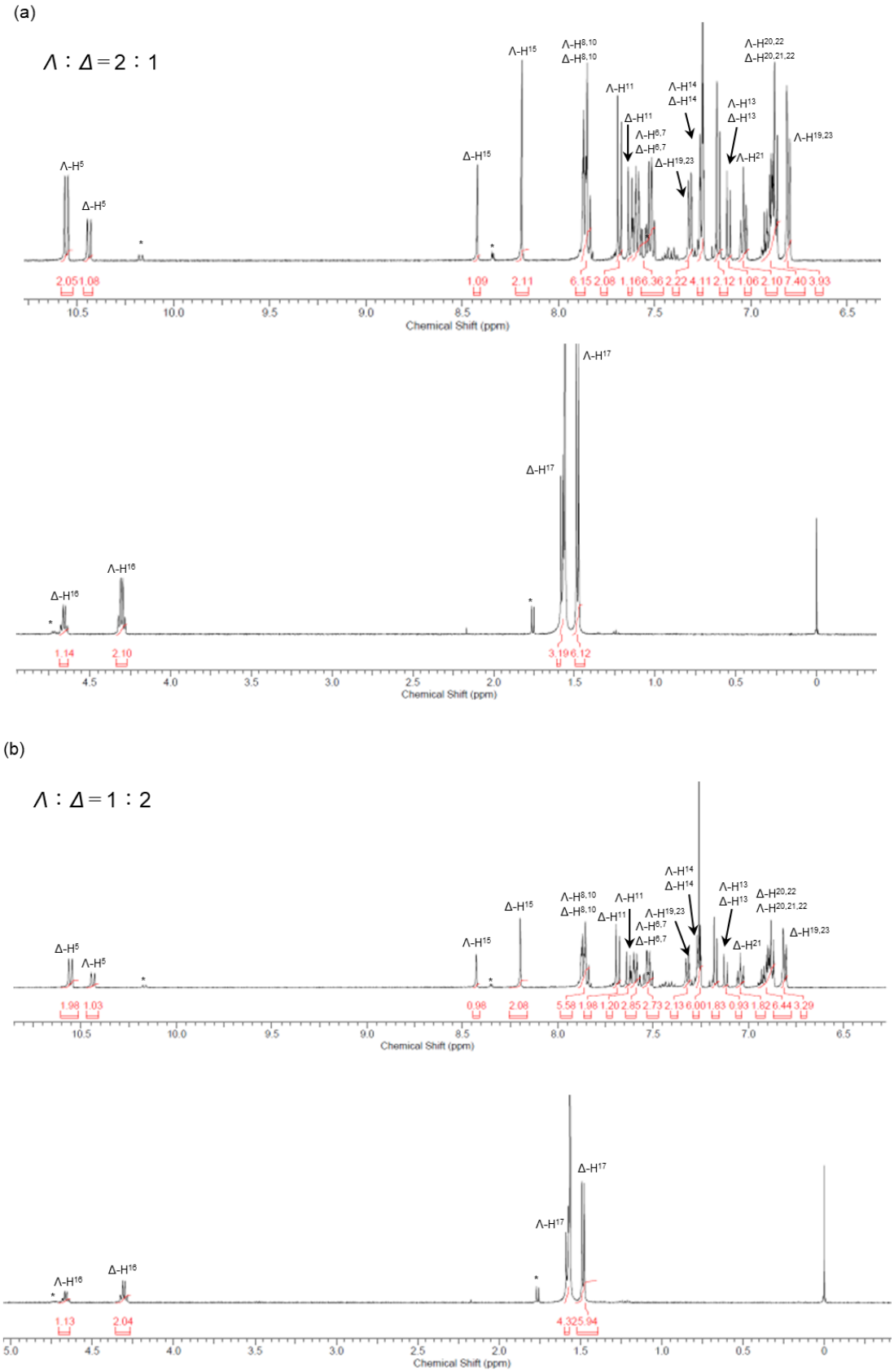


Fig. S4 ^{1}H NMR spectra of (a) (*S*,*S*)-**2** and (b) (*R*,*R*)-**2** in $CDCl_3$ (500 MHz, 298 K). Asterisked peaks correspond to the free ligand in the sample.

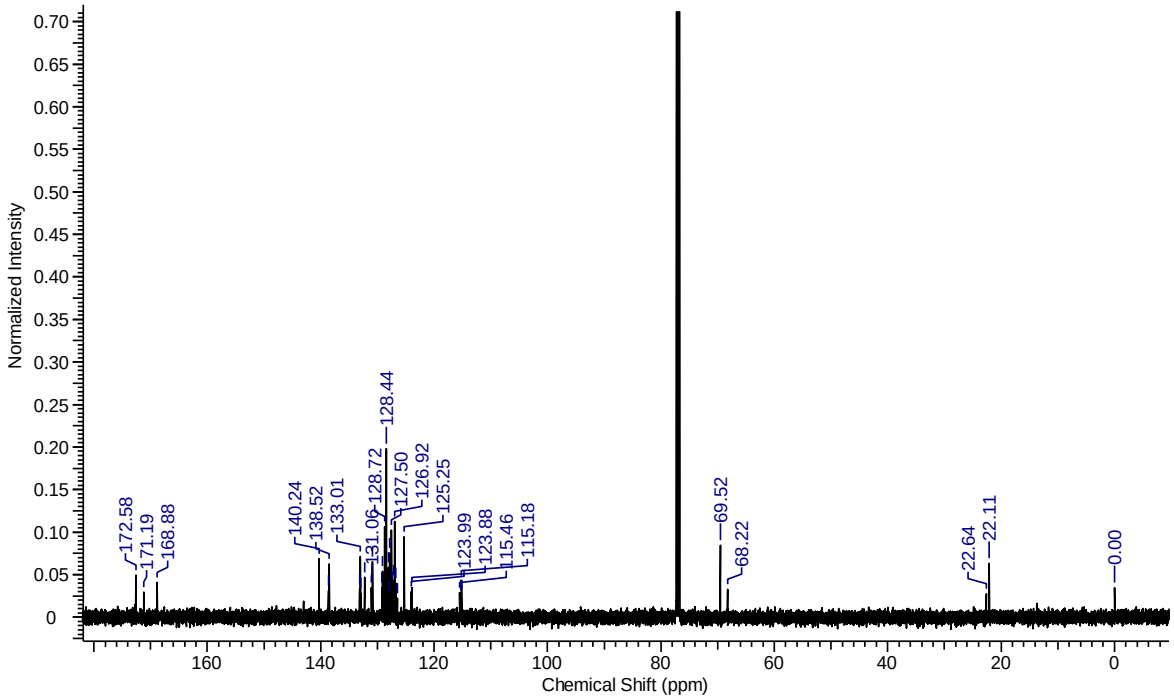


Fig. S5 ^{13}C NMR spectrum of (*S*,*S*)-**2** in $CDCl_3$ (125 MHz, 298 K).

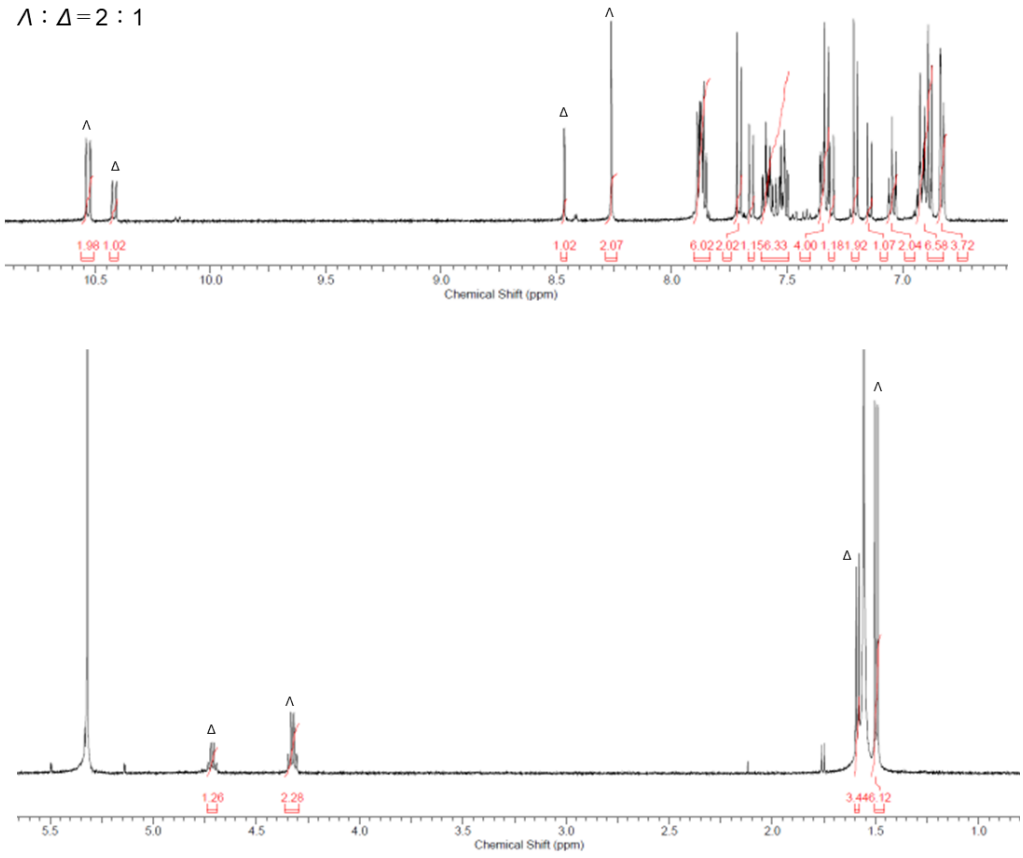


Fig. S6 ^{1}H NMR spectrum of (*S*,*S*)-**2** in CD_2Cl_2 (500 MHz, 298 K).

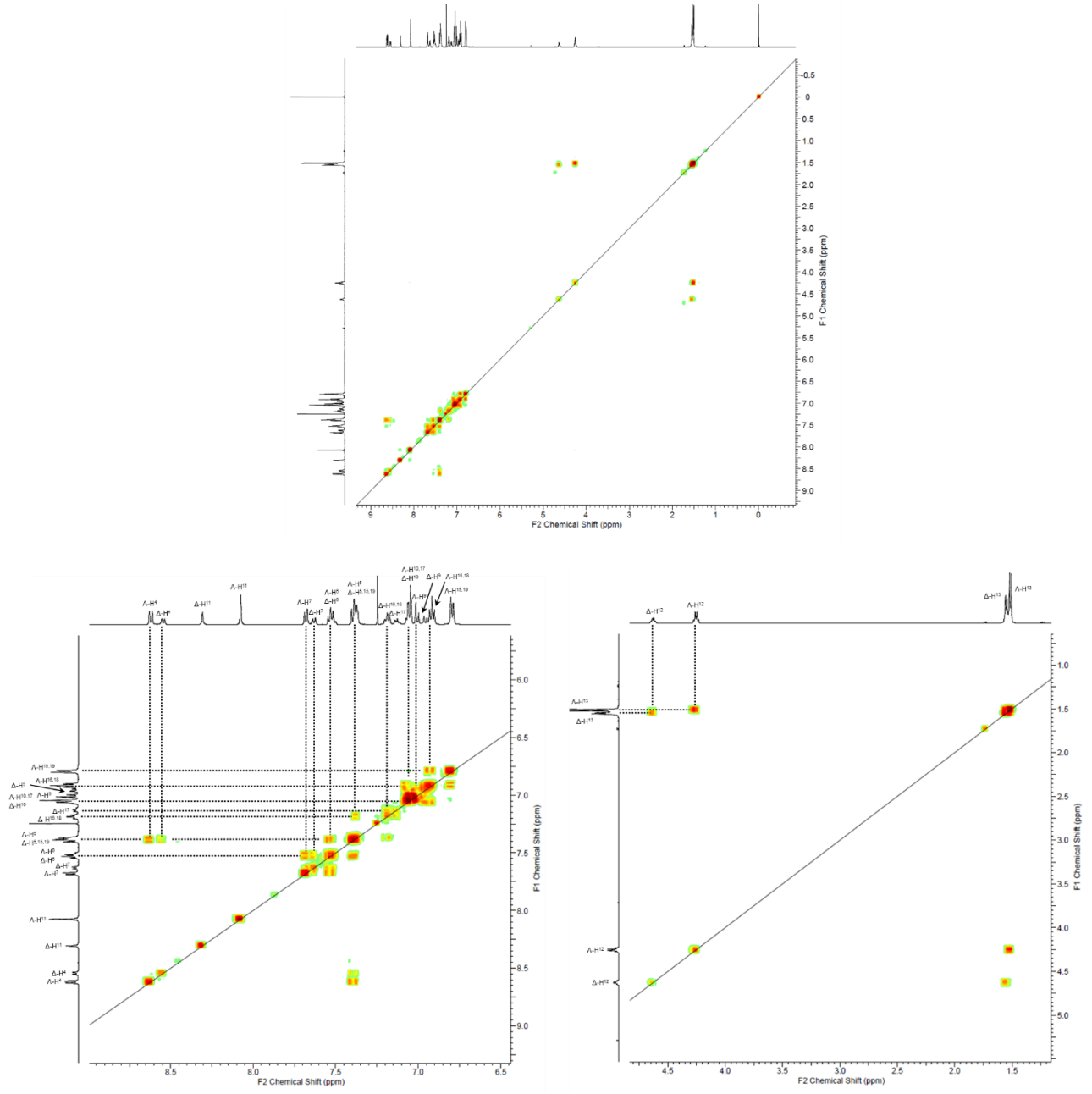


Fig. S7 gCOSY spectra of (*S*,*S*)-**1** in $CDCl_3$ (500 MHz, 298 K). Whole spectrum (upper) and enlarged spectra (lower).

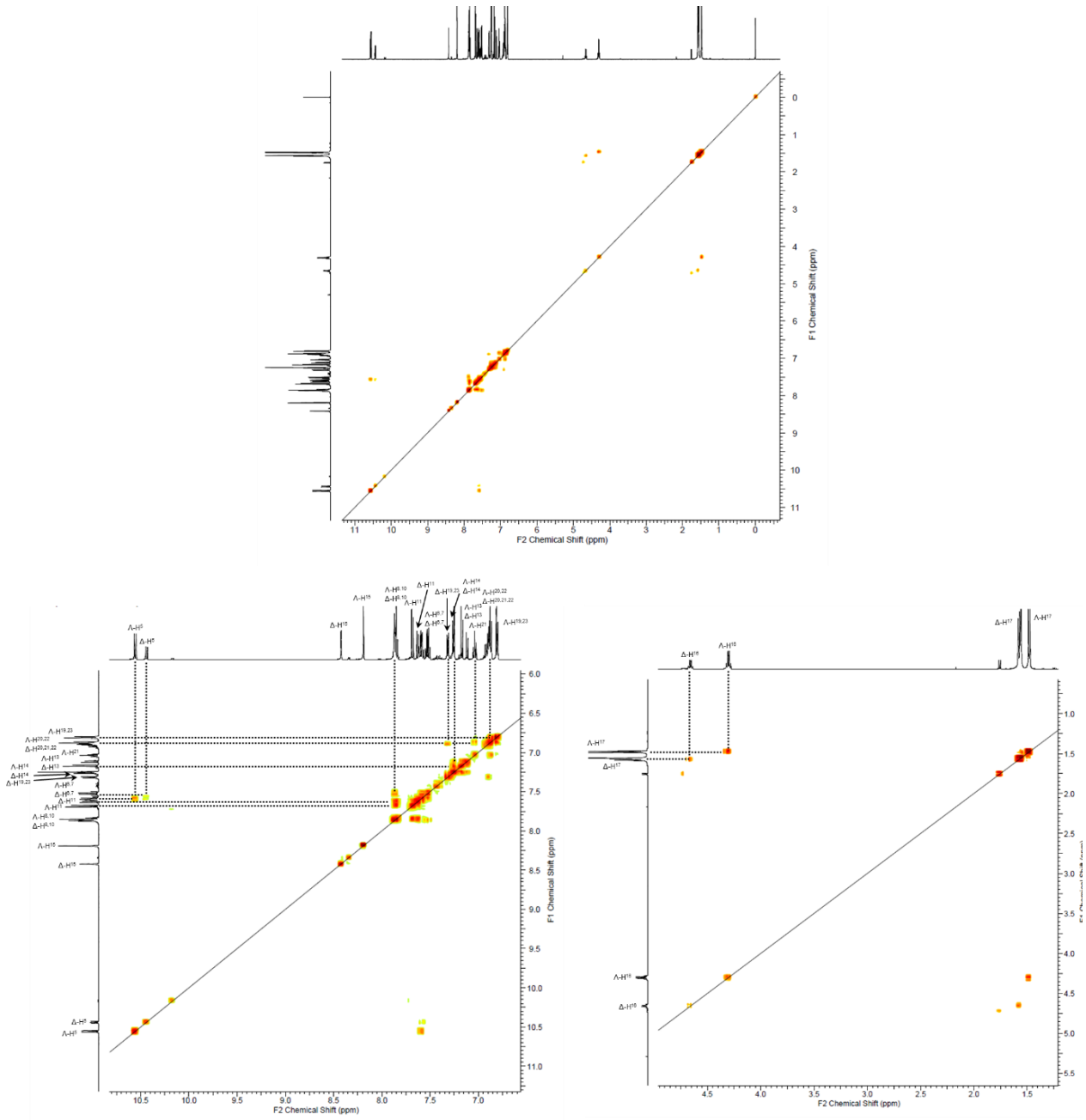


Fig. S8 gCOSY spectra of (*S*,*S*)-**2** in $CDCl_3$ (500 MHz, 298 K). Whole spectrum (upper) and enlarged spectra (lower).

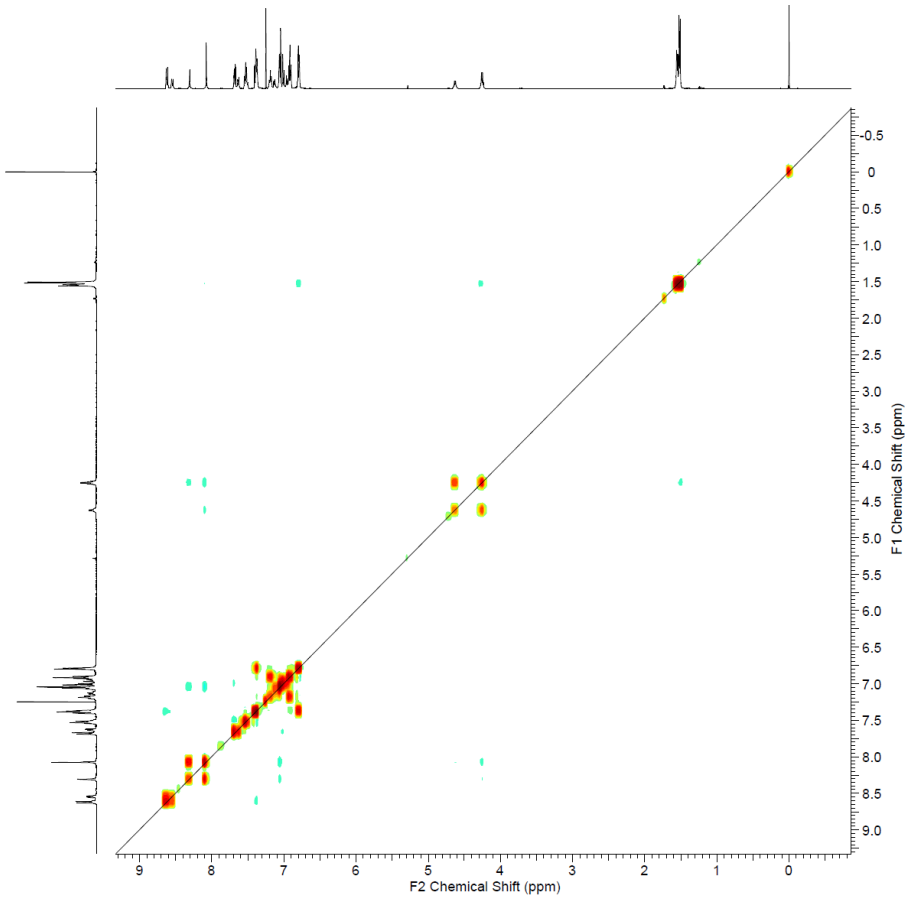


Fig. S9 NOESY spectrum of (*S*,*S*)-**1** in $CDCl_3$ (500 MHz, 298 K).

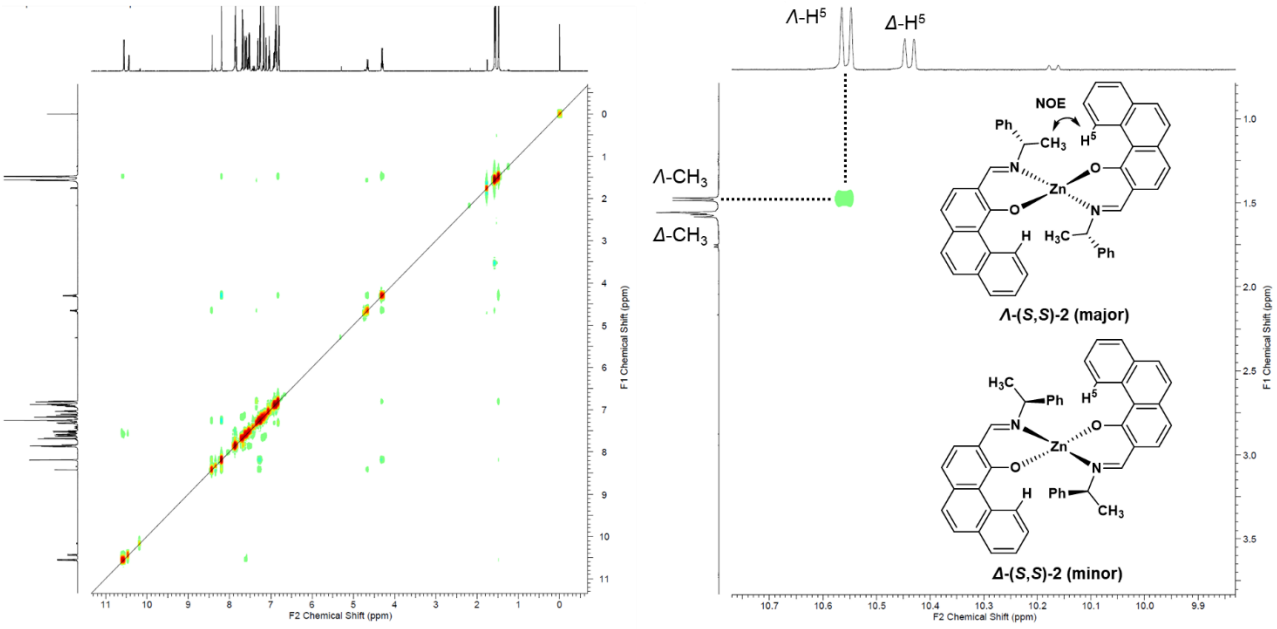


Fig. S10 NOESY spectra of (*S*,*S*)-**2** in $CDCl_3$ (500 MHz, 298 K). Whole spectrum (left) and enlarged spectrum (right).

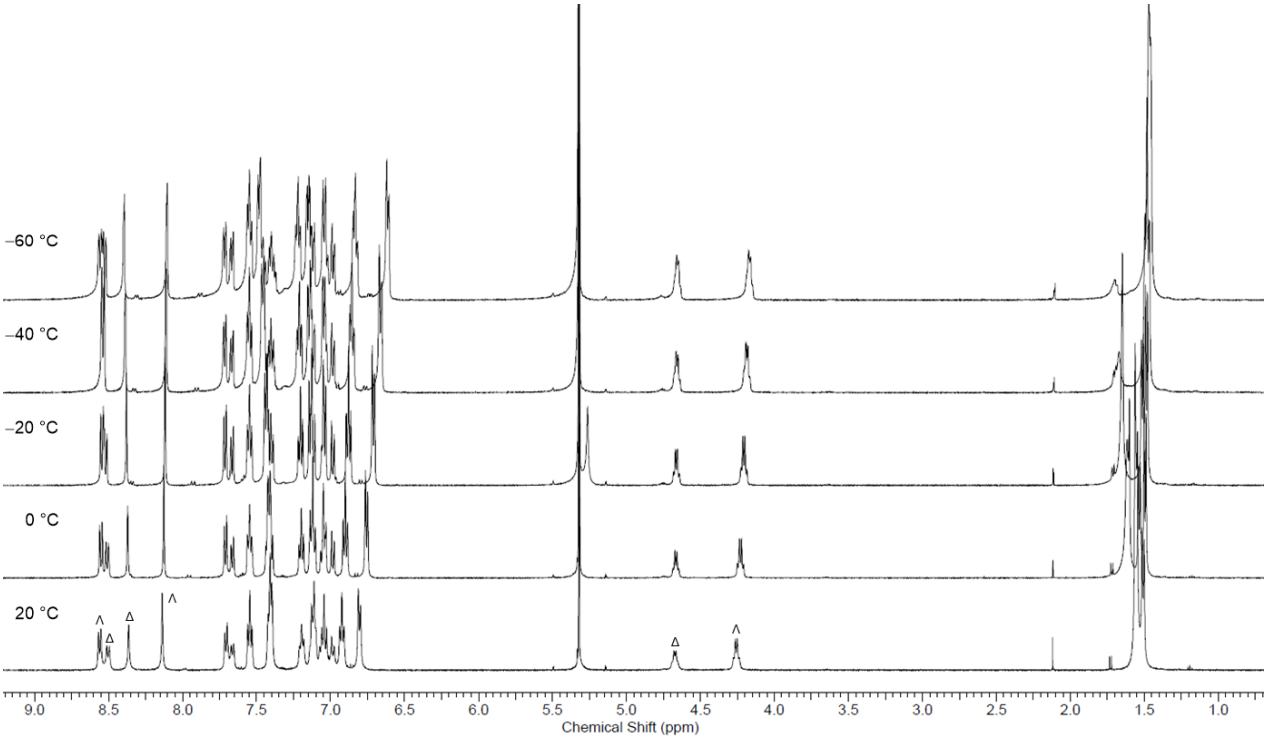


Fig. S11 ^{1}H NMR spectra of (*S*,*S*)-**1** in CD_2Cl_2 (500 MHz) at variable temperature.

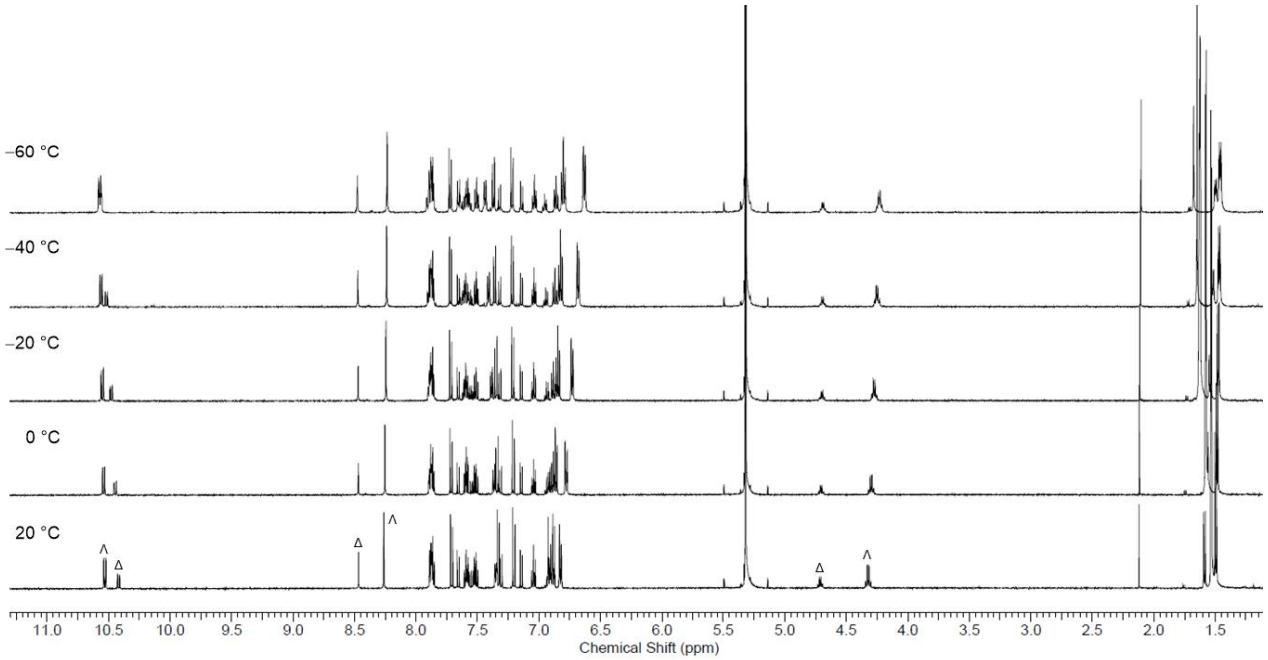


Fig. S12 ^{1}H NMR spectra of (*S*,*S*)-**2** in CD_2Cl_2 (500 MHz) at variable temperature.

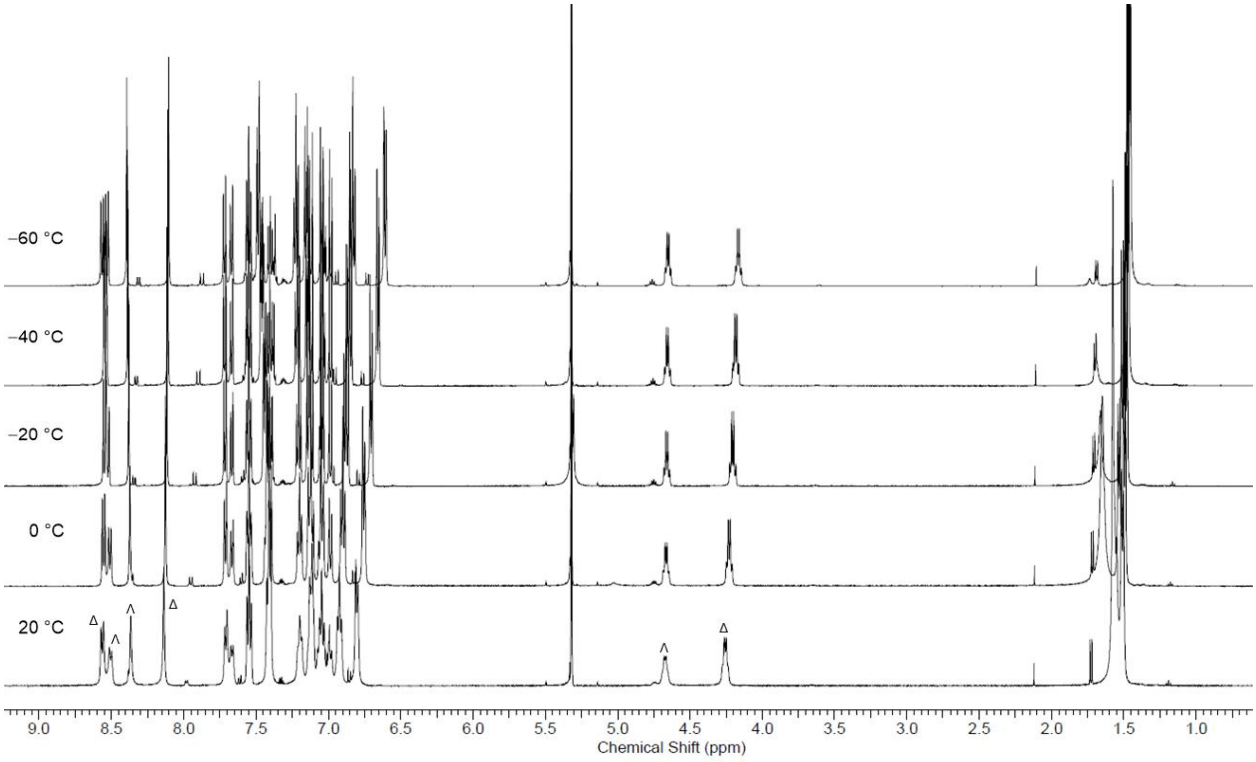


Fig. S13 ^{1}H NMR spectra of (*R*,*R*)-**1** in CD_2Cl_2 (500 MHz) at variable temperature.

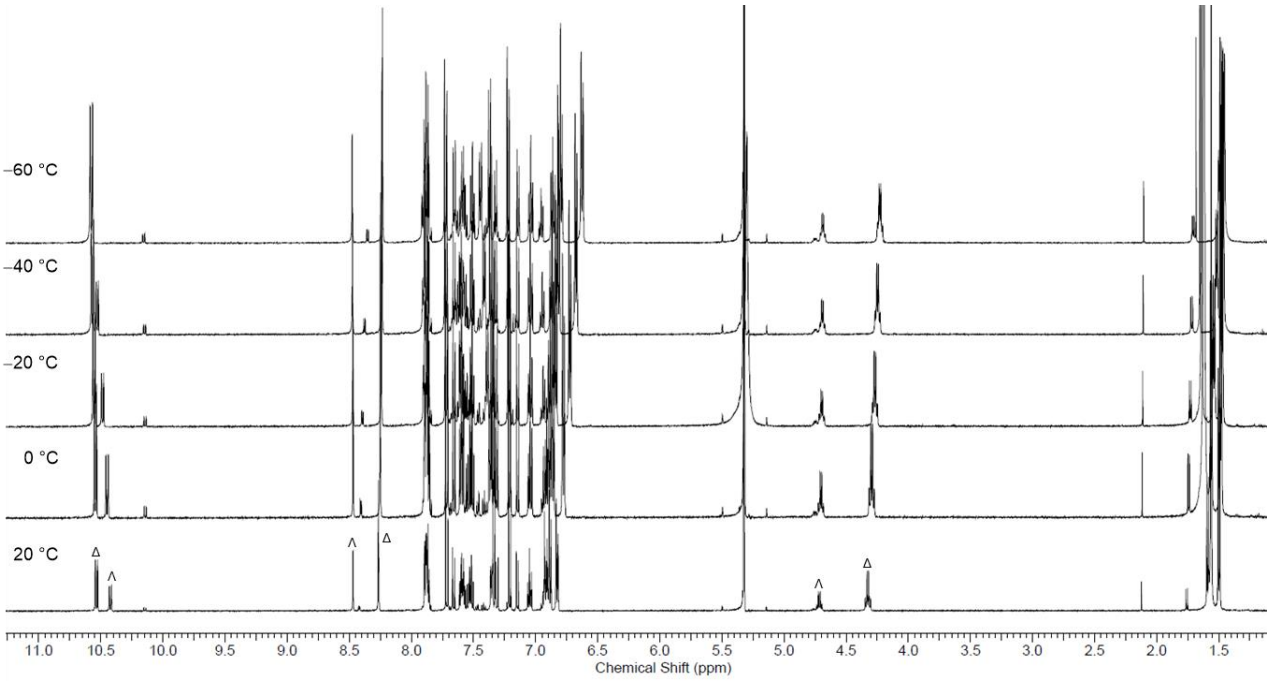


Fig. S14 ^{1}H NMR spectra of (*R*,*R*)-**2** in CD_2Cl_2 (500 MHz) at variable temperature.

3. Single Crystal X-ray Diffraction Analysis

Crystals suitable for XRD studies were analyzed using Rigaku RAXIS-RAPID imaging plate diffractometer using Mo-K_α radiation (graphite monochromated, λ = 0.71073 Å, fine focus tube, ω-scan) and Rigaku XtaLAB mini2 benchtop X-ray crystallography system equipped with a Mo rotating-anode X-ray generator with monochromated Mo-K_α radiation (λ = 0.71073 Å). The molecular structures and packings in crystals *Δ*-(*S*,*S*)-**1**, *Λ*-(*R*,*R*)-**1**, *Λ*-(*S*,*S*)-**2** and *Δ*-(*R*,*R*)-**2** were solved by direct methods and refined using the full-matrix least-squares method. In subsequent refinements, the function $\Sigma\omega(F_o^2–F_c^2)^2$ was minimized, where F_o and F_c are the observed and calculated structure factor amplitudes, respectively. The positions of non-hydrogen atoms were found from difference Fourier electron density maps and refined anisotropically. All calculations were performed using the Crystal Structure crystallographic or CrysAlisPro program software package, and illustrations were drawn by using ORTEP.

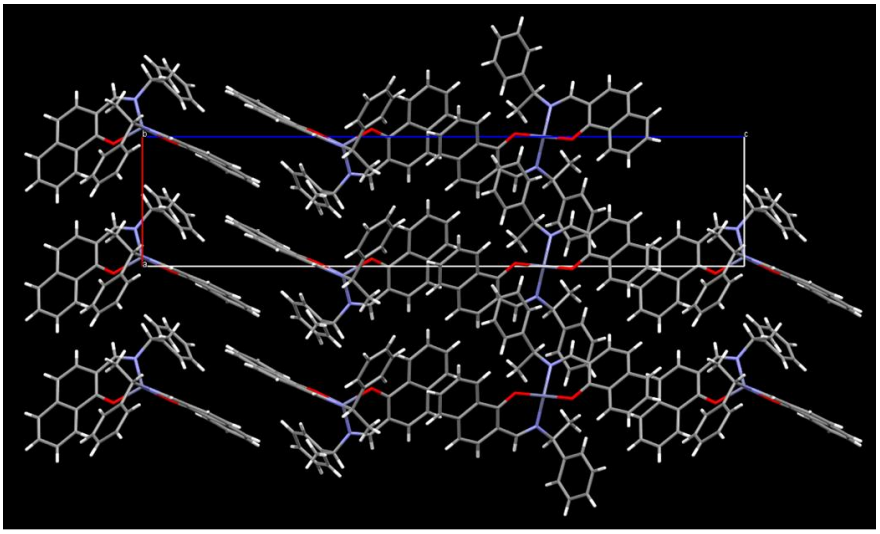


Fig. S15 The *b*-axis projections of packing structure of *Δ*-(*S*,*S*)-**1**.

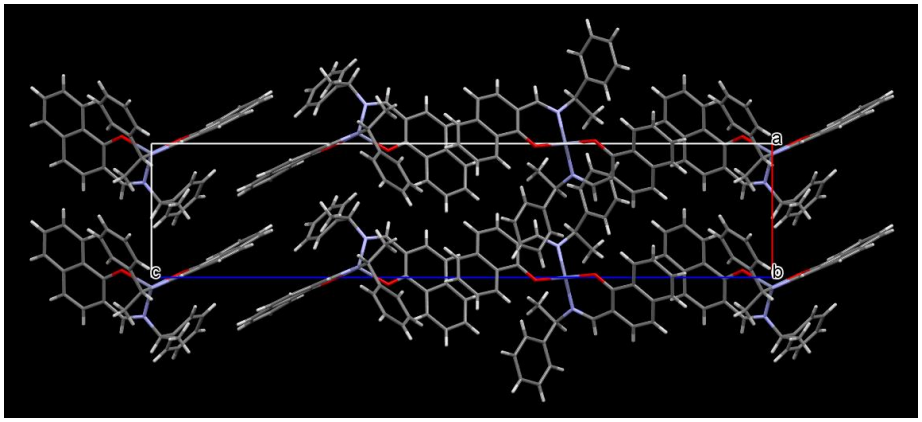


Fig. S16 The *b*-axis projections of packing structure of *Λ*-(*R*,*R*)-**1**.

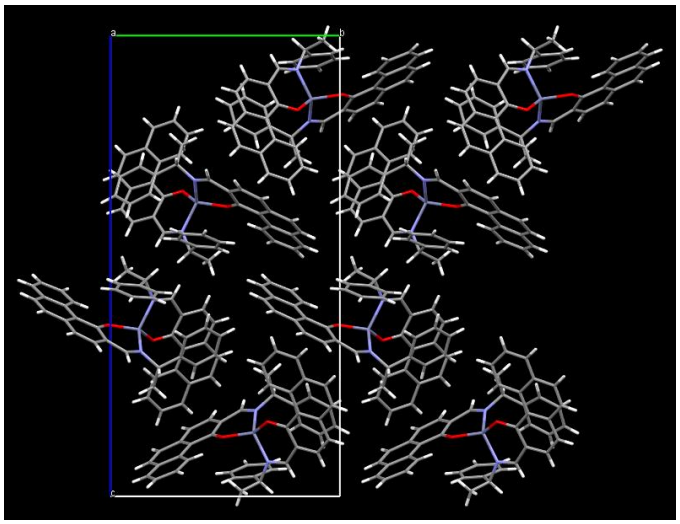


Fig. S17 The *c*-axis projections of packing structure of *Λ*-(*S*,*S*)-**2**.

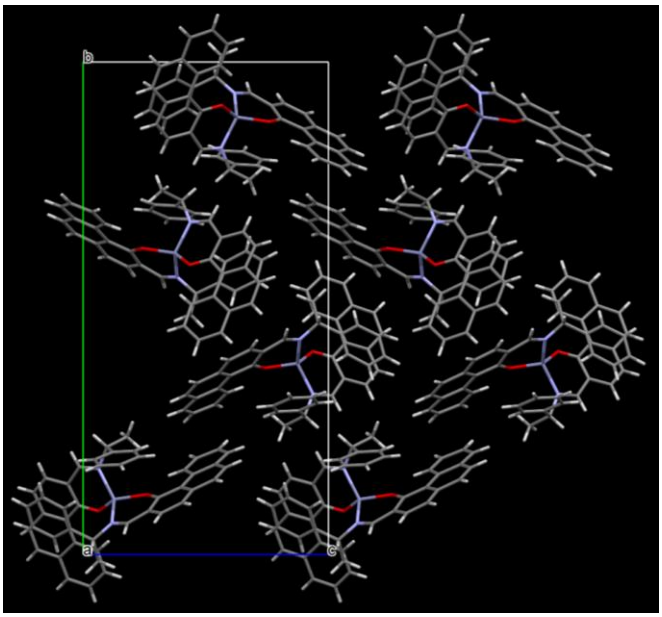


Fig. S18 The *a*-axis projections of packing structure of *Δ*-(*R*,*R*)-**2**.

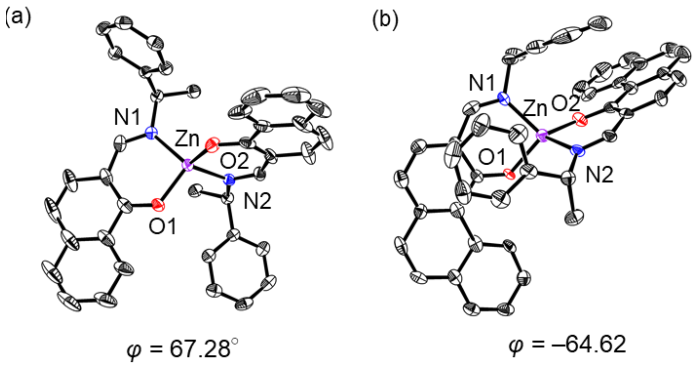


Fig. S19 ORTEP drawings of (a) *Λ*-(*R*,*R*)-**1** and (b) *Δ*-(*R*,*R*)-**2**. Thermal ellipsoids are shown at 50% probability level. Hydrogen atoms are omitted for clarity. The dihedral angles of tetrahedral geometry O(1)–N(1)–O(2)–N(2) (*φ*) are given under each structure.

Table S1. Crystal data and structural refinement details for complexes *Δ*-(*S*,*S*)-**1**, *Λ*-(*R*,*R*)-**1**, *Λ*-(*S*,*S*)-**2** and *Δ*-(*S*,*S*)-**2**.

	Δ-(*S*,*S*)-**1**	*Λ*-(*R*,*R*)-**1**	*Λ*-(*S*,*S*)-**2**	*Δ*-(*R*,*R*)-**2**
Formula	$C_{38}H_{32}N_2O_2Zn$	$C_{38}H_{32}N_2O_2Zn$	$C_{46}H_{36}N_2O_2Zn$	$C_{46}H_{36}N_2O_2Zn$
M_F	614.085	614.085	714.206	714.206
T [K]	173.15	113.15	173.15	173.15
Crystal color, habit	yellow, plate	yellow, plate	yellow, plate	yellow, plate
Crystal size [mm]	0.283×0.154×0.123	0.330×0.264×0.183	0.215×0.086×0.068	0.215×0.086×0.068
Crystal system	trigonal	trigonal	orthorhombic	orthorhombic
Space group	$P3_121$ (#152)	$P3_221$ (#154)	$P2_12_12_1$ (#19)	$P2_12_12_1$ (#19)
a [Å]	8.6360(5)	8.6028(2)	8.6130(5)	8.6225(9)
b [Å]	8.6360(5)	8.6028(2)	14.1657(8)	28.466(2)
c [Å]	34.785(2)	34.6337(8)	28.4939(15)	14.1674(11)
α [°]	90	90	90	90
β [°]	90	90	90	90
γ [°]	120	120	90	90
V [Å^3]	2246.7(2)	2219.78(12)	3476.5(3)	3477.4(5)
Z	3	3	4	4
D_{calcd} [g cm^{-3}]	1.362	1.378	1.365	1.364
Abs coeff (mm^{-1})	0.858	0.868	0.750	0.749
Abs correct	multi-scan	multi-scan	multi-scan	multi-scan
Transmiss max/min	1.0000/0.87065	1.0000/0.91994	1.0000/0.73360	1.0000/0.70332
F (000)	961.5	960.0	1490.2	1488.0
θ range (°)	5.44–51.98	5.468–60.946	4.06–50	4.056–60.942
Rflns/unique	10148/2858	30053/4401	33792/6125	31897/10053
R_{int}	0.0351	0.0412	0.0792	0.1916
Data/params	2858/310/305	4401/0/196	6125/0/462	10053/7/462
Largest diff. peak and hole (e Å^{-3})	0.62/–0.49	0.34/–0.78	0.81/–0.55	0.94/–0.70
R_1 (I > 2σ(I))[a]	0.0366	0.0390	0.0509	0.1377
wR_2 (all reflections)[b]	0.0595	0.0711	0.0908	0.1399
Goodness of fit	1.067	1.095	1.054	1.011
Flack Parameter	0.002(7)	–0.007(4)	0.001(7)	–0.04(2)
CCDC No.	2159108	2174594	2159109	2174595

[a] $R_1 = \Sigma(|F_o|-|F_c|)/ \Sigma(|F_o|)$. [b] $wR_2 = [w(F_o^2-F_c^2)^2]/wF_o^2)^2]^{1/2}$.

4. Photophysical Properties

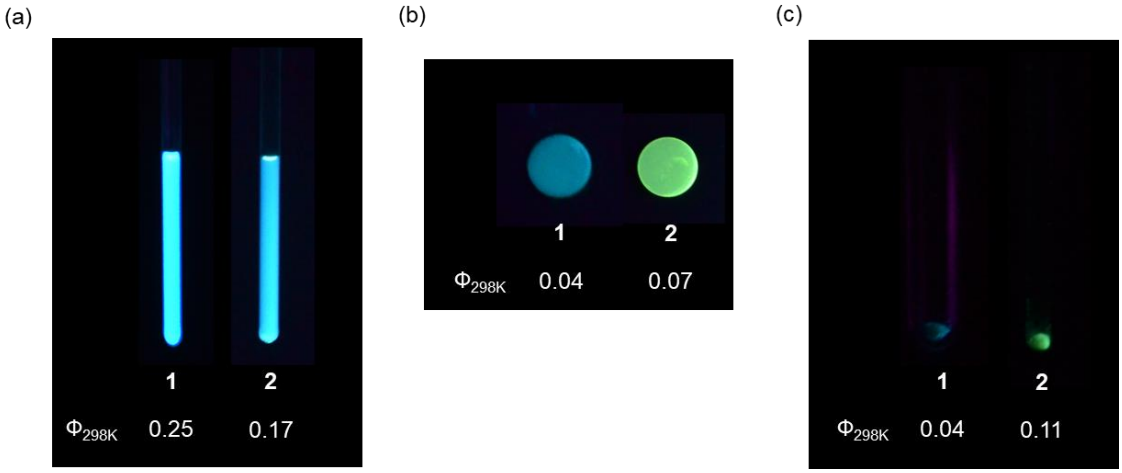


Fig. S20 Photographs of (a) CH_2Cl_2 solutions (2.0×10^{-4} M), (b) KBr-dispersed pellet and (c) crystals of (*S*,*S*)-**1** and (*S*,*S*)-**2** at 298 K under UV illumination at 365 nm.

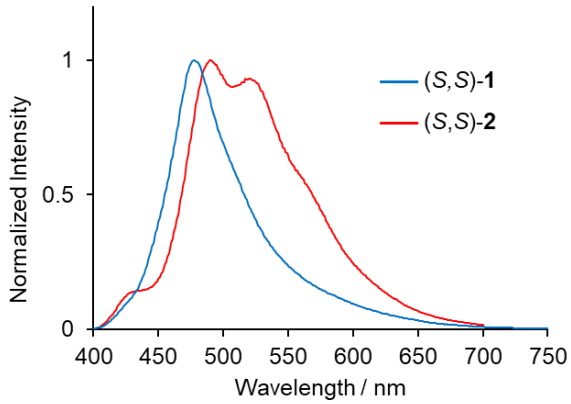


Fig. S21 Normalized emission spectra of crystals of (*S*,*S*)-**1** and (*S*,*S*)-**2** ((*S*,*S*)-**1**: λ_{ex} = 350 nm, (*S*,*S*)-**2**: λ_{ex} = 400 nm).

Table S2. Photophysical data for complexes (*S*,*S*)-**1** and (*S*,*S*)-**2**.

	Solution[a]			KBr-dispersed pellet		Crystal	
Compound	λ_{abs} [nm]	λ_{max} [nm][b]	$\Phi^{[b,d]}$	λ_{max} [nm][c]	$\Phi^{[b,d]}$	λ_{max} [nm][c]	$\Phi^{[b,d]}$
(*S*,*S*)-**1**	398, 413	462	0.25	491	0.04	478	0.04
(*S*,*S*)-**2**	408, 426	469	0.17	484, 509	0.07	489, 517	0.11

[a] Data were obtained from a 2.0×10^{-4} M solution in CH_2Cl_2 at 298 K. [b] λ_{ex} = 350 nm. [c] λ_{ex} = 350 (**1**), 400 nm (**2**). [d] Luminescent quantum efficiencies measured using the absolute method with an integrating sphere.

5. Computational Methods

All calculations were carried out based on DFT with the CAM-B3LYP exchange-correlation functional, using the Gaussian 16W program package.[S3] The basis set used was 6-31+G(d,p) for all atoms. Molecular orbitals and their eigenvalues for *Δ*-(*S*,*S*)-**1** and *Λ*-(*S*,*S*)-**2** were estimated using the optimized geometries determined by the DFT calculations using initial geometries obtained from XRD analysis. An initial structure with opposite configuration at the metal, *Λ*-(*S*,*S*)-**1** and *Δ*-(*S*,*S*)-**2**, was obtained by mirror inversion of the optimized structure of *Δ*-(*S*,*S*)-**1** and *Λ*-(*S*,*S*)-**2**, followed by manual inversion of the carbon chirality centers only. The singlet–singlet (*E*(Sn)) transition energies were estimated by time-dependent (TD) DFT calculation (CAM-B3LYP/6-31+G(d,p)).

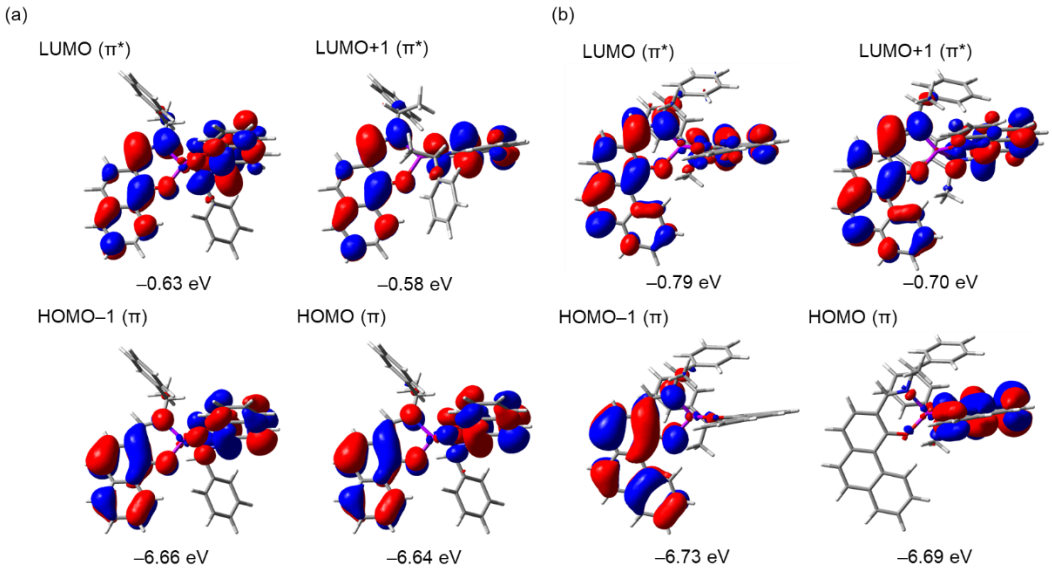


Fig. S22 Molecular orbitals and eigenvalues for the frontier orbitals of (a) *Δ*-(*S*,*S*)-**1** and (b) *Λ*-(*S*,*S*)-**2** estimated from DFT calculations (CAM-B3LYP/6-31+G(d,p)) on the basis of the optimized geometries in the ground states.

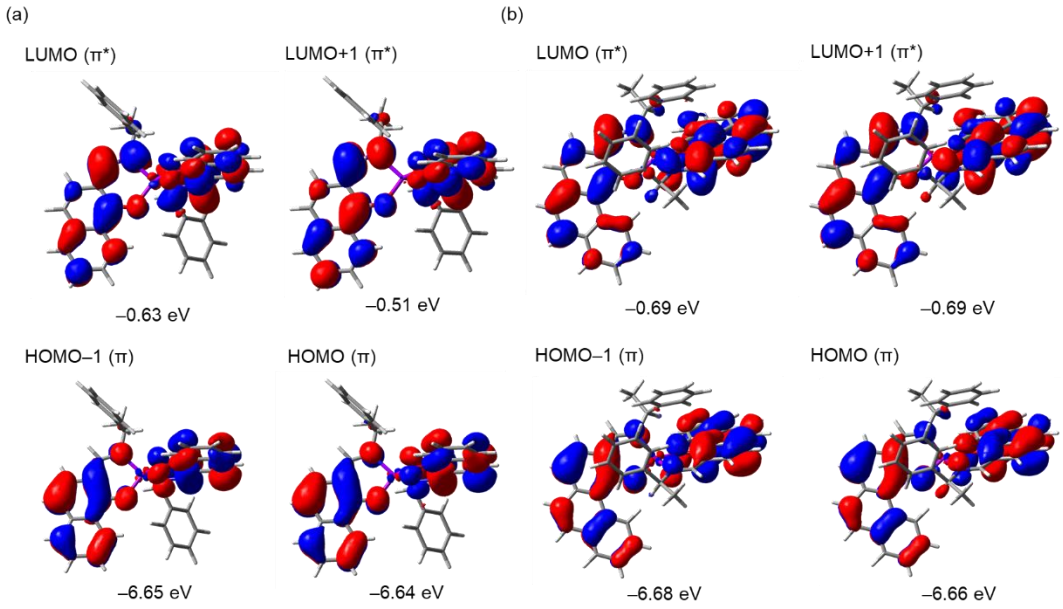


Fig. S23 Molecular orbitals and eigenvalues for the frontier orbitals of (a) *Λ*-(*S*,*S*)-**1** and (b) *Δ*-(*S*,*S*)-**2** estimated from DFT calculations (CAM-B3LYP/6-31+G(d,p)) on the basis of the optimized geometries in the ground states.

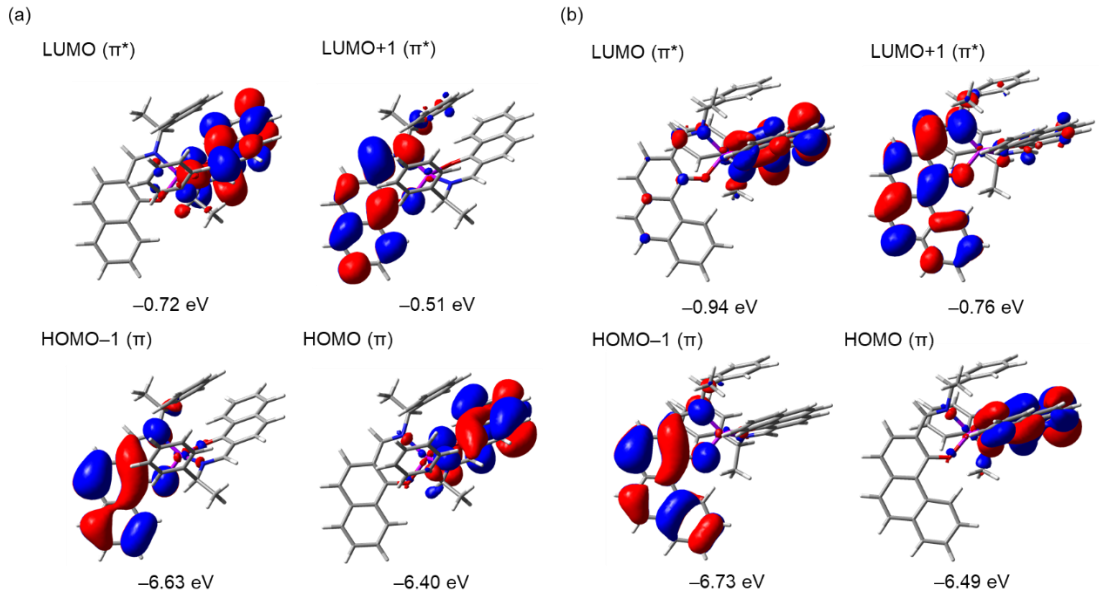


Fig. S24 Molecular orbitals and eigenvalues for the frontier orbitals of (a) *Δ*-(*S*,*S*)-**1** and (b) *Λ*-(*S*,*S*)-**2** estimated from DFT calculations (CAM-B3LYP/6-31+G(d,p)) on the basis of the optimized geometries in the S_1 excited states.

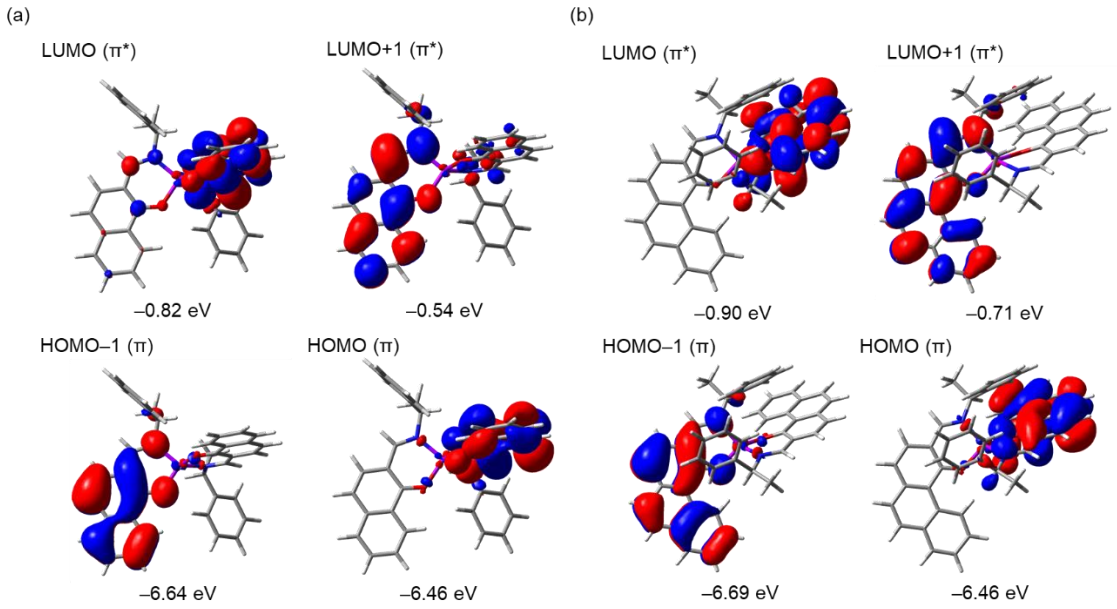


Fig. S25 Molecular orbitals and eigenvalues for the frontier orbitals of (a) *Λ*-(*S*,*S*)-**1** and (b) *Δ*-(*S*,*S*)-**2** estimated from DFT calculations (CAM-B3LYP/6-31+G(d,p)) on the basis of the optimized geometries in the S_1 excited states.

Table S3. Selected data for excitation energy, major configuration, coefficient, and oscillator strength for **1** and **2** (for the geometries optimized in the S_0 state).[a]

Compound	State	Excitation energy (eV)	Major configuration[b]	Coefficient	Oscillator strength
Δ-(*S*,*S*)-**1**	S_1	3.54 (350 nm)	HOMO→LUMO+1	0.527	0.122
	S_2	3.57 (347 nm)	HOMO→LUMO	0.527	0.265
Λ-(*S*,*S*)-**2**	S_1	3.48 (356 nm)	HOMO→LUMO+1	0.438	0.217
	S_2	3.51 (353 nm)	HOMO-1→LUMO	0.477	0.276
Λ-(*S*,*S*)-**1**	S_1	3.55 (349 nm)	HOMO→LUMO+1	0.520	0.123
	S_2	3.59 (345 nm)	HOMO→LUMO	0.524	0.280
Δ-(*S*,*S*)-**2**	S_1	3.47 (357 nm)	HOMO-1→LUMO HOMO→LUMO+1	0.487 0.476	0.0156
	S_2	3.47 (357 nm)	HOMO-1→LUMO HOMO→LUMO+1	0.487 0.476	0.0156

[a] Estimated by TD-DFT (CAM-B3LYP/6-31+G(d,p)) calculations based on the optimized geometries. [b] Molecular orbitals are shown in Fig. S20 and S21.

Table S4. Selected data for excitation energy, major configuration, coefficient, and oscillator strength for **1** and **2** (for the geometries optimized in the S_1 state).[a]

Compound	State	Excitation energy (eV)	Major configuration[b]	Coefficient	Oscillator strength
Δ-(*S*,*S*)-**1**	S_1	3.19 (389 nm)	HOMO→LUMO	0.689	0.156
Λ-(*S*,*S*)-**2**	S_1	3.13 (396 nm)	HOMO→LUMO	0.674	0.219
Λ-(*S*,*S*)-**1**	S_1	3.19 (388 nm)	HOMO→LUMO	0.684	0.180
Δ-(*S*,*S*)-**2**	S_1	3.12 (398 nm)	HOMO→LUMO	0.685	0.213

[a] Estimated by TD-DFT (CAM-B3LYP/6-31+G(d,p)) calculations based on the optimized geometries. [b] Molecular orbitals are shown in Fig. S22 and S23.

Table S5. Calculated transition dipole moments and chiroptical properties for **1** and **2** (for the geometries optimized in the S_0 state).[a]

Compound	State	$\|\boldsymbol{\mu}_e\|$[b] / 10^{-20} esu·cm	$\|\boldsymbol{\mu}_m\|$[c] / 10^{-20} erg·G^{-1}	$\cos(\theta_{e,m})$ [d]	g_{abs}[e]
Δ-(*S*,*S*)-**1**	S_1	300.84	2.457	-1	-3.27×10^{-2}
	S_2	442.18	2.146	0.9982	1.94×10^{-2}
Λ-(*S*,*S*)-**2**	S_1	405.35	2.945	0.9434	2.74×10^{-2}
	S_2	455.87	2.658	-0.9361	2.18×10^{-2}
Λ-(*S*,*S*)-**1**	S_1	301.91	2.556	1	3.39×10^{-2}
	S_2	453.55	1.919	-0.996	-1.69×10^{-2}
Δ-(*S*,*S*)-**2**	S_1	344.25	3.393	-1	-3.94×10^{-2}
	S_2	508.53	2.080	0.9928	1.62×10^{-2}

[a] Calculated at the CAM-B3LYP/6-31+G(d,p) level of theory. [b] Transition electric dipole moment (TEDM). [c] Transition magnetic dipole moment (TMDM). [d] $\cos(\theta_{e,m})$ represents the angle of TEDM and TMDM. [e] Dissymmetry factor (g_{abs}) was calculated follows: $g_{abs} = 4R/(D + G)$, where *R*, *D*, and *G* represent the rotatory, electric dipole, magnetic dipole strength ($R = |\boldsymbol{\mu}_e||\boldsymbol{\mu}_m|\cos\theta$, $D = |\boldsymbol{\mu}_e|^2$, $G = |\boldsymbol{\mu}_m|^2$)

Table S6. Calculated transition dipole moments and chiroptical properties for **1** and **2** (for the geometries optimized in the S_1 state).[a]

Compound	State	$\|\boldsymbol{\mu}_e\|$[b] / 10^{-20} esu·cm	$\|\boldsymbol{\mu}_m\|$[c] / 10^{-20} erg·G^{-1}	$\cos(\theta_{e,m})$ [d]	g_{lum}[e]
Δ-(*S*,*S*)-**1**	S_1	358.96	2.385	-0.2455	-6.52×10^{-3}
Λ-(*S*,*S*)-**2**	S_1	430.26	2.748	0.0948	2.42×10^{-3}
Λ-(*S*,*S*)-**1**	S_1	385.35	2.285	0.03629	8.61×10^{-4}
Δ-(*S*,*S*)-**2**	S_1	424.21	2.878	-0.2125	-5.77×10^{-3}

[a] Calculated at the CAM-B3LYP/6-31+G(d,p) level of theory. [b] Transition electric dipole moment (TEDM). [c] Transition magnetic dipole moment (TMDM). [d] $\cos(\theta_{e,m})$ represents the angle of TEDM and TMDM. [e] Dissymmetry factor (g_{lum}) was calculated follows: $g_{abs} = 4R/(D + G)$, where *R*, *D*, and *G* represent the rotatory, electric dipole, magnetic dipole strength ($R = |\boldsymbol{\mu}_e||\boldsymbol{\mu}_m|\cos\theta$, $D = |\boldsymbol{\mu}_e|^2$, $G = |\boldsymbol{\mu}_m|^2$)

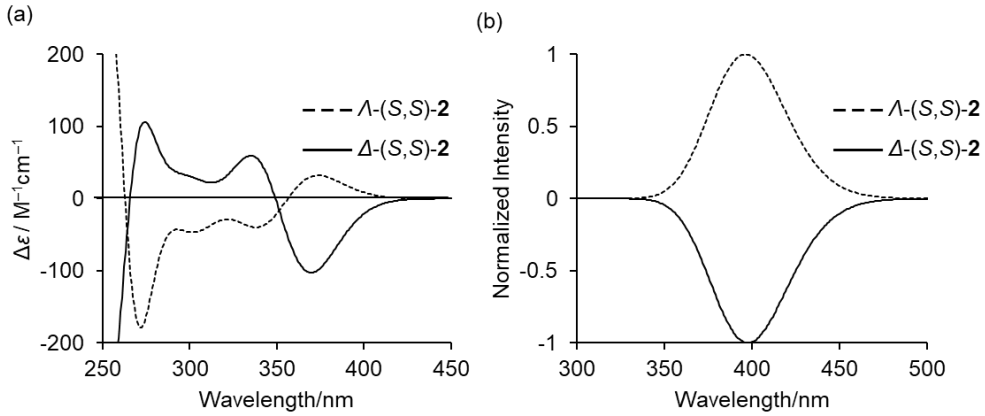


Fig. S26 Theoretical (a) CD and (b) CPL spectra of *Δ*-(*S*,*S*)-**2** and *Λ*-(*S*,*S*)-**2** estimated by TD-DFT calculation (CAM-B3LYP/6-31+G(d,p)).

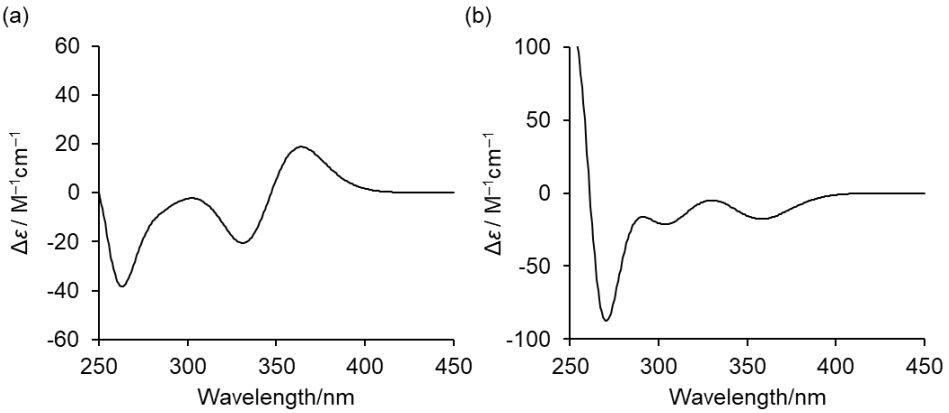


Fig. S27 Theoretical CD spectra of (a) (*S*,*S*)-**1** and (b) (*S*,*S*)-**2** simulated by 2 : 1 ratio of *Λ*-(*S*,*S*) and *Δ*-(*S*,*S*)-isomer estimated by TD-DFT calculation (CAM-B3LYP/6-31+G(d,p)).

6. Cartesian Coordinates (in Å)

Table S7. Cartesian coordinates (in angstrom) of *Δ*-(*S*,*S*)-**1** in S_0 state[a].

atom	x	y	z
Zn	-0.000001	-0.000003	-0.365121
O	1.623526	0.33089	0.62738
N	-0.014672	1.768877	-1.318927
C	-2.336272	4.426589	-1.981517
H	-1.848878	4.748601	-2.898343
C	-1.112252	2.23061	-2.198868
H	-0.662018	2.804491	-3.019088
C	2.129935	2.469602	-0.319655
C	-2.065314	3.160281	-1.465241
C	0.97336	2.592822	-1.153431
H	0.92948	3.533405	-1.71466
C	-3.227335	5.283769	-1.33891
H	-3.426839	6.266281	-1.755104
C	3.561364	1.422936	1.388126
C	2.379012	1.37557	0.544757
C	-2.698957	2.760883	-0.285134
H	-2.494642	1.780562	0.135789
C	-1.843649	1.034653	-2.802498
H	-1.152465	0.393895	-3.356546
H	-2.621132	1.380971	-3.487467
H	-2.326762	0.435949	-2.025561
C	3.061403	3.559004	-0.358424
H	2.847082	4.384114	-1.033035
C	3.820314	0.373668	2.294649
H	3.111349	-0.444329	2.345591
C	-3.854704	4.879472	-0.166439
H	-4.548389	5.543769	0.339056
C	4.453886	2.518447	1.312459
C	-3.586622	3.616112	0.357047
H	-4.073622	3.292916	1.271809
C	4.936062	0.399962	3.09911
H	5.124561	-0.408439	3.798099
C	5.595667	2.518164	2.145365
H	6.284564	3.355877	2.08752
C	4.179553	3.593293	0.408629
H	4.867184	4.430868	0.356504
C	5.833385	1.482367	3.0188
H	6.714415	1.500618	3.652962
O	-1.623524	-0.3309	0.627385
N	0.014668	-1.76888	-1.318932
C	2.336279	-4.426582	-1.981517
H	1.848886	-4.7486	-2.898341

C	1.112247	-2.230611	-2.198875
H	0.662013	-2.804497	-3.019093
C	-2.129939	-2.469606	-0.319661
C	2.065315	-3.160273	-1.465246
C	-0.973366	-2.592824	-1.153438
H	-0.929488	-3.533404	-1.714672
C	3.227349	-5.283753	-1.338907
H	3.426858	-6.266266	-1.755096
C	-3.561364	-1.422945	1.388127
C	-2.379012	-1.375577	0.544757
C	2.698958	-2.760865	-0.285142
H	2.494639	-1.780543	0.135776
C	1.843637	-1.034652	-2.802511
H	1.152449	-0.393899	-3.35656
H	2.62112	-1.380968	-3.487481
H	2.326748	-0.435944	-2.025577
C	-3.06141	-3.559006	-0.358435
H	-2.847091	-4.384113	-1.03305
C	-3.82031	-0.373681	2.294656
H	-3.111343	0.444313	2.345602
C	3.854718	-4.879447	-0.166439
H	4.548407	-5.543737	0.339057
C	-4.453888	-2.518453	1.312455
C	3.586629	-3.616086	0.357041
H	4.073629	-3.292883	1.271801
C	-4.936057	-0.399976	3.099118
H	-5.124554	0.408421	3.798112
C	-5.595668	-2.518172	2.145363
H	-6.284568	-3.355883	2.087514
C	-4.179559	-3.593296	0.408619
H	-4.867192	-4.430869	0.356491
C	-5.833383	-1.482379	3.018803
H	-6.714413	-1.500631	3.652967

[a] The geometry was optimized by DFT calculation (CAM-B3LYP/6-31+G(d,p)).

Table S8. Cartesian coordinates (in angstrom) of *Λ*-(*S*,*S*)-**2** in S_0 state[a].

atom	x	y	z
Zn	0.020543	-0.251668	0.012424
O	-1.624398	0.756949	-0.061535
O	1.704569	0.703735	-0.016733
N	0.289831	-0.956978	1.870025
N	-0.294495	-1.216044	-1.719892
C	-5.176449	3.140229	0.512389
C	2.670577	0.705604	0.844848
C	-6.282159	2.81776	-0.334046
H	-7.218207	3.349404	-0.188178
C	-2.628655	0.622882	-0.865359
C	-3.933774	2.463956	0.352885
C	4.948952	1.35866	1.490705
C	-1.530219	-2.621989	1.788723
C	-4.276332	4.514418	2.297702
H	-4.399663	5.292978	3.043669
C	4.026866	2.353157	-0.577152
C	-2.7589	-2.341229	1.190765
H	-3.219244	-1.368544	1.318748
C	-1.445566	-1.096547	-2.299581
H	-1.583053	-1.661093	-3.229214
C	-3.734083	-0.486639	-2.765338
H	-3.681015	-1.205027	-3.579412
C	1.41945	-0.775867	2.472267
H	1.515501	-1.211081	3.474422
C	3.873255	1.476883	0.581748
C	1.395305	-3.035332	-1.568011
C	-4.87943	0.212861	-2.547629
H	-5.754003	0.062574	-3.171486
C	-0.787515	-1.608267	2.644071
H	-0.314226	-2.166485	3.463314
C	-2.870165	2.879171	1.194888
H	-1.907806	2.407982	1.085932
C	2.589025	-0.058024	2.045246
C	-3.824071	1.425171	-0.668623
C	-4.937507	1.172245	-1.501419
C	2.363364	-2.700562	-0.619059
H	2.658533	-1.666006	-0.485612
C	-2.594083	-0.311969	-1.939317
C	3.002059	2.628363	-1.518555
H	2.037539	2.168075	-1.38561
C	-6.163011	1.885781	-1.305942
H	-6.999211	1.654986	-1.95886

C	-3.038879	3.874026	2.134383
H	-2.194876	4.164887	2.752347
C	-5.325136	4.147403	1.489541
H	-6.290922	4.635951	1.584032
C	6.180722	2.045332	1.245756
H	6.987635	1.919902	1.961222
C	5.273838	3.009606	-0.77935
C	-1.678625	-0.528991	3.258479
H	-1.093527	0.081292	3.951429
H	-2.507015	-0.981595	3.809959
H	-2.083779	0.135188	2.492088
C	3.211097	3.474448	-2.586771
H	2.395855	3.661941	-3.278879
C	-2.84664	-4.561233	0.248701
H	-3.360252	-5.313681	-0.341704
C	1.73922	-1.015411	-3.073954
H	1.229616	-0.360854	-3.786343
H	2.520399	-1.56765	-3.60294
H	2.207885	-0.383616	-2.316774
C	0.736458	-1.986809	-2.446651
H	0.231668	-2.525304	-3.259156
C	1.054944	-4.37889	-1.726758
H	0.304803	-4.656388	-2.462308
C	4.84657	0.564007	2.664115
H	5.693931	0.513467	3.339413
C	-0.968452	-3.88683	1.598869
H	-0.006754	-4.1181	2.048813
C	-1.618958	-4.850938	0.838831
H	-1.165751	-5.827905	0.706711
C	-3.411521	-3.302833	0.423065
H	-4.365385	-3.062651	-0.035669
C	3.693651	-0.103139	2.934996
H	3.604837	-0.691615	3.844688
C	5.464595	3.862226	-1.887505
H	6.432535	4.340082	-2.010217
C	6.341147	2.82496	0.153154
H	7.281843	3.336984	-0.02851
C	4.452923	4.095505	-2.78737
H	4.608294	4.755819	-3.634525
C	2.623927	-5.022813	-0.014726
H	3.106269	-5.791648	0.580821
C	2.968419	-3.684665	0.155921
H	3.720703	-3.401992	0.885771
C	1.665193	-5.36827	-0.961723
H	1.393248	-6.408992	-1.1087

[a] The geometry was optimized by DFT calculation (CAM-B3LYP/6-31+G(d,p)).

Table S9. Cartesian coordinates (in angstrom) of *Λ*-(*S*,*S*)-**1** in S_0 state[a].

atom	x	y	z
Zn	0.000001	0.000003	0.230893
O	-1.713218	-0.118637	-0.659127
N	-0.137503	-1.761819	1.146525
C	1.41751	-4.759985	2.219849
H	0.88239	-4.802134	3.162574
C	0.952083	-2.242498	2.034722
C	-2.280012	-2.326216	0.084589
C	1.550578	-3.551453	1.539095
C	-1.129419	-2.560094	0.903665
H	-1.099534	-3.554428	1.360895
C	1.978581	-5.930211	1.708096
H	1.866268	-6.862446	2.252806
C	-3.711822	-1.058094	-1.465305
C	-2.506847	-1.138707	-0.655883
C	2.26301	-3.534097	0.334837
H	2.373161	-2.594492	-0.200731
C	-3.23848	-3.38993	0.016676
H	-3.034976	-4.290627	0.590505
C	-3.964072	0.096689	-2.234866
H	-3.234363	0.897157	-2.207001
C	2.680495	-5.902598	0.509837
H	3.118984	-6.812346	0.112337
C	-4.634198	-2.130979	-1.492475
C	2.822758	-4.697196	-0.176146
H	3.374776	-4.664359	-1.110137
C	-5.100045	0.194523	-3.004734
H	-5.283894	1.085493	-3.596332
C	-5.795178	-2.004096	-2.288618
H	-6.50598	-2.82512	-2.309809
C	-4.370644	-3.310054	-0.726265
H	-5.079162	-4.1312	-0.755368
C	-6.025042	-0.867127	-3.027904
H	-6.921642	-0.788289	-3.635082
O	1.71321	0.118621	-0.65915
N	0.137516	1.761846	1.146481
C	-1.417483	4.760039	2.219749
H	-0.882352	4.802211	3.162467
C	-0.952059	2.242548	2.034679
C	2.280013	2.326217	0.084507
C	-1.55056	3.551491	1.539027
C	1.129429	2.560116	0.903591
H	1.09955	3.554461	1.360797

C	-1.97856	5.930254	1.707975
H	-1.86624	6.862502	2.25266
C	3.711804	1.058058	-1.465373
C	2.506839	1.138691	-0.655939
C	-2.263006	3.534106	0.334777
H	-2.373164	2.594488	-0.200766
C	3.238482	3.38993	0.016558
H	3.034984	4.290641	0.590368
C	3.964045	-0.096744	-2.23491
H	3.234336	-0.89721	-2.207018
C	-2.680488	5.902611	0.509724
H	-3.118982	6.81235	0.112208
C	4.634181	2.130942	-1.492579
C	-2.82276	4.697193	-0.176227
H	-3.374788	4.664333	-1.110211
C	5.100009	-0.194596	-3.004788
H	5.283852	-1.08558	-3.596368
C	5.795152	2.004039	-2.288732
H	6.505954	2.825063	-2.309951
C	4.370637	3.310035	-0.726394
H	5.079155	4.13118	-0.755525
C	6.025007	0.867053	-3.027994
H	6.9216	0.7882	-3.63518
C	-0.485426	2.249666	3.488526
H	0.338177	2.951298	3.649177
H	-1.305538	2.520516	4.158556
H	-0.129077	1.254552	3.765344
C	0.485466	-2.249581	3.488574
H	-0.338135	-2.951209	3.649252
H	1.305586	-2.520414	4.158602
H	0.12912	-1.25446	3.765372
H	-1.739759	1.488712	1.945208
H	1.739781	-1.488664	1.945224

[a] The geometry was optimized by DFT calculation (CAM-B3LYP/6-31+G(d,p)).

Table S10. Cartesian coordinates (in angstrom) of *Δ*-(*S*,*S*)-**2** in S_0 state[a].

atom	x	y	z
Zn	0.000041	-0.097275	-0.000112
O	-1.740492	-0.923736	-0.145991
O	1.740581	-0.923718	0.145276
N	0.026339	0.632479	1.864617
N	-0.026587	0.634026	-1.864156
C	-5.70404	-2.518629	0.454224
C	2.65876	-0.717756	1.034674
C	-6.675123	-2.160989	-0.532188
H	-7.697859	-2.502386	-0.399738
C	-2.658881	-0.716766	-1.034936
C	-4.352641	-2.091751	0.314824
C	4.984397	-0.965256	1.792874
C	-1.805821	2.2697	1.664771
C	-5.190778	-3.703331	2.508868
H	-5.503073	-4.315433	3.348884
C	4.352924	-2.091078	-0.316306
C	-3.07509	2.189594	1.092629
H	-3.635549	1.261742	1.161169
C	-1.108149	0.581206	-2.567924
H	-1.074503	0.974276	-3.585633
C	-3.430309	0.271707	-3.153156
H	-3.20059	0.844558	-4.048078
C	1.107709	0.578736	2.568612
H	1.073885	0.970815	3.586694
C	3.989624	-1.266173	0.834465
C	1.805642	2.271074	-1.663495
C	-4.690928	-0.197742	-2.951362
H	-5.481387	-0.005177	-3.668825
C	-1.250847	1.091917	2.448876
C	-3.442737	-2.52818	1.312478
H	-2.406466	-2.24821	1.225251
C	2.396384	0.042737	2.210629
C	-3.989678	-1.265446	-0.835043
C	-4.984715	-0.963389	-1.79282
C	3.074681	2.190297	-1.09089
H	3.634851	1.262286	-1.159635
C	-2.396798	0.045046	-2.210115
C	3.443309	-2.526359	-1.314727
H	2.406989	-2.246603	-1.227401
C	-6.327301	-1.427684	-1.612768
H	-7.063231	-1.169016	-2.367993
C	-3.851491	-3.309477	2.372786

H	-3.118337	-3.626657	3.108264
C	-6.097272	-3.310753	1.553706
H	-7.13867	-3.611815	1.625963
C	6.327042	-1.429304	1.61263
H	7.062754	-1.171545	2.368379
C	5.704382	-2.517716	-0.455875
C	3.852388	-3.306317	-2.375895
H	3.119443	-3.622649	-3.111945
C	-2.911964	4.472158	0.334971
H	-3.341263	5.328187	-0.176156
C	1.250595	1.093717	-2.448222
C	1.089143	3.463282	-1.549211
H	0.089148	3.536232	-1.967248
C	4.69029	-0.200999	2.952253
H	5.480547	-0.00931	3.670173
C	-1.088938	3.461718	1.550695
H	-0.088745	3.534105	1.968353
C	-1.639466	4.557159	0.895143
H	-1.072646	5.479731	0.819865
C	-3.626934	3.282921	0.430257
H	-4.61432	3.200836	-0.012651
C	3.429633	0.268263	3.154231
H	3.199682	0.840088	4.049748
C	6.097952	-3.308455	-1.556233
H	7.139387	-3.609368	-1.628583
C	6.675185	-2.161262	0.531242
H	7.697967	-2.502467	0.398651
C	5.191738	-3.699905	-2.512121
H	5.504295	-4.310944	-3.352814
C	2.912034	4.472587	-0.33233
H	3.341422	5.32825	0.179336
C	3.626641	3.283138	-0.427838
H	4.613827	3.200536	0.015418
C	1.639807	4.558266	-0.892983
H	1.073279	5.481006	-0.81757
C	-1.229336	1.397417	3.946967
H	-0.594153	2.254258	4.190376
H	-2.245119	1.648317	4.25966
H	-0.901381	0.534307	4.533625
H	-1.939452	0.255486	2.290666
H	1.939189	0.257208	-2.290429
C	1.22902	1.399894	-3.946161
H	2.244812	1.650752	-4.258857
H	0.900836	0.537094	-4.533146
H	0.593966	2.256949	-4.189157

[a] The geometry was optimized by DFT calculation (CAM-B3LYP/6-31+G(d,p)).

Table S11. Cartesian coordinates (in angstrom) of *Δ*-(*S*,*S*)-**1** in S_1 state[a].

atom	x	y	z
Zn	0.128246	-0.606705	-0.276643
O	-1.555385	-1.620873	-0.492401
O	1.932296	-1.195106	-0.670185
N	0.360013	-0.63207	1.711675
N	-0.282519	0.727508	-1.667159
C	-5.117301	-3.550886	0.468337
C	2.901558	-1.305533	0.176098
C	-6.334444	-3.079265	-0.053028
H	-7.264513	-3.584204	0.182249
C	-2.648389	-1.129881	-0.964037
C	-3.917912	-2.920232	0.175894
C	5.327776	-1.758436	0.524946
C	-1.539608	0.822723	2.292691
C	4.390617	-1.849814	-1.728882
C	-2.912647	0.856574	2.048809
H	-3.468018	-0.074719	1.977032
C	-1.494441	0.826117	-2.189441
H	-1.663126	1.544333	-2.989901
C	-3.884254	0.460516	-2.346158
H	-3.907394	1.326646	-3.002372
C	1.519982	-0.861117	2.238193
H	1.592363	-0.882403	3.326894
C	4.216962	-1.641503	-0.34447
C	1.226176	2.642813	-1.32201
C	-5.084835	-0.180226	-2.055131
H	-6.006762	0.190319	-2.493086
C	-0.849672	-0.507138	2.546912
C	2.764861	-1.123467	1.573893
C	-3.887806	-1.77558	-0.650134
C	-5.129926	-1.303448	-1.195693
C	2.461094	2.647219	-0.673886
H	3.136649	1.806662	-0.806961
C	-2.649825	0.060991	-1.824117
C	-6.327459	-1.964372	-0.881617
H	-7.256032	-1.591482	-1.305245
C	6.588806	-2.076799	-0.028964
H	7.443376	-2.166326	0.635551
C	5.62822	-2.161843	-2.242822
C	-2.86812	3.265288	1.968093
H	-3.382261	4.213166	1.843263
C	0.843816	1.482655	-2.233068
C	0.365326	3.726168	-1.130527

H	-0.610296	3.731503	-1.607733
C	5.148315	-1.560499	1.929911
H	6.001414	-1.657427	2.593269
C	-0.835687	2.025553	2.358284
H	0.238005	2.016302	2.521915
C	-1.49539	3.239259	2.199758
H	-0.932005	4.165004	2.247415
C	-3.575456	2.070028	1.888205
H	-4.643678	2.078481	1.695738
C	3.91503	-1.266259	2.41519
H	3.779549	-1.128074	3.485238
C	6.737575	-2.273668	-1.382263
H	7.713698	-2.518855	-1.789546
C	1.97789	4.794678	0.311891
H	2.27037	5.63146	0.938585
C	2.836488	3.714453	0.139616
H	3.802847	3.700327	0.634115
C	0.738296	4.795567	-0.325962
H	0.059806	5.633061	-0.194178
C	-0.654201	-0.72979	4.047829
H	-0.020645	0.038577	4.500969
H	-1.630798	-0.67156	4.533067
H	-0.23021	-1.714877	4.263924
H	-1.521468	-1.290479	2.178694
H	1.687236	0.783988	-2.215274
C	0.668604	1.94137	-3.68305
H	1.618902	2.345768	-4.039964
H	0.387778	1.10286	-4.326695
H	-0.077713	2.732558	-3.793286
H	-5.113643	-4.427223	1.109488
H	-2.981749	-3.29953	0.56835
H	3.521358	-1.762894	-2.370094
H	5.751711	-2.323336	-3.308813

[a] The geometry was optimized by DFT calculation (CAM-B3LYP/6-31+G(d,p)).

Table S12. Cartesian coordinates (in angstrom) of *Λ*-(*S*,*S*)-**2** in S_1 state[a].

atom	x	y	z
Zn	0.055974	0.328285	0.040028
O	-1.568726	-0.785887	0.186217
O	1.723999	-0.651636	0.050011
N	0.20949	0.864148	-1.878299
N	-0.28966	1.348572	1.688667
C	-5.111466	-3.189961	-0.440036
C	2.653754	-0.698262	-0.848828
C	-6.26187	-2.81366	0.313031
H	-7.19451	-3.340228	0.139709
C	-2.612738	-0.621155	0.911842
C	-3.851627	-2.522938	-0.241002
C	4.909688	-1.373051	-1.549014
C	-1.690243	2.435643	-1.813077
C	-4.110006	-4.667351	-2.091124
H	-4.202291	-5.482196	-2.802349
C	4.090078	-2.233375	0.619756
C	-2.971024	2.175994	-1.325696
H	-3.449283	1.223404	-1.523033
C	-1.458105	1.226025	2.296811
H	-1.606988	1.832841	3.193993
C	-3.755943	0.613652	2.695981
H	-3.76743	1.378857	3.466951
C	1.315281	0.654623	-2.51628
H	1.359511	1.0179	-3.550184
C	3.876031	-1.43897	-0.587501
C	1.427458	3.11507	1.465156
C	-4.913061	-0.124726	2.460634
H	-5.801536	0.076299	3.051508
C	-0.913505	1.433268	-2.651902
H	-0.483503	1.988014	-3.497441
C	-2.741419	-3.011498	-0.979133
H	-1.775289	-2.5606	-0.823415
C	2.512005	-0.016773	-2.092705
C	-3.786957	-1.423851	0.703082
C	-4.968795	-1.129468	1.478303
C	2.423092	2.704859	0.575645
H	2.724785	1.664013	0.541884
C	-2.58691	0.414438	1.960817
C	3.112457	-2.448237	1.624928
H	2.139685	-2.001406	1.507157
C	-6.176272	-1.828781	1.256723
H	-7.043228	-1.561461	1.854123

C	-2.866396	-4.051149	-1.87697
H	-1.989786	-4.397343	-2.415125
C	-5.206413	-4.241331	-1.376932
H	-6.171289	-4.720266	-1.515399
C	6.157537	-2.033761	-1.314942
H	6.930896	-1.95024	-2.072358
C	5.350697	-2.867746	0.807977
C	-1.756235	0.290977	-3.217595
H	-1.144898	-0.32035	-3.88631
H	-2.604673	0.680371	-3.786573
H	-2.129216	-0.35922	-2.422761
C	3.377527	-3.218708	2.736999
H	2.597311	-3.360996	3.478477
C	-3.067998	4.364309	-0.313695
H	-3.604096	5.11283	0.261449
C	1.701586	1.204737	3.12548
H	1.155098	0.594689	3.849942
H	2.462218	1.784053	3.657232
H	2.201776	0.52899	2.428367
C	0.728362	2.137916	2.395874
H	0.212204	2.74118	3.154627
C	1.081899	4.466842	1.497336
H	0.311945	4.803121	2.186374
C	4.748419	-0.657476	-2.766124
H	5.565698	-0.644161	-3.479218
C	-1.106726	3.673778	-1.531894
H	-0.103731	3.888033	-1.891222
C	-1.787332	4.63166	-0.791242
H	-1.315342	5.586822	-0.586338
C	-3.6549	3.132662	-0.578969
H	-4.649773	2.909447	-0.20691
C	3.577663	-0.01953	-3.030065
H	3.443688	0.507618	-3.971243
C	5.599033	-3.642786	1.960802
H	6.5756	-4.106039	2.070521
C	6.373433	-2.738938	-0.181965
H	7.325952	-3.231964	-0.009588
C	4.631928	-3.819402	2.920554
H	4.831651	-4.419794	3.802296
C	2.690394	4.965778	-0.227481
H	3.183727	5.681516	-0.877687
C	3.044196	3.619897	-0.268943
H	3.815194	3.277957	-0.952515
C	1.708196	5.388099	0.663592
H	1.43106	6.436866	0.712576

[a] The geometry was optimized by DFT calculation (CAM-B3LYP/6-31+G(d,p)).

Table S13. Cartesian coordinates (in angstrom) of *Λ*-(*S*,*S*)-**1** in S_1 state[a].

atom	x	y	z
Zn	0.128246	-0.606705	-0.276643
O	-1.555385	-1.620873	-0.492401
O	1.932296	-1.195106	-0.670185
N	0.360013	-0.63207	1.711675
N	-0.282519	0.727508	-1.667159
C	-5.117301	-3.550886	0.468337
C	2.901558	-1.305533	0.176098
C	-6.334444	-3.079265	-0.053028
H	-7.264513	-3.584204	0.182249
C	-2.648389	-1.129881	-0.964037
C	-3.917912	-2.920232	0.175894
C	5.327776	-1.758436	0.524946
C	-1.539608	0.822723	2.292691
C	4.390617	-1.849814	-1.728882
C	-2.912647	0.856574	2.048809
H	-3.468018	-0.074719	1.977032
C	-1.494441	0.826117	-2.189441
H	-1.663126	1.544333	-2.989901
C	-3.884254	0.460516	-2.346158
H	-3.907394	1.326646	-3.002372
C	1.519982	-0.861117	2.238193
H	1.592363	-0.882403	3.326894
C	4.216962	-1.641503	-0.34447
C	1.226176	2.642813	-1.32201
C	-5.084835	-0.180226	-2.055131
H	-6.006762	0.190319	-2.493086
C	-0.849672	-0.507138	2.546912
C	2.764861	-1.123467	1.573893
C	-3.887806	-1.77558	-0.650134
C	-5.129926	-1.303448	-1.195693
C	2.461094	2.647219	-0.673886
H	3.136649	1.806662	-0.806961
C	-2.649825	0.060991	-1.824117
C	-6.327459	-1.964372	-0.881617
H	-7.256032	-1.591482	-1.305245
C	6.588806	-2.076799	-0.028964
H	7.443376	-2.166326	0.635551
C	5.62822	-2.161843	-2.242822
C	-2.86812	3.265288	1.968093
H	-3.382261	4.213166	1.843263
C	0.843816	1.482655	-2.233068
C	0.365326	3.726168	-1.130527

H	-0.610296	3.731503	-1.607733
C	5.148315	-1.560499	1.929911
H	6.001414	-1.657427	2.593269
C	-0.835687	2.025553	2.358284
H	0.238005	2.016302	2.521915
C	-1.49539	3.239259	2.199758
H	-0.932005	4.165004	2.247415
C	-3.575456	2.070028	1.888205
H	-4.643678	2.078481	1.695738
C	3.91503	-1.266259	2.41519
H	3.779549	-1.128074	3.485238
C	6.737575	-2.273668	-1.382263
H	7.713698	-2.518855	-1.789546
C	1.97789	4.794678	0.311891
H	2.27037	5.63146	0.938585
C	2.836488	3.714453	0.139616
H	3.802847	3.700327	0.634115
C	0.738296	4.795567	-0.325962
H	0.059806	5.633061	-0.194178
C	-0.654201	-0.72979	4.047829
H	-0.020645	0.038577	4.500969
H	-1.630798	-0.67156	4.533067
H	-0.23021	-1.714877	4.263924
H	-1.521468	-1.290479	2.178694
H	1.687236	0.783988	-2.215274
C	0.668604	1.94137	-3.68305
H	1.618902	2.345768	-4.039964
H	0.387778	1.10286	-4.326695
H	-0.077713	2.732558	-3.793286
H	-5.113643	-4.427223	1.109488
H	-2.981749	-3.29953	0.56835
H	3.521358	-1.762894	-2.370094
H	5.751711	-2.323336	-3.308813

[a] The geometry was optimized by DFT calculation (CAM-B3LYP/6-31+G(d,p)).

Table S14. Cartesian coordinates (in angstrom) of *Δ*-(*S*,*S*)-**2** in S_1 state[a].

atom	x	y	z
Zn	0.052484	-0.050008	-0.097443
O	-1.636043	-1.001993	-0.508504
O	1.795138	-0.876917	-0.043516
N	-0.071317	0.196933	1.878068
N	-0.00804	1.038945	-1.733401
C	-5.63892	-2.544549	0.104347
C	2.650085	-0.879898	0.92784
C	-6.661713	-1.964603	-0.699995
H	-7.686358	-2.292176	-0.558613
C	-2.624775	-0.572804	-1.204065
C	-4.264521	-2.149371	-0.055242
C	4.926986	-1.280452	1.761966
C	-1.982719	1.750992	1.871306
C	-5.021094	-4.139492	1.833844
H	-5.302872	-4.896965	2.558523
C	4.457283	-1.885461	-0.589276
C	-3.301166	1.743589	1.41487
H	-3.870702	0.818592	1.436127
C	-1.103238	1.086184	-2.470096
H	-1.078187	1.667086	-3.390302
C	-3.45045	0.880641	-3.002362
H	-3.287173	1.633832	-3.76799
C	0.972652	-0.000494	2.615457
H	0.869653	0.151574	3.690819
C	4.003126	-1.355519	0.694725
C	1.824048	2.603415	-1.249283
C	-4.731592	0.373486	-2.816189
H	-5.542965	0.733394	-3.44158
C	-1.388217	0.491516	2.478064
C	-3.306186	-2.823401	0.746693
H	-2.263875	-2.581997	0.620468
C	2.293556	-0.421559	2.229564
C	-3.946013	-1.106688	-1.014555
C	-5.018358	-0.588823	-1.828029
C	3.078614	2.409949	-0.672205
H	3.634789	1.503589	-0.893999
C	-2.372943	0.474209	-2.2142
C	3.623514	-2.079439	-1.721009
H	2.578287	-1.832173	-1.642508
C	-6.347052	-1.030938	-1.648306
H	-7.121316	-0.606576	-2.281105
C	-3.672494	-3.786911	1.664237

H	-2.904836	-4.281808	2.250717
C	-5.979434	-3.528087	1.05938
H	-7.025453	-3.801145	1.163648
C	6.288138	-1.68014	1.569997
H	6.968129	-1.600851	2.412706
C	5.823855	-2.25973	-0.732243
C	4.117003	-2.587096	-2.904322
H	3.440457	-2.725017	-3.742322
C	-3.162817	4.090911	0.885665
H	-3.619472	4.999365	0.505619
C	1.265303	1.582381	-2.230074
C	1.112158	3.763939	-0.938712
H	0.122283	3.915591	-1.359246
C	4.54153	-0.810904	3.045452
H	5.28037	-0.785381	3.839239
C	-1.255957	2.940498	1.816071
H	-0.220575	2.958732	2.143493
C	-1.84325	4.103693	1.329343
H	-1.265707	5.021795	1.293778
C	-3.89016	2.905424	0.925138
H	-4.915343	2.880211	0.569773
C	3.260198	-0.413078	3.267036
H	2.960743	-0.068852	4.25371
C	6.304508	-2.769032	-1.95731
H	7.354666	-3.038566	-2.027108
C	6.720932	-2.137451	0.373901
H	7.757426	-2.431513	0.235049
C	5.470395	-2.93098	-3.037113
H	5.849552	-3.326286	-3.97402
C	2.910831	4.520768	0.481371
H	3.331927	5.266221	1.148712
C	3.620469	3.361023	0.189648
H	4.596286	3.19081	0.633408
C	1.653048	4.718873	-0.085835
H	1.092703	5.621442	0.139054
C	-1.427837	0.56425	4.005568
H	-0.825193	1.390383	4.395125
H	-2.460618	0.741525	4.312524
H	-1.09784	-0.369215	4.470569
H	-2.027629	-0.343275	2.169897
H	1.96561	0.737455	-2.229272
C	1.245505	2.150537	-3.650516
H	2.260741	2.454377	-3.915174
H	0.916114	1.404817	-4.379518
H	0.607623	3.035116	-3.73668

[a] The geometry was optimized by DFT calculation (CAM-B3LYP/6-31+G(d,p)).

7. References

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