Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

An Axially Chiral 1,1′-Biazulene and Its π-Extended Derivative: Synthesis, Structures and Properties

Chaolumen,[ab] Hideto Ito *[ab] and Kenichiro Itami *[abc]

[a] *JST, ERATO, Itami Molecular Nanocarbon Project, Nagoya University, Nagoya 464-8602, Japan.*
[b] *Graduate School of Science, Nagoya University, Nagoya 464-8602, Japan.*
[c] *Institute of Transformative Bio-Molecules (WPI-ITbM) Nagoya University, Nagoya 464-8602, Japan.*

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1. General

Unless otherwise noted, all materials including dry solvents were obtained from commercial suppliers and used without further purification. Azulene-2-yl-boronic acid pinacol ester[1] and 2,6-diphenyliodobenzene[2] were synthesized according to procedures reported in the literatures. Azulene was purchased from TCI. Unless otherwise noted, all reactions were performed with dry solvents under an atmosphere of nitrogen in oven-dried glassware with standard vacuum-line techniques. All work-up and purification procedures were carried out with reagent-grade solvents in air.

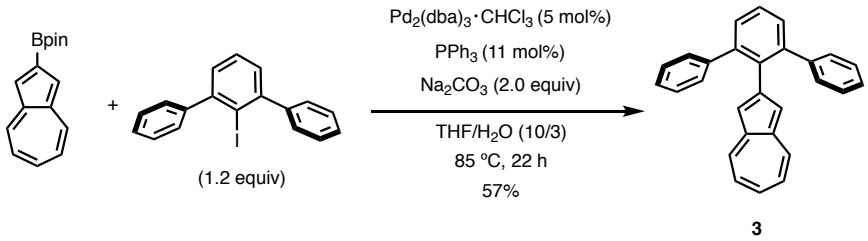
Analytical thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F_{254} precoated plates (0.25 mm). The developed chromatogram was analyzed by UV lamp (254 nm and 365 nm). Flash column chromatography was performed with E. Merck silica gel 60 (230–400 mesh). High-resolution mass spectra (HRMS) were obtained from a JMS-T100GCV (EI). Melting points were measured on an MPA100 Optimelt automated melting point system. Preparative gel permeation chromatography (GPC) was performed with a JAI LC-9204 instrument equipped with JAIGEL-1H/JAIGEL-2H columns using chloroform as an eluent. Chiral HPLC analysis was conducted on a Shimadzu Prominence 2000 instrument equipped with CHIRALPAK® ID column (10 mm × 250 mm). Nuclear magnetic resonance (NMR) spectra were recorded on a JEOL ECS-600 (^{1}H 600 MHz, ^{13}C 150 MHz) spectrometer and a JEOL ECA 600II with Ultra COOL probe (^{1}H 600 MHz, ^{1}H 150 MHz). Chemical shifts for ^{1}H NMR are expressed in parts per million (ppm) relative to tetramethylsilane (δ 0.00 ppm) or $CDCl_3$ (δ 7.26 ppm). Chemical shifts for ^{13}C NMR are expressed in ppm relative to $CDCl_3$ (δ 77.0 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, ddd = doublet of doublet of doublets, t = triplet, td = triplet of doublets, q = quartet, m = multiplet), coupling constant (Hz), and integration. Cyclic voltammetry (CV) was performed on a BAS ALS620A electrochemical analyzer. The CV cell consisted of a glassy carbon electrode, a Pt wire counter electrode, and a titanium reference electrode. The measurements were carried out under a nitrogen atmosphere using a CH_2Cl_2 solution of a sample with a concentration of 1 mM and 0.1 M tetrabutylammonium hexafluorophosphate (n-$Bu_4N^+PF_6^-$) as a supporting electrolyte. The redox potentials were calibrated with ferrocene as an internal standard. UV-vis absorption spectra were measured with a Shimadzu UV-3150 spectrometer. Circular dichroism spectra were measured with a JASCO FT/IR6100. Thermogravimetry and differential thermal analyses (TG-DTA) were performed on Rigaku ThermoMass Photonization.

2. Computational Methods

The Gaussian 09 program[3] running on a SGI Altix4700 system was used for optimization (B3LYP/6-31G(d)).[4] Structures were optimized without any symmetry assumptions. Zero-point energy, enthalpy, and Gibbs free energy at 298.15 K and 1 atm were estimated from the gas-phase studies. Harmonic vibration frequency calculation at the same level was performed to verify all stationary points as local minima (with no imaginary frequency) or transition states (with one imaginary frequency). Visualization of the results was performed by use of GaussView 5.0.9 software. Optical transitions with oscillator strength were calculated at the TD-CAM-B3LYP/6-31G* using the optimized structures at the B3LYP/6-31G* level.

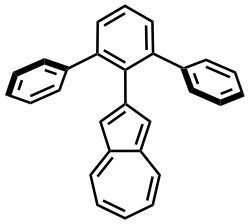
3. Synthesis

Synthesis of 2-Terphenyl Azulene 3



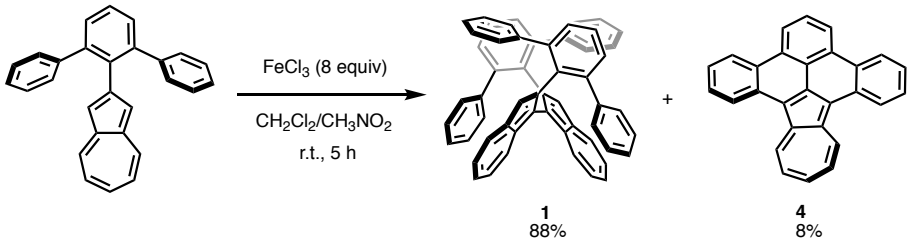
To a mixture of azulene-2-ylboronic acid pinacol ester (33 mg, 130 μmol), 2,6-diphenyliodobenzene (55 mg, 156 μmol), $Pd_2(dba)_3 \cdot CHCl_3$ (7 mg, 7 μmol), PPh_3 (4 mg, 14.3 μmol) and Na_2CO_3 (28 mg, 260 μmol) were added degassed THF (1 mL) and distilled water (0.3 mL) in a Schlenk tube, and the solution was stirred at 85 °C for 22 h. After cooling to room temperature, to the resulting mixture was added distilled water. The aqueous layer was extracted with CH_2Cl_2 and the combined organic layers were washed with brine. After drying with Na_2SO_4, the solution was filtered and evaporated under reduced pressure. Then, the crude product was purified by GPC using CH_3Cl as eluent to give **3** (26 mg, 74 μmol) in 57% yield as a blue solid.

2-([1,1':3',1''-terphenyl]-2'-yl)azulene (3)



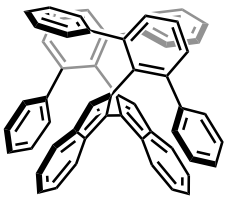
Mp 170−172 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.92 (d, J = 9.6 Hz, 2H), 7.52–7.47 (m, 3H), 7.39 (t, J = 9.6, Hz, 1H), 7.11–7.06 (m, 10H), 6.97 (t, J = 9.6, Hz, 2H), 6.76 (s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 149.57, 142.40, 142.13, 139.37, 135.83,135.54, 135.33, 129.76, 129.66, 127.52, 127.48, 126.20, 122.51, 120.97. HRMS (EI^+) m/z calcd for $C_{28}H_{20}$ $[M]^+$: 356.1565, found: 356.1560.

Synthesis of 1,1'-Biazulene Derivative 1 and π-Extended Azulene Derivative 4



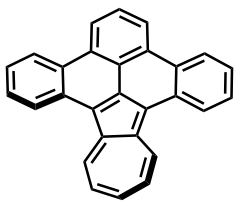
2-Terphenyl azulene **3** (59 mg 140 μmol) was dissolved in dry dichloromethane (2 mL) in a 10 mL Schlenk flask. After stirring for 5 min under nitrogen, the solution of anhydrous iron (III) chloride (182 mg, 1.12 mmol) in dry nitromethane (0.8 mL) was added through a syringe. The solution was stirred at room temperature for 5 h under nitrogen. Excessive water and methanol were added to the solution. The aqueous layer was extracted with CH_2Cl_2 and the combined organic layers were washed with brine. After drying with Na_2SO_4, the solution was filtered and evaporated under the reduced pressure. Then, the crude product was purified by silica gel column chromatography using CH_2Cl_2/hexane (1:4) as an eluent. In the first fraction, **4** was obtained in 8% yield (4 mg, 11 μmol) as a yellow solid. In the second fraction, **1** was obtained in 88% yield (45 mg, 63 μmol) as a blue solid. Single crystals of **1** and **4** for the X-ray diffraction analyses were obtained by recrystallizations from $CHCl_3$/hexane and $CHCl_3$/hexane, respectively.

rac-2,2'-Di([1,1':3',1''-terphenyl]-2'-yl)-1,1'-biazulene (1)



Mp >300 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.88 (d, *J* = 9.6 Hz, 2H), 7.24–7.17 (m, 6H), 7.16–7.13 (m, 2H), 7.12–7.09 (m, 4H), 7.06 (dd, *J* = 7.2, 4.2 Hz, 2H), 6.89 (t, *J* = 9.6, Hz, 2H), 6.84 (s, 2H), 6.75–6.72 (m, 2H), 6.54–6.51 (m, 8H), 6.27 (dd, *J* = 8.4, 1.5 Hz, 4H), 6.20 (t, *J* = 9.6 Hz, 2H), 6.08 (d, *J* = 9.6 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 149.49, 143.43, 143.05, 142.69, 142.09, 140.41, 138.04, 135.46, 135.02, 134.95, 134.88, 131.01, 130.09, 129.94, 129.06, 127.72, 127.24, 127.08, 126.56, 125.82, 125.30, 124.33, 122.71, 121.87. HRMS (EI$^+$) *m*/*z* calcd for $C_{56}H_{38}$ $[M]^+$: 710.2974, found: 710.2970.

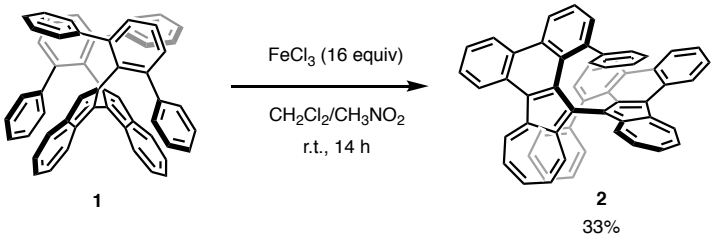
Azuleno[1,2,3-*fg*]benzo[*op*]tetracene (4)



Mp 285−287 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.88 (d, *J* = 9.6 Hz, 2H), 9.15 (d, *J* = 7.2 Hz, 2H), 8.89 (d, *J* = 8.4 Hz, 2H), 8.81 (d, *J* = 7.8 Hz, 2H), 8.09 (t, *J* = 7.8 Hz, 1H), 8.07 (t, *J* = 9.6 Hz, 1H), 7.83–7.80 (m, 2H), 7.77–7 (m, 2H), 7.69–7.67 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 137.36, 136.28, 135.16, 131.25, 130.89, 130.10, 128.01, 125.15, 124.91,

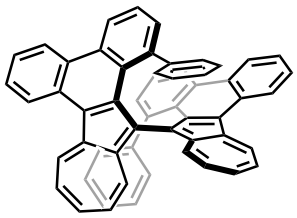
124.86, 124.06, 123.34, 120.67, 117.45 (two sp^2 carbon signals were overlapped with other signals). HRMS (EI): *m*/*z* calcd for $C_{28}H_{16}$ $[M]^+$: 352.1252, found: 352.1256.

Synthesis of π-Extended 1,1′-Biazulene Derivative 2



1,1′-Diazulene derivative **1** (45 mg 63 μmol) was dissolved in dry dichloromethane (2 mL) in a 10 mL Schlenk flask. After stirring for 5 min under nitrogen, the solution of anhydrous iron (III) chloride (162 mg, 1.00 mmol) in dry nitromethane (0.8 mL) was added through a syringe. The solution was stirred at room temperature for 14 h under nitrogen. Excessive water and methanol were added to the solution. The aqueous layer was extracted with CH_2Cl_2 and the combined organic layers were washed with brine. After drying with Na_2SO_4, the solution was filtered and evaporated under the reduced pressure. Then, the crude product was purified by GPC using CH_3Cl as an eluent to afford product **2** in 33% yield (15 mg, 22 μmol) as a green solid. Single crystal of **2** for the X-ray diffraction analysis was obtained by the recrystallization from $CHCl_3$/hexane.

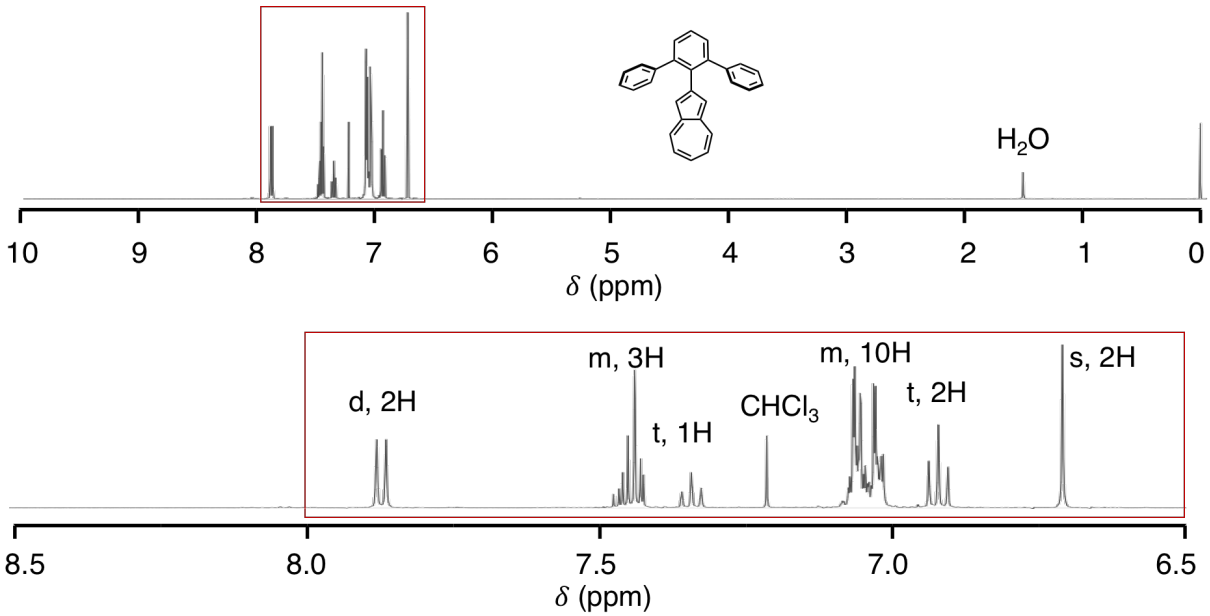
rac-1,1'-Diphenyl-14,14'-biazuleno[1,2-*l*]phenanthrene (2)



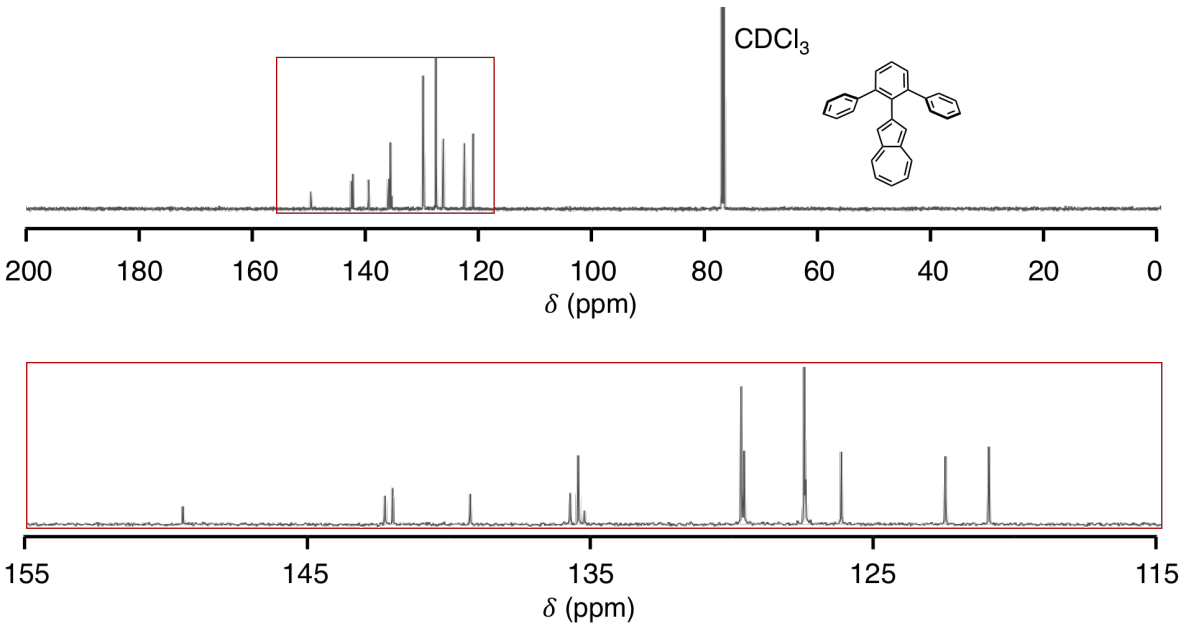
Mp >300 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ 9.29 (d, *J* = 9.6 Hz, 2H), 8.96 (d, *J* = 7.8 Hz, 2H), 8.67 (d, *J* = 7.8 Hz, 2H), 8.27 (d, *J* = 7.8 Hz, 2H), 7.82–7.80 (m, 2H), 7.68 (t, *J* = 6.6 Hz, 2H), 7.51 (t, *J* = 9.6 Hz, 2H), 7.46 (d, *J* = 10.2 Hz, 2H), 7.39 (t, *J* = 9.9 Hz, 2H), 7.14 (t, *J* = 8.1 Hz, 2H), 6.76 (t, *J* = 9.3 Hz, 2H), 6.36 (dd, *J* = 7.2, 1.2 Hz, 2H), 6.24 (d, *J* = 7.8 Hz, 2H), 6.11–6,09 (m, 2H), 6.05–6.02 (m, 2H), 6.89–6.86 (m, 2H), 5.39 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 142.54, 141.39, 139.75, 138.31, 137. 87, 136.82, 136.14, 134.32, 133.16, 130.54, 129.83, 129.02, 128.58, 127.54, 127.31, 127.17, 126.91, 126.01, 124.88, 124.80, 124.54, 124.28, 124.17, 123.13, 123.06, 122.83, 120.01 (one sp^2 carbon signal was overlapped with other signals). HRMS (EI^+): *m*/*z* calcd. for $C_{56}H_{34}$ $[M]^+$: 706.2661, found 706.2660.

4. NMR Spectra

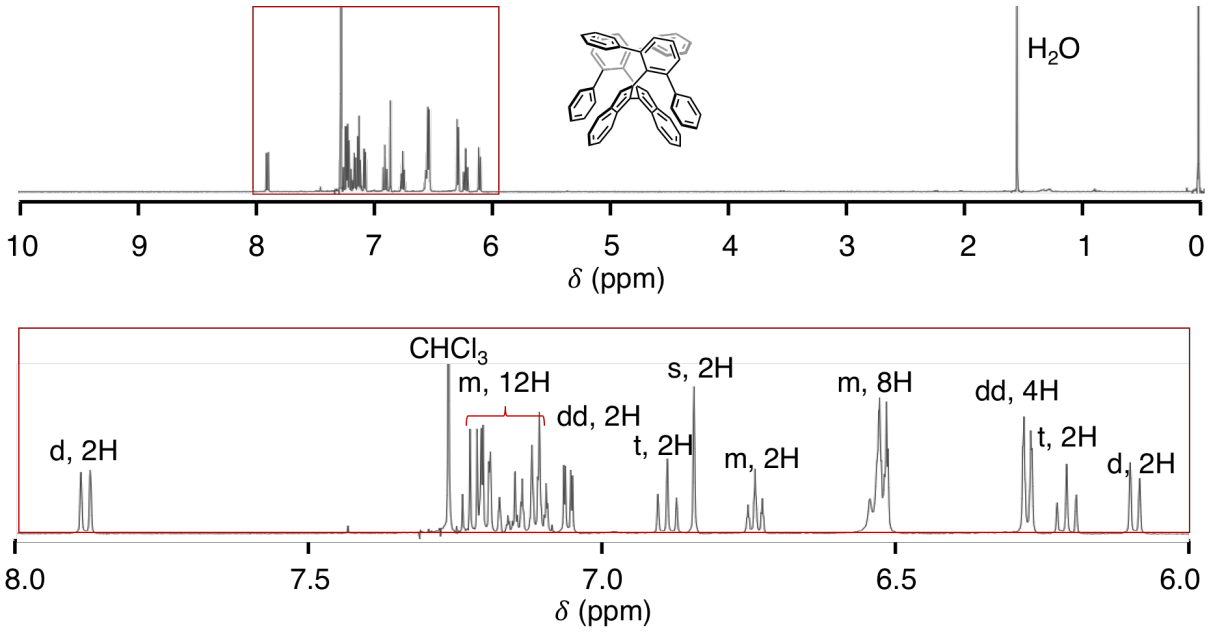
^{1}H NMR spectrum of **3** (600 MHz, $CDCl_3$)



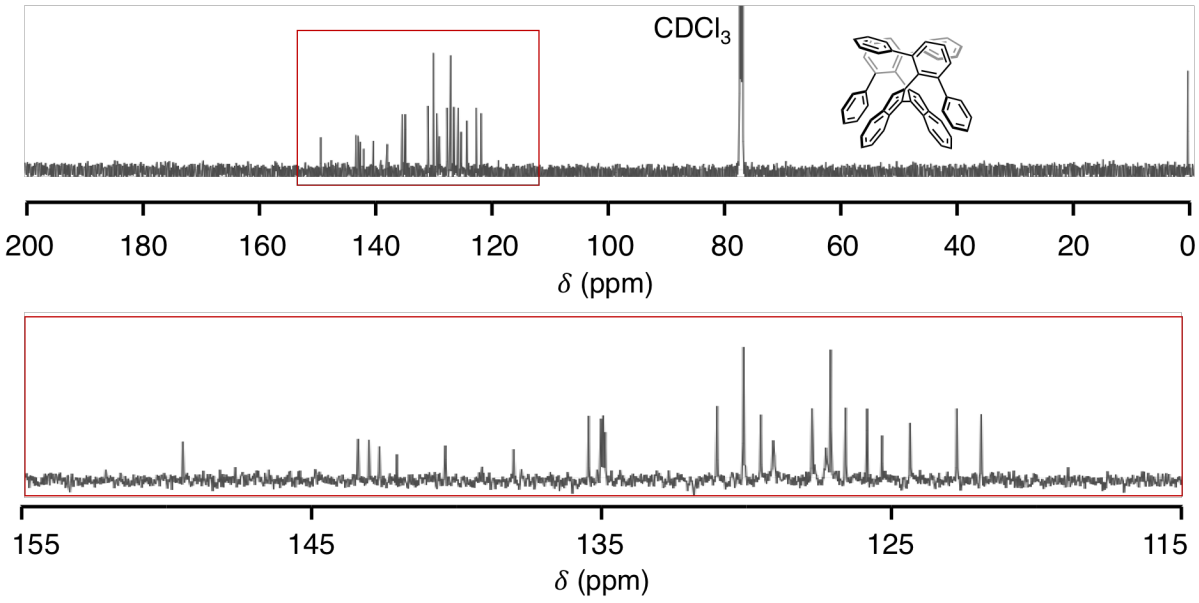
^{13}C NMR spectrum of **3** (150 MHz, $CDCl_3$)



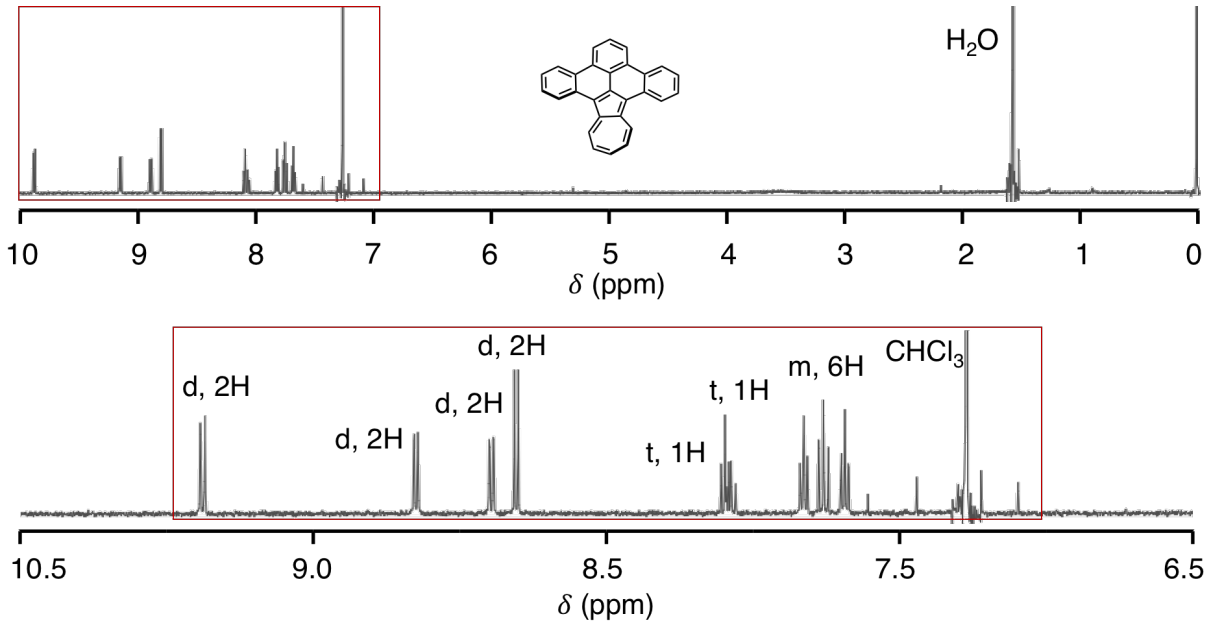
^{1}H NMR spectrum of **1** (600 MHz, $CDCl_3$)



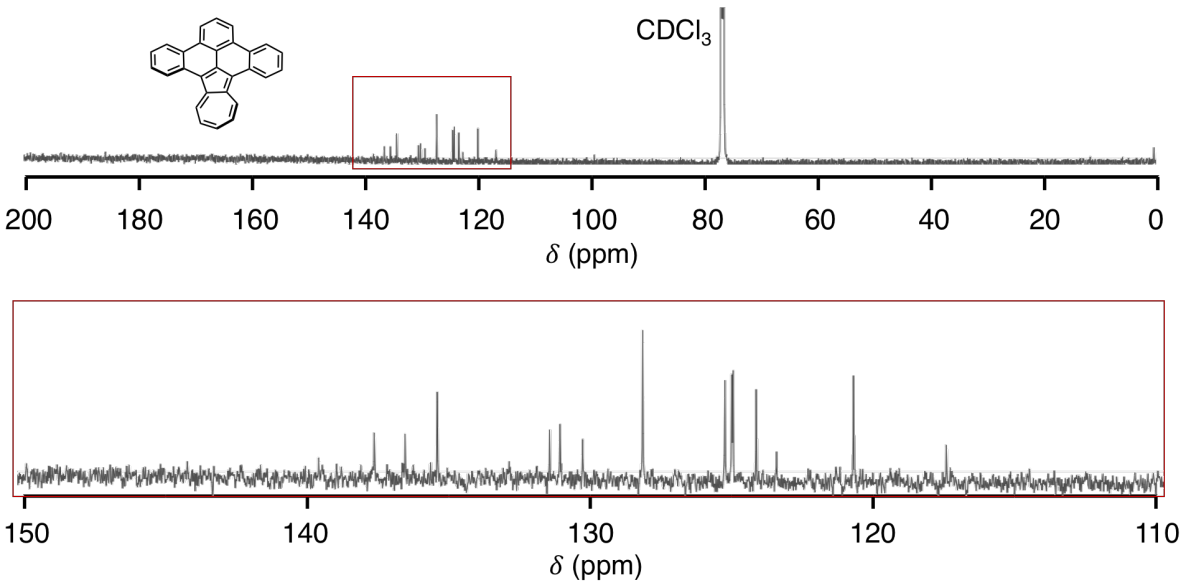
^{13}C NMR spectrum of **1** (150 MHz, $CDCl_3$)



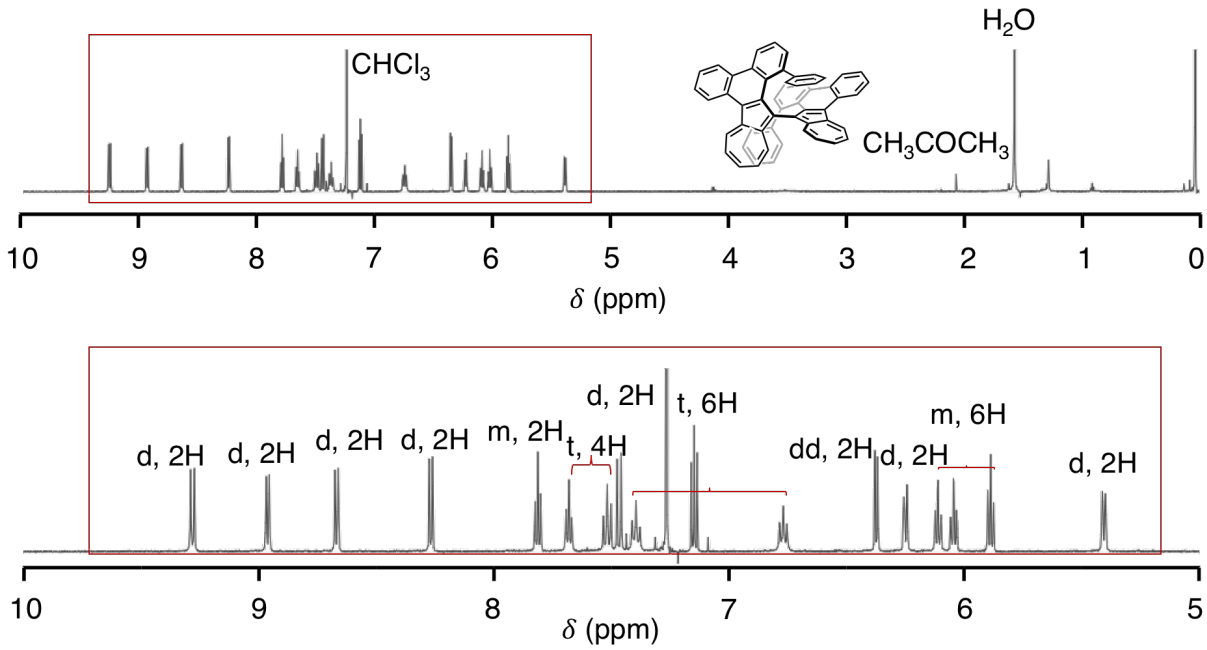
^{1}H NMR spectrum of **4** (600 MHz, $CDCl_3$)



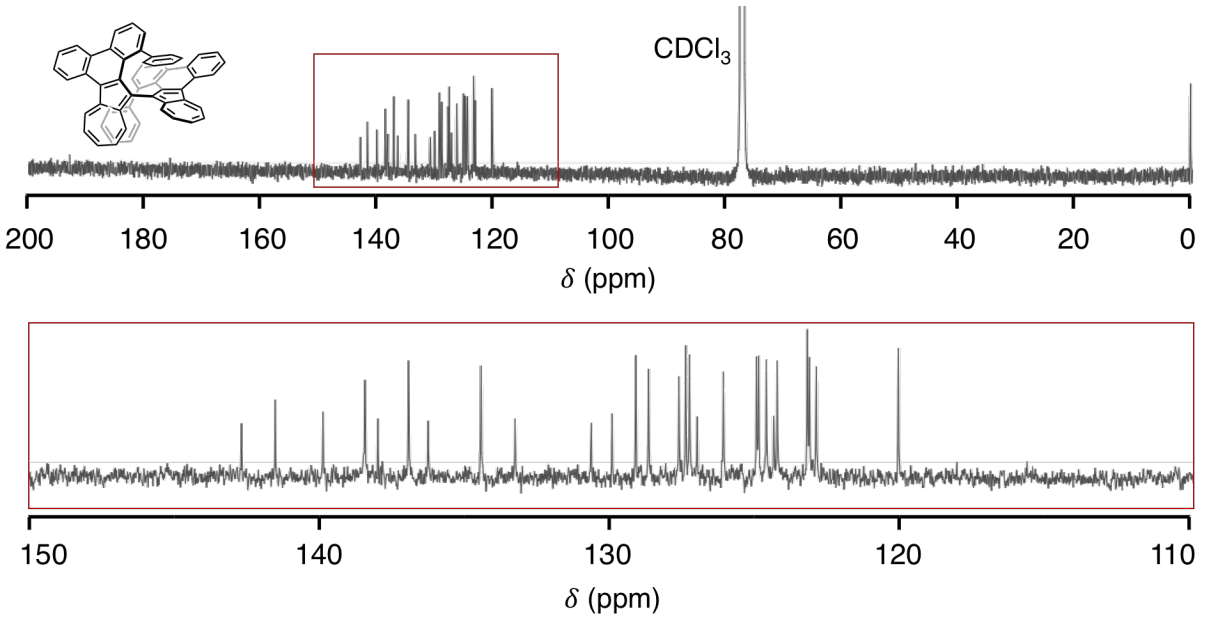
^{13}C NMR spectrum of **4** (150 MHz, $CDCl_3$)



^{1}H NMR spectrum of **2** (600 MHz, $CDCl_3$)



^{13}C NMR spectrum of **2** (150 MHz, $CDCl_3$)



5. X-ray Crystallographic Analysis

Details of the crystal data and a summary of the intensity data collection parameters for **1**,**2**, and **3** are listed in Table S1. A suitable crystal, obtained by crystallization from chloroform solution, was mounted with mineral oil on a MiTeGen MicroMounts and transferred to the goniometer of a Rigaku PILATUS diffractometer. Graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) was used. The structures were solved by direct methods with (SIR-97)[5] and refined by full-matrix least-squares techniques against F^2 (SHELXL- 2014/7)[6] by using Yadokari-XG software package.[7] The intensities were corrected for Lorentz and polarization effects. The non- hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using AFIX instructions.

Table S1 Crystallographic Data and Structure Refinement Details of **1**, **2**, and **4**

	1 (CCDC 1899599)	**2** (CCDC 1899597)	**4** (1899598)
formula	$C_{56}H_{38}$	$C_{56}H_{34}$	$C_{28}H_{16}$
fw	710.86	706.83	352.41
T (K)	123(2)	123(2)	123(2)
λ (Å)	0.71073	0.71073	0.71073
cryst syst	Monoclinic	Monoclinic	Orthorhombic
space group	$P2_1/a$	$C2/c$	$P\mathrm{na}2_1$
a (Å)	20.704(2)	16.1839(6)	19.4033(7)
b (Å)	9.6416(8)	17.6048(3)	5.3758(2)
c (Å)	20.416(2)	14.1755(4)	15.7105(6)
α (deg)	90	90	90
β (deg)	111.978(2)	118.502(3)	90
γ (deg)	90	90	90
V (Å^3)	3779.3(6)	3549.3(2)	1638.7(11)
Z	4	4	4
D_{calc} (g·cm^{-3})	1.249	1.323	1.428
μ (mm^{-1})	0.071	0.075	0.081
F(000)	1496	1480	736
cryst size (mm)	0.20 × 0.15 × 0.15	0.15 × 0.10 × 0.10	0.20 × 0.10 × 0.05
θ range (deg)	3.13–25.00	2.31–24.99	2.10–25.00
reflns collected	40422	12726	16785
indep reflns/R_{int}	6644/0.0250	3124/0.0163	2883/0.0394
params	505	253	253
GOF on F^2	1.049	1.074	1.220
R_1, wR_2 [$I>2\sigma(I)$]	0.0322, 0.0792	0.0322, 0.0893	0.0320, 0.0805
R_1, wR_2 (all data)	0.0377, 0.0825	0.0354, 0.0914	0.0462, 0.1145

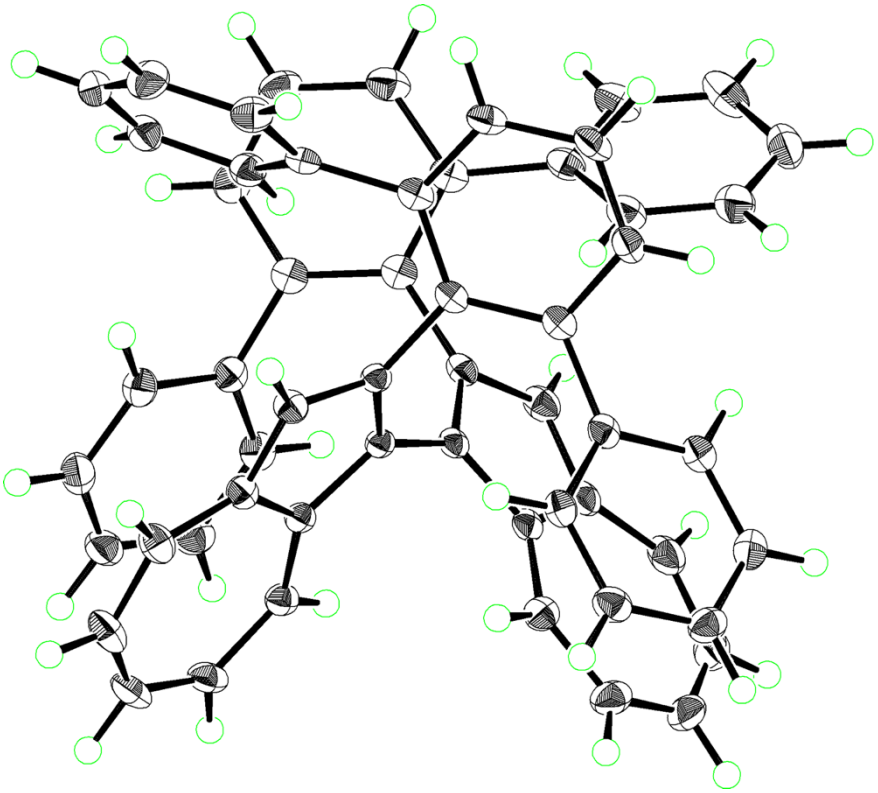


Fig. S1 ORTEP drawing of **1** (50% probability for thermal ellipsoids).

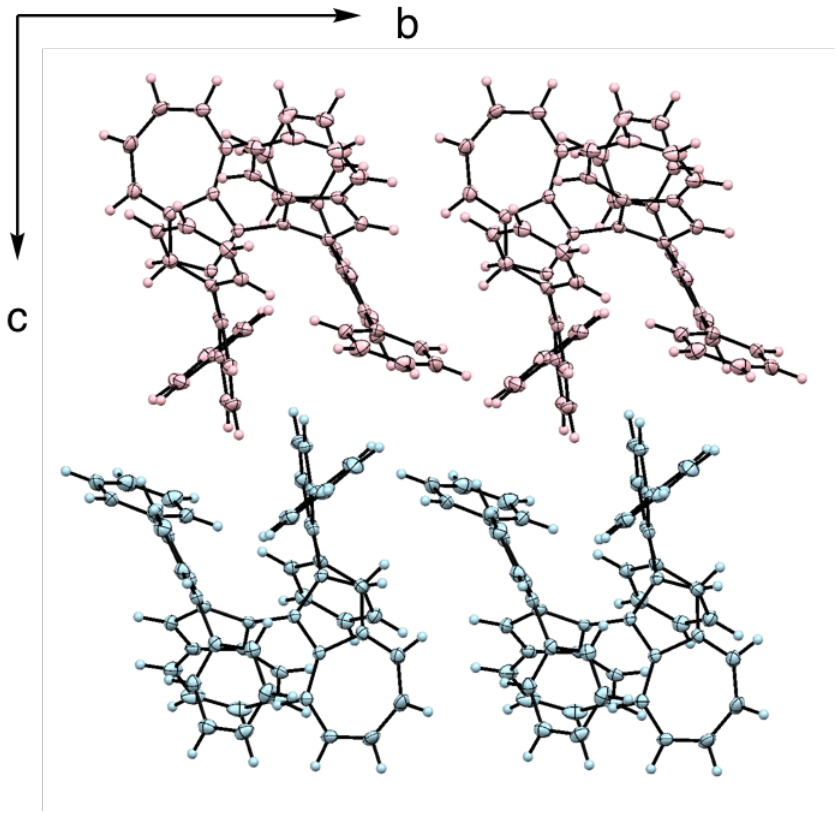


Fig. S2 Packing structure of **1**.

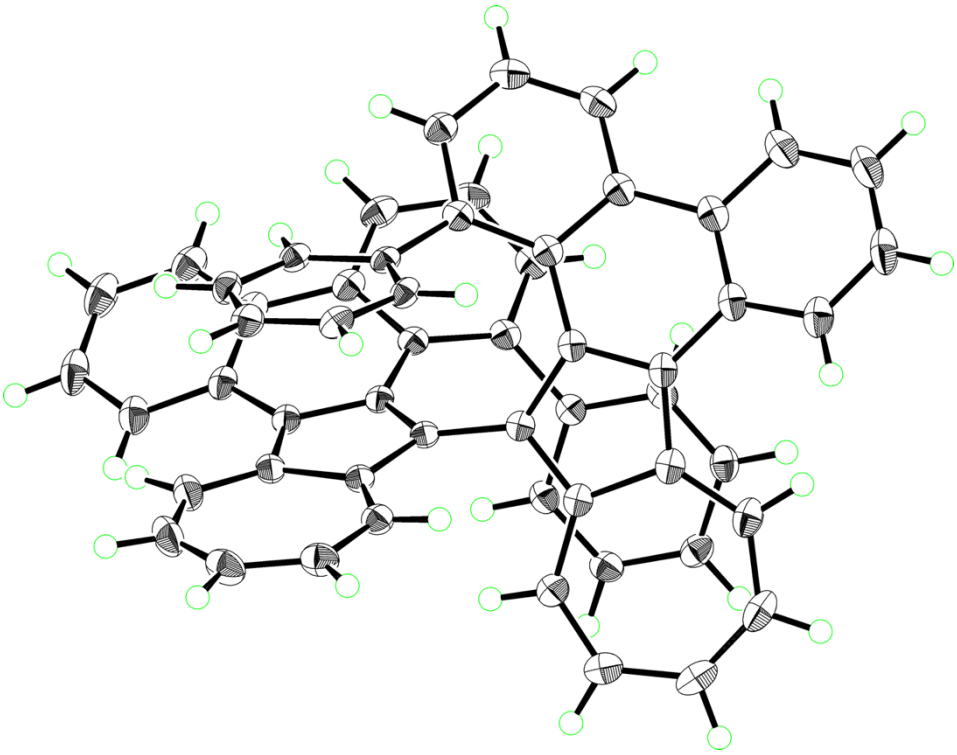


Fig. S3 ORTEP drawing of **2** (50% probability for thermal ellipsoids).

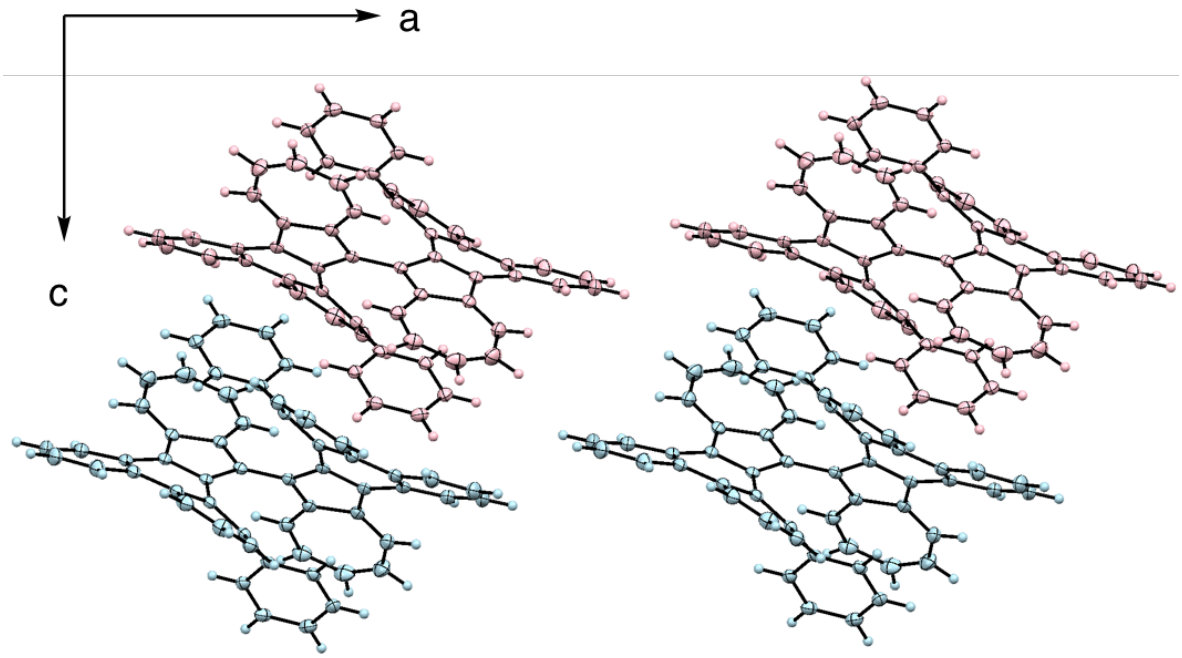


Fig. S4 Packing structure of **2**.

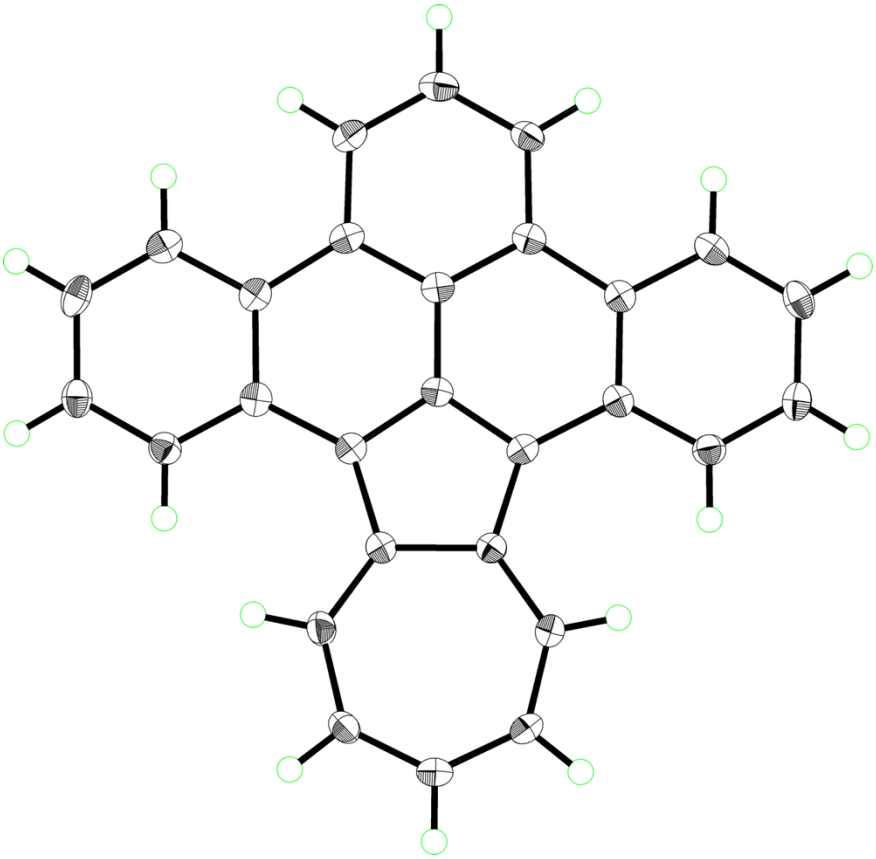


Fig. S5 ORTEP drawing of **4** (50% probability for thermal ellipsoids).

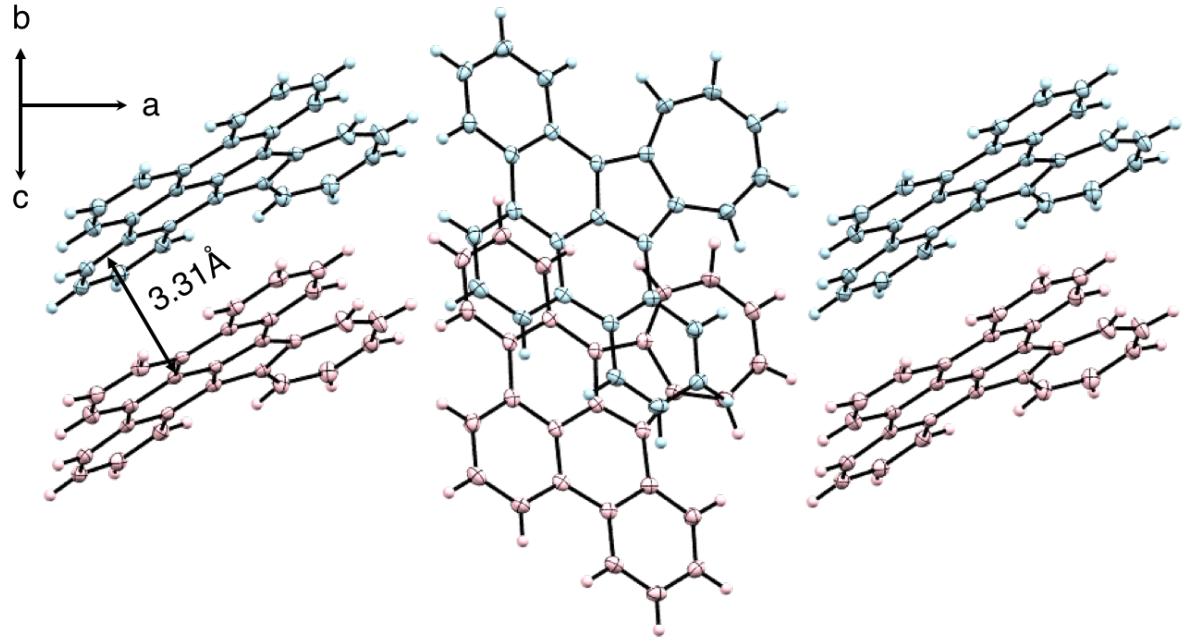


Fig. S6 Packing structure of **4**.

6. Optical resolution by HPLC

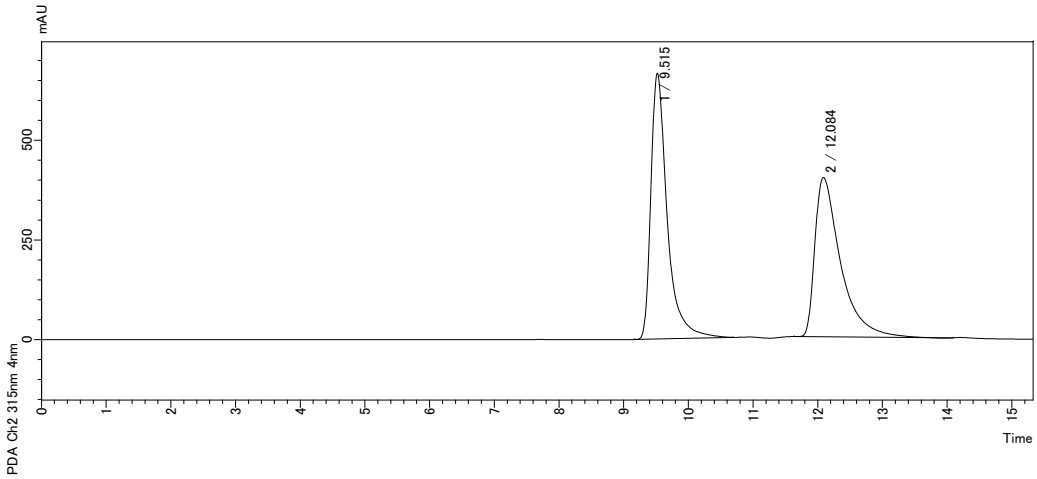


Fig. S7 Chromatograms for the resolution of **1** using UV (315 nm) detectors in *n*-hexane/CH_2Cl_2 (70:30, v/v) at the flow rate of 0.6 mL/min. Optical resolution was carried out with a DAICEL CHIRALPAK-ID column (0.46(i.d.) × 25 cm) at 30 °C.

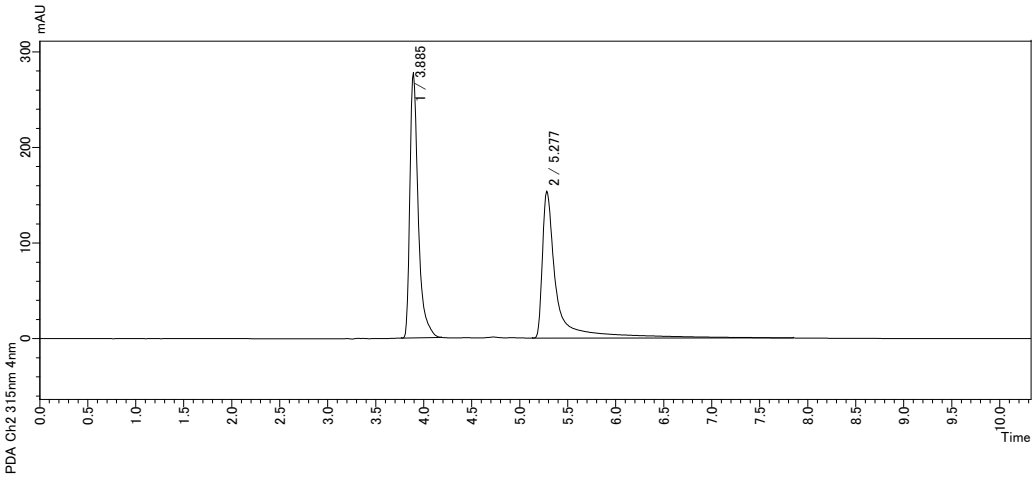


Fig. S8 Chromatograms for the resolution of **2** using UV (315 nm) detectors in *n*-hexane/CH_2Cl_2 (50:50, v/v) at the flow rate of 1.0 mL/min. Optical resolutions were carried out with a DAICEL CHIRALPAK-ID column (0.46(i.d.) × 25 cm) at 40 °C.

Table S2 The dissymmetry factor $|g_{CD}|$ of **1**.

Wavelength	256	308	337	596 (*R*-**1**)	626 (*S*-**1**)
$\|\Delta\varepsilon\|$	48.9	74.4	29.5	1.7	0.4
$\|g_{CD}\|$	5.4 X × 10^{-4}	1.0 × 10^{-3}	9.4 × 10^{-4}	2.8 × 10^{-3}	7.4 × 10^{-4}

$|g_{CD}| = |\Delta\varepsilon / \varepsilon|$

Table S3 The dissymmetry factor $|g_{CD}|$ of **2**.

Wavelength	282	333	358	404	686 (*R*-**2**)	666 (*S*-**2**)
$\|\Delta\varepsilon\|$	37.7	18.0	17.8	33.1	0.3	0.3
$\|g_{CD}\|$	5.0 × 10^{-4}	1.5 × 10^{-3}	2.2 × 10^{-4}	1.2 × 10^{-3}	5.5 × 10^{-4}	7.0 × 10^{-4}

$|g_{CD}| = |\Delta\varepsilon / \varepsilon|$

7. Cyclic voltammograms

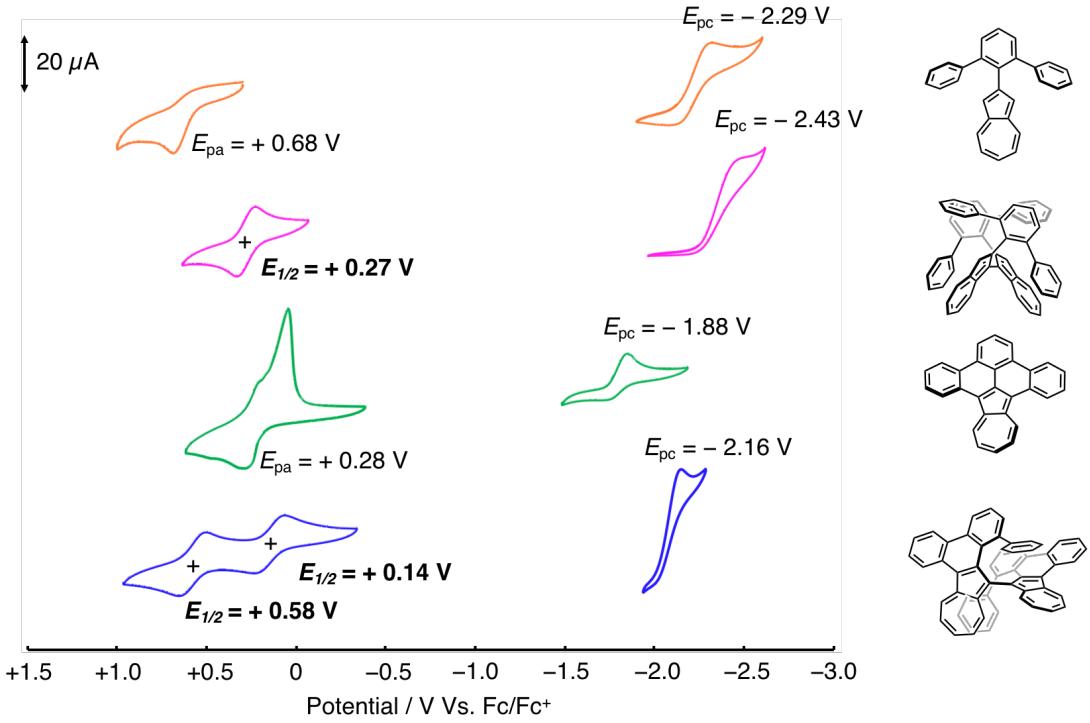


Fig. S9 Cyclic voltammograms of **3**, **1**, **4** and **1** in CH_2Cl_2 (1 mM), measured with *n*-Bu_4NPF_6 (0.1 M) as a supporting electrolyte at a scan rate of 100 mV s^{-1}.

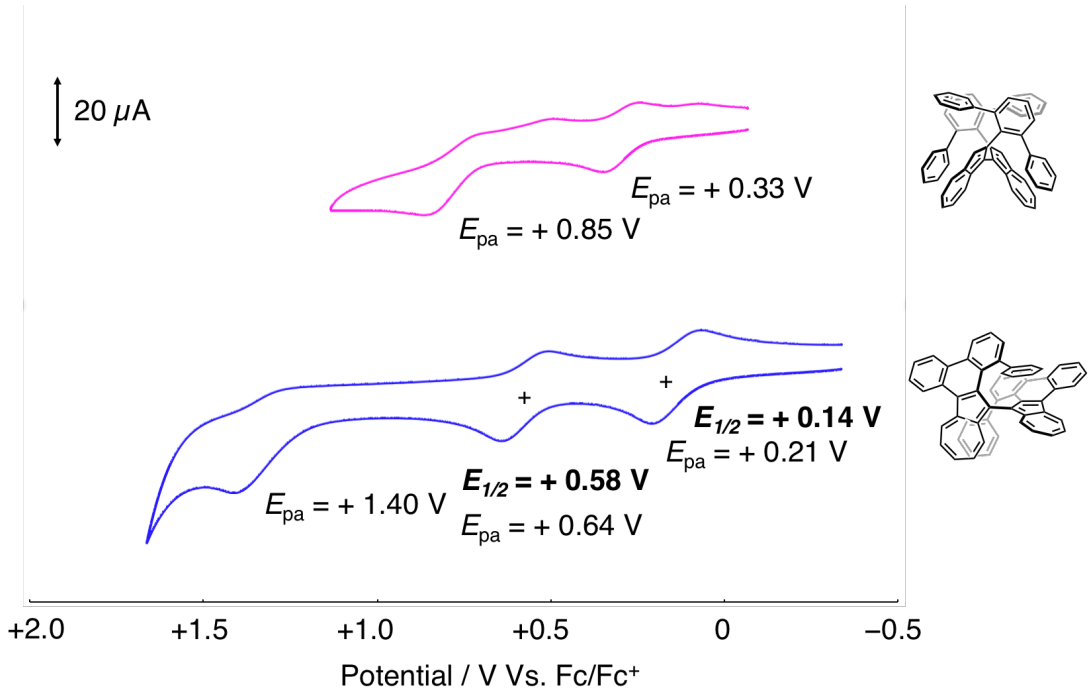


Fig. S10 Full oxidation waves of **1** and **3** in CH_2Cl_2 (1 mM), measured with *n*-Bu_4NPF_6 (0.1 M) as a supporting electrolyte at a scan rate of 100 mV s^{-1}.

8. DFT calculations

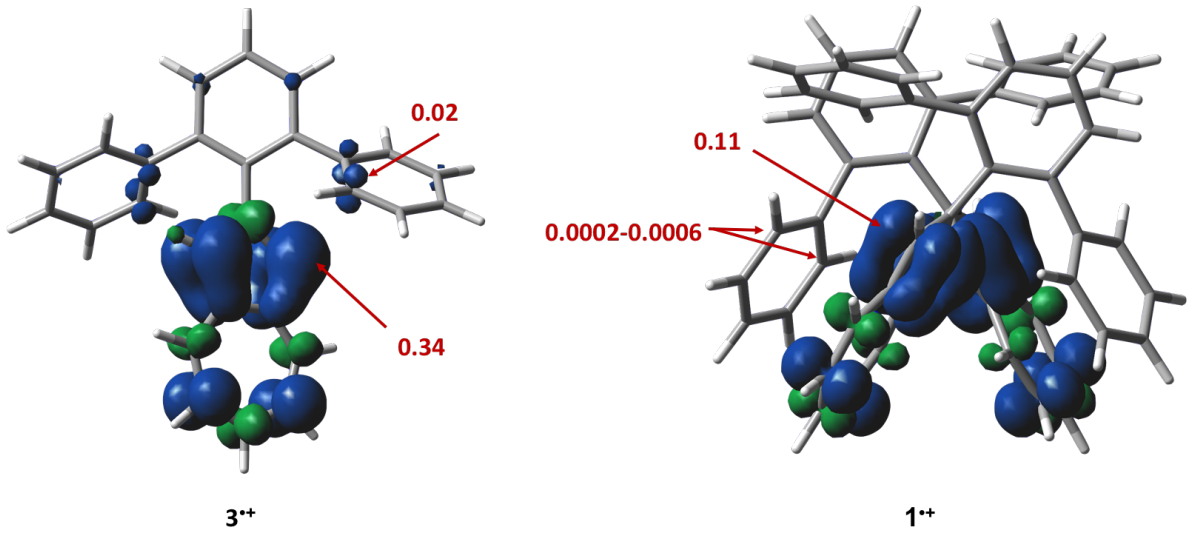


Fig. S11 Mulliken spin densities of radical cation intermediates **3**•+ and **1**•+ calculated at the UB3LYP/6-311G** level of theory.

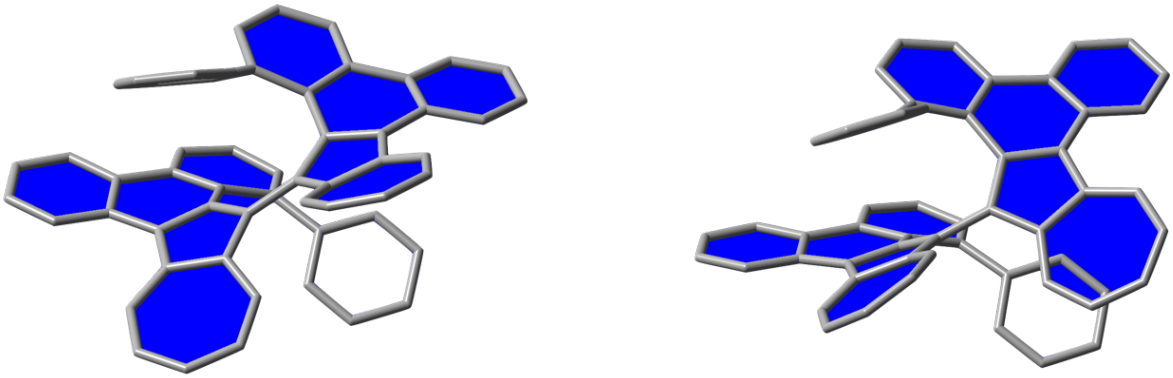


Fig. S12 Relative energies calculated at the B3LYP/6-31G* level of theory.

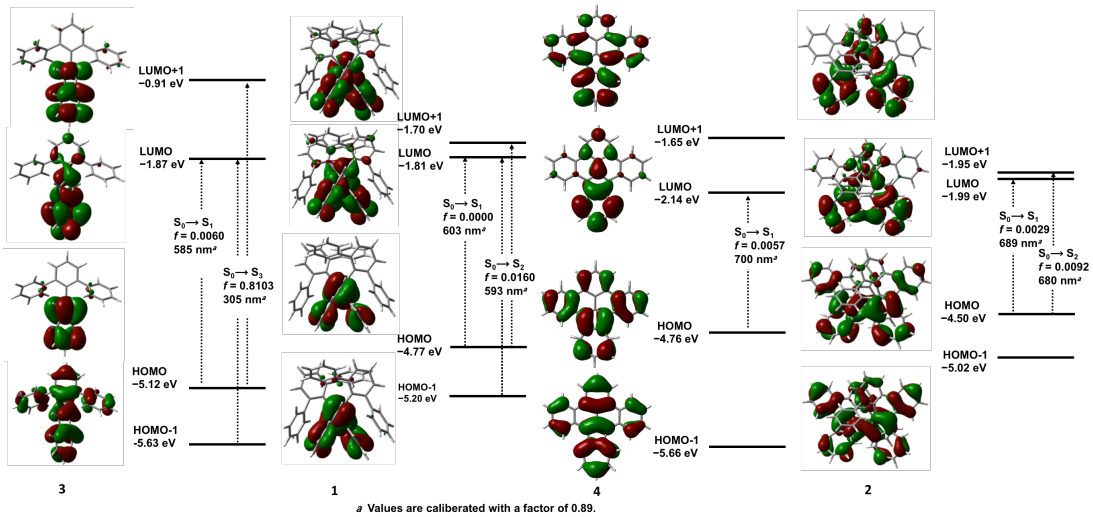


Fig. S13 Pictorial representation of the frontier orbitals, a plot of HOMO and LUMO energy levels for **3**, **1**, **4** and **2** (B3LYP/6-31G*), and optical transition with oscillator strength (TD-CAM-B3LYP/6-31G*//B3LYP/6-31G*).

Table S4 TD-DFT vertical one-electron excitations of **1**.

Compound	Excitation [nm][a]	Oscillator strength (f)	Description
1	603	0.0000	H→L
	593	0.0162	H–1→L, H→L+1
	329	0.3698	H–3→L, H→L+2
	303	0.4317	H–3→L+1, H–1→L+2

H: HOMO. L: LUMO. Excitations 1, 2, 7 and 12 are listed in this order. [a] Values are caliberated with a factor of 0.89.

Table S5 TD-DFT vertical one-electron excitations of **2**.

Compound	Excitation [nm][a]	Oscillator strength (f)	Description
2	689	0.0029	H→L
	680	0.0092	H–1→L, H→L+1
	378	0.4035	H–3→L, H–2→L+1, H→L+2
	342	0.4864	H–2→L, H–1→ L+2, H→ L+4

H: HOMO. L: LUMO. Excitations 1, 2, 8 and 14 are listed in this order. [a] Values are caliberated with a factor of 0.89.

Table S6 TD-DFT vertical one-electron excitations of **3**.

Compound	Excitation [nm][a]	Oscillator strength (f)	Description
3	585	0.0060	H→L
	306	0.8103	H-1→L, H→L+1

H: HOMO. L: LUMO. Excitations 1 and 3 are listed in this order. [a] Values are caliberated with a factor of 0.89.

Table S7 TD-DFT vertical one-electron excitations of **4**.

Compound	Excitation [nm][a]	Oscillator strength (f)	Description
4	700	0.0057	H→L
	354	0.4602	H-1→L, H→L+2

H: HOMO. L: LUMO. Excitations 1 and 4 are listed in this order. [a] Values are caliberated with a factor of 0.89.

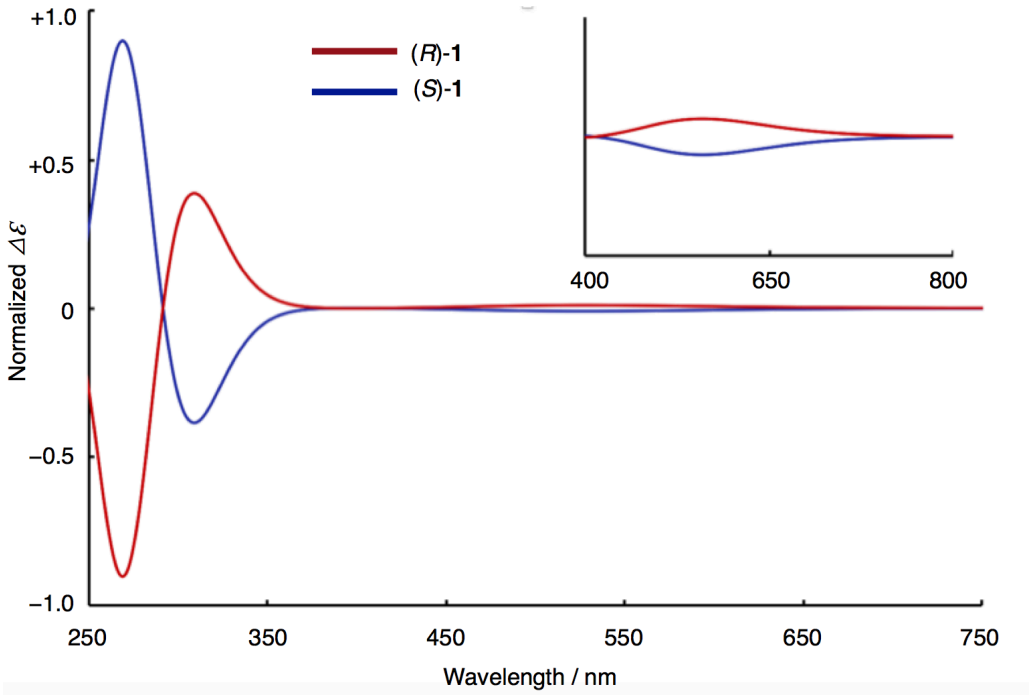


Fig. S14 Simulated CD spectra of (*R*)-**1** and (*S*)-**1** based on TD-DFT calculations at the TD-CAM-B3LYP/6-31G*//B3LYP/6-31G* level of theory.

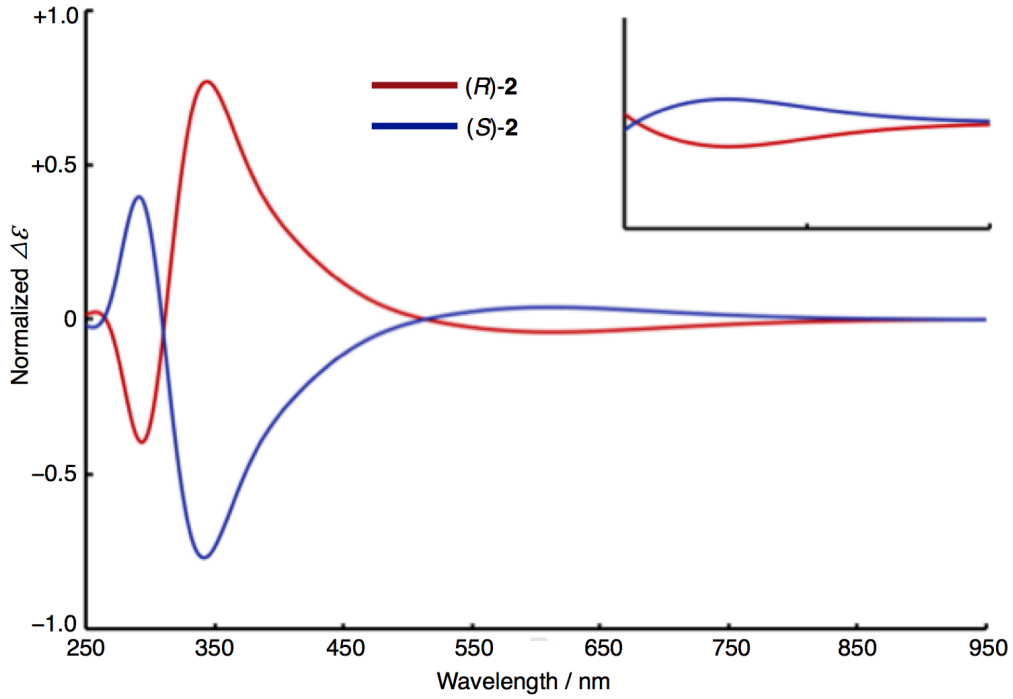


Fig. S15 Simulated CD spectra of (*R*)-**2** and (*S*)-**2** based on TD-DFT calculations at the TD-CAM-B3LYP/6-31G*//B3LYP/6-31G* level of theory.

9. TG-DTA Analysis

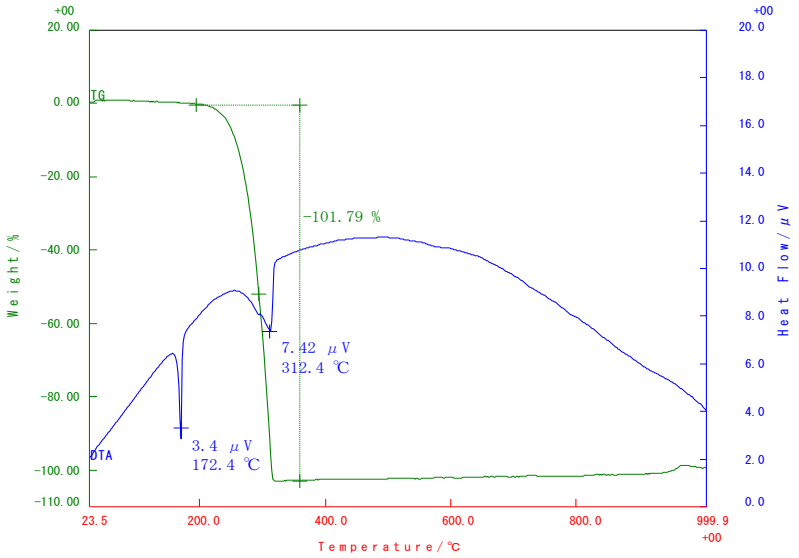


Fig. S16 Thermogravimetric and differential thermal analyses of **3** heating at 20 °C/min under He.

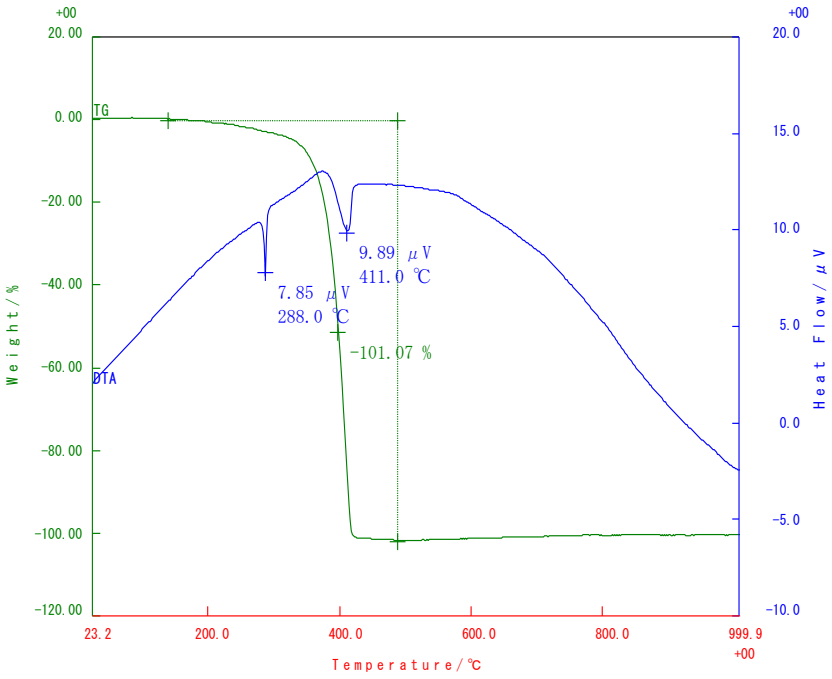


Fig. S17 Thermogravimetric and differential thermal analyses of **4** heating at 20 °C/min under He.

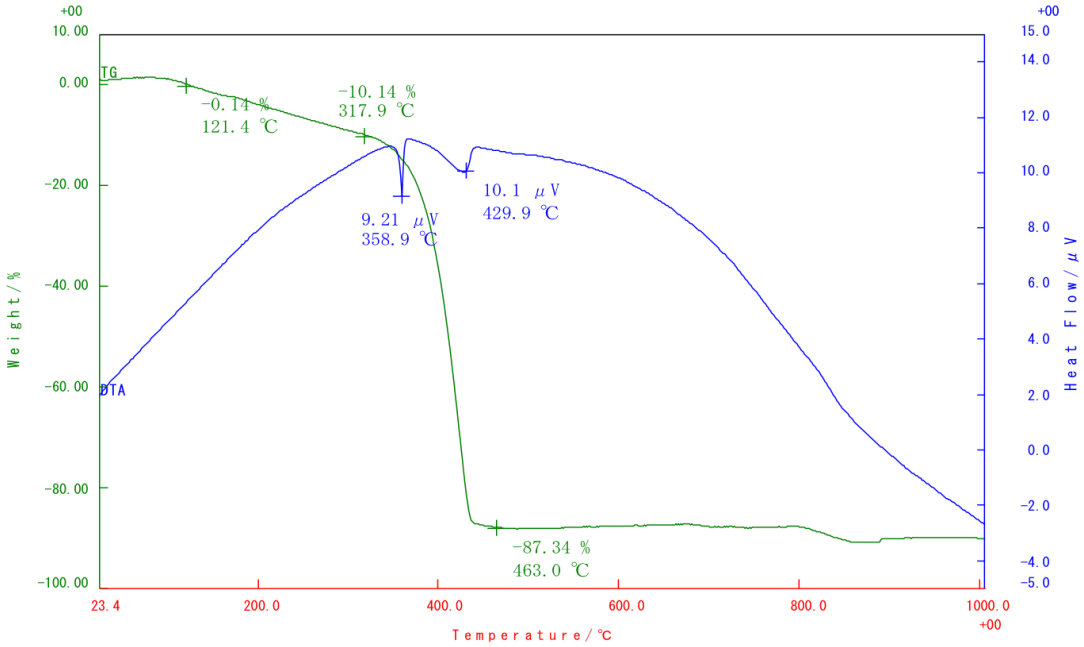


Fig. S18 Thermogravimetric and differential thermal analyses of **1** heating at 20 °C/min under He.

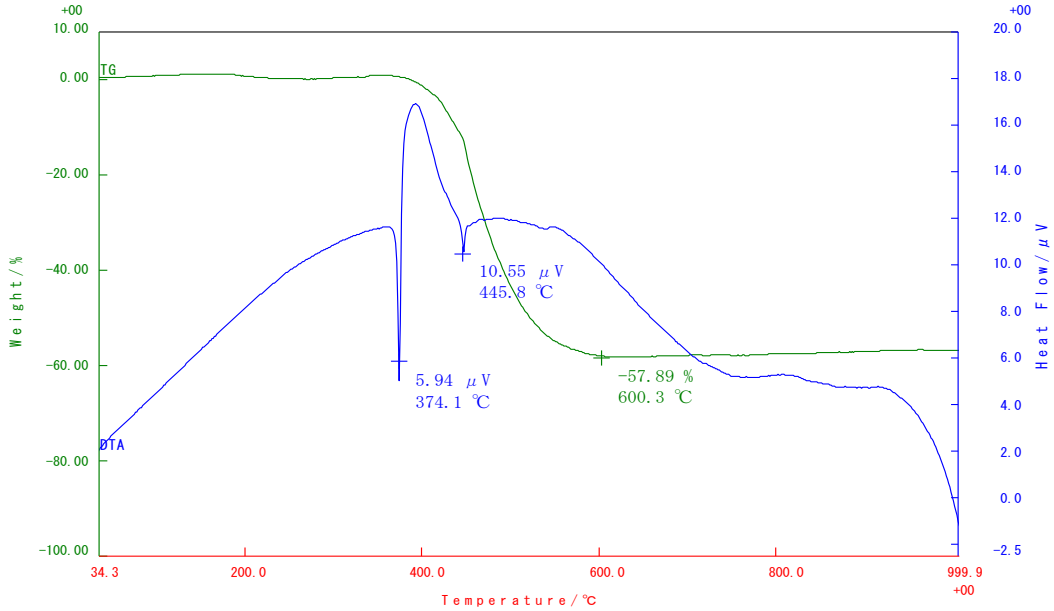


Fig. S19 Thermogravimetric and differential thermal analyses of **2** heating at 20 °C/min under He.

10. Optimized Geometries

Table S8 Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree) calculated by B3LYP/6-31G* level of theory ((*R*)-**1**, (*S*)-**2**, *twisted*-**2**, **3**) and by UB3LYP/6-311G** level of theory ($\mathbf{1}^{\bullet+}$, $\mathbf{3}^{\bullet+}$).[a]

structure	*E*	*E* + *ZPE*	*H*	*G*
(*R*)-**1**	-2156.79241524	-2156.034182	-2155.990043	-2155.990043
(*S*)-**2**	-2154.41445378	-2153.657392	-2153.656448	-2153.769551
twisted-**2**	-2154.37753406	-2153.661056	-2153.619883	-2153.732200
3	-1078.99968485	-1078.610759	-1078.588422	-1078.662898
$\mathbf{1}^{\bullet+}$	-2157.06174034	-2156.306474	-2156.262217	-2156.384833
$\mathbf{3}^{\bullet+}$	-1079.00336473	-1078.616546	-1078.594088	-1078.669166

[a] *E*: electronic energy; *ZPE*: zero-point energy; *H* (= $E + ZPE + E_{vib} + E_{rot} + E_{trans} + RT$): sum of electronic and thermal enthalpies; *G* (= $H - TS$): sum of electronic and thermal free energies.

Table S9 Cartesian coordinates of optimized structures calculated by B3LYP/6-31G* or UB3LYP/6-311G** level of theory.

3

C	0.74160500	4.68450800	1.02886600
C	0.00369400	5.27853500	0.00007200
C	-0.73505300	4.68551600	-1.02878900
C	-0.92890000	3.32735800	-1.29528300
C	-0.43616300	2.22009700	-0.60791600
C	0.43917600	2.21951100	0.60804300
C	0.93352800	3.32601900	1.29536500
C	-0.67293100	0.87671200	-0.92955000
C	0.00002400	0.05310900	0.00010900
C	0.67406500	0.87575100	0.92972800
C	-0.00098800	-1.43143500	0.00011400
C	1.22173500	-2.15147100	-0.02546000
C	1.19884100	-3.55405100	-0.01500700
C	-0.00264800	-4.25438900	0.00028000
C	-1.20329900	-3.55261300	0.01544600
C	-1.22458300	-2.15000300	0.02571600
C	-2.56081300	-1.48716200	0.10867700
C	2.55873100	-1.49019500	-0.10866100
C	2.86916900	-0.58175100	-1.13348300
C	4.14265000	-0.02405100	-1.23021100
C	5.13238500	-0.35996200	-0.30359300
C	4.83840100	-1.26234100	0.71911200
C	3.56458900	-1.82502900	0.81176800
C	-3.56713800	-1.82143200	-0.81145500
C	-4.84028300	-1.25719500	-0.71908300
C	-5.13314700	-0.35377800	0.30302800
C	-4.14295600	-0.01841600	1.22935400
C	-2.87013100	-0.57766800	1.13290700
H	1.23411700	5.37223800	1.71295000
H	0.00443600	6.36757900	0.00006100
H	-1.22655900	5.37397300	-1.71286500
H	-1.55310800	3.09906800	-2.15909800
H	1.55745800	3.09685800	2.15914800
H	-1.28049000	0.52789000	-1.75549600
H	1.28115100	0.52615000	1.75569800
H	2.14193300	-4.09192400	-0.05146700
H	-0.00330800	-5.34110800	0.00037100
H	-2.14701000	-4.08939400	0.05199800
H	2.10652600	-0.31573100	-1.85885800
H	4.36334200	0.67348900	-2.03404700
H	6.12424000	0.07788000	-0.37923500
H	5.59950000	-1.52933500	1.44791100
H	3.33821200	-2.52241000	1.61429500
H	-3.34166100	-2.51961300	-1.61353900
H	-5.60172500	-1.52378000	-1.44767400
H	-6.12447800	0.08528900	0.37843800
H	-4.36276900	0.67989900	2.03275800
H	-2.10715300	-0.31206600	1.85807800

(*R*)-1

C	-0.43880700	0.89551300	-0.59970600
C	-0.45507800	0.01602500	-1.72812100
C	-1.45480300	0.42962200	-2.63139700
C	-2.06507700	1.59217000	-2.15589900
C	-3.06167200	2.31053100	-2.81797700
C	-3.69057000	3.49715500	-2.44351200
C	-3.48652100	4.25612700	-1.28503200
C	-2.62450800	4.02285700	-0.21316300
C	-1.71728500	2.97370300	-0.01590700
C	-1.41976400	1.89898700	-0.84775800
C	0.43951900	0.89529000	0.59960500
C	0.45512500	0.01588900	1.72808600
C	1.45516600	0.42885000	2.63134800
C	2.06604400	1.59112000	2.15587600
C	3.06293800	2.30904800	2.81799100
C	3.69246500	3.49534100	2.44348700
C	3.48892500	4.25430100	1.28490100
C	2.62687200	4.02137700	0.21298600
C	1.71907100	2.97270700	0.01577400
C	1.42092700	1.89823700	0.84770100
C	0.44162800	-1.13217200	-2.04958900
C	1.81511400	-0.92178100	-2.34705600
C	2.63554000	-2.02341100	-2.64311700
C	2.12430700	-3.31496000	-2.68499000
C	0.76390600	-3.51324700	-2.48220400

C	-0.09278200	-2.44219500	-2.18409300
C	2.44604100	0.42366800	-2.50603800
C	1.89911000	1.38223700	-3.37539100
C	2.58009300	2.56800200	-3.65207600
C	3.82137000	2.82191100	-3.06515700
C	4.37002600	1.88472900	-2.18848600
C	3.68945800	0.69912000	-1.91358800
C	-1.55196600	-2.75649400	-2.09738700
C	-2.15921900	-3.43104400	-3.17092200
C	-3.50966200	-3.77831600	-3.13115000
C	-4.27840500	-3.46568100	-2.00939800
C	-3.68378000	-2.80312000	-0.93406000
C	-2.33597600	-2.44811000	-0.97764600
C	-0.44223700	-1.13180000	2.04960700
C	-1.81560500	-0.92072300	2.34707600
C	-2.63658000	-2.02192400	2.64319000
C	-2.12602600	-3.31372800	2.68510400
C	-0.76571700	-3.51270300	2.48234800
C	0.09149100	-2.44208500	2.18421200
C	-2.44587300	0.42503700	2.50591700
C	-1.89873300	1.38323100	3.37553900
C	-2.57923800	2.56927500	3.65218900
C	-3.82024400	2.82382000	3.06498400
C	-4.36911600	1.88699200	2.18807400
C	-3.68900000	0.70113100	1.91317600
C	1.55052900	-2.75708400	2.09762700
C	2.15758600	-3.43134000	3.17143000
C	3.50784500	-3.77931400	3.13159500
C	4.27654500	-3.46771300	2.00951900
C	3.68207900	-2.80545200	0.93391200
C	2.33446700	-2.44970400	0.97757600
H	-1.68866500	-0.06556000	-3.56624100
H	-3.38251400	1.88294500	-3.76794700
H	-4.43497000	3.88000500	-3.13836700
H	-4.09644400	5.15500800	-1.20484700
H	-2.66615000	4.75333100	0.59137400
H	-1.16400100	3.00696600	0.91860600
H	1.68871900	-0.06645600	3.56620100
H	3.38349100	1.88136200	3.76801300
H	4.43696900	3.87788500	3.13839700
H	4.09931800	5.15285800	1.20465900
H	2.66899200	4.75173000	-0.59163600
H	1.16577500	3.00620500	-0.91873600
H	3.67911900	-1.84509900	-2.88570100
H	2.77475600	-4.15628500	-2.90818200
H	0.34423600	-4.51281500	-2.54623400
H	0.94543800	1.18605700	-3.85400000
H	2.14433600	3.28788900	-4.34044000
H	4.35553700	3.74191400	-3.28828300
H	5.32786500	2.07749100	-1.71260000
H	4.12016100	-0.02043400	-1.22264800
H	-1.56654300	-3.66995300	-4.05022100
H	-3.95913400	-4.29199000	-3.97730800
H	-5.33009400	-3.73796800	-1.97243800
H	-4.26713500	-2.56875200	-0.04755300
H	-1.88670500	-1.94020600	-0.13348500
H	-3.68006400	-1.84306500	2.88577700
H	-2.77691400	-4.15470200	2.90834400
H	-0.34654900	-4.51248300	2.54640200
H	-0.94529700	1.18651500	3.85439700
H	-2.14334000	3.28886600	4.34077100
H	-4.35403200	3.74406500	3.28802400
H	-5.32672700	2.08028600	1.71194400
H	-4.11989500	-0.01820500	1.22212300
H	1.56489400	-3.66957500	4.05091100
H	3.95721600	-4.29275000	3.97795200
H	5.32810800	-3.74048900	1.97256400
H	4.26535000	-2.57191800	0.04713100
H	1.88524900	-1.94209900	0.13321300

(*S*)-2

C	4.08651400	2.33974700	-0.63733600
C	4.30727700	3.67710800	-0.25029300
C	3.49195500	4.51193000	0.49867300
C	2.20392900	4.25943500	1.00254300
C	1.39383200	3.15346300	0.78727200
C	1.64383900	1.98389800	0.04912900
C	2.96817300	1.53866500	-0.46500000
C	0.69960000	0.97764100	-0.22655900
C	1.39612200	-0.08080100	-0.91434300
C	2.79091100	0.18494500	-0.90042200
C	0.90211800	-1.29406200	-1.54783000
C	3.75065500	-0.87803100	-1.12011800
C	-0.40376100	-1.43627200	-2.11803500
C	-0.84853100	-2.71031900	-2.47305500
C	-0.01546300	-3.82609900	-2.36624500
C	1.31115400	-3.65548200	-2.01616100
C	1.81380700	-2.39197000	-1.64236400
C	3.25056500	-2.18596300	-1.40623900
C	4.17287700	-3.24965400	-1.50681300
C	5.53469600	-3.06392300	-1.33606000
C	6.02180400	-1.78826300	-1.02721400
C	5.14276100	-0.72506500	-0.91228500
C	-1.23362000	-0.29480400	-2.60119100
C	1.23353800	-0.29444600	2.60124700
C	-5.14275900	-0.72476000	0.91219700
C	-6.02184300	-1.78791600	1.02719600
C	-5.53479400	-3.06356000	1.33619600
C	-4.17299100	-3.24931700	1.50704000
C	-3.25063800	-2.18566700	1.40639900
C	-1.81390300	-2.39169600	1.64264800
C	-1.31132200	-3.65516100	2.01669900
C	0.01526200	-3.82576200	2.36692100
C	0.84836600	-2.70999500	2.47359200
C	0.40367300	-1.43599700	2.11829500
C	-3.75066700	-0.87774800	1.12010500
C	-0.90216600	-1.29383900	1.54799600
C	-2.79087200	0.18517400	0.90035500
C	-1.39609600	-0.08063300	0.91435200
C	-0.69950000	0.97770400	0.22648600
C	-2.96804900	1.53887300	0.46482600
C	-1.64367100	1.98400200	-0.04928000
C	-1.39356700	3.15351300	-0.78747500
C	-2.20358900	4.25952200	-1.00283600
C	-3.49161900	4.51212000	-0.49903000
C	-4.30701600	3.67738700	0.24995300

C	-4.08634600	2.34003500	0.63708000
C	-0.64051100	0.72526800	-3.36600900
C	-1.42170900	1.68960800	-4.00097600
C	-2.81301200	1.65849800	-3.88572300
C	-3.41421000	0.65695500	-3.12277600
C	-2.63397200	-0.31091800	-2.49103500
C	2.63389900	-0.31062800	2.49122400
C	3.41410200	0.65740300	3.12276600
C	2.81285800	1.65918400	3.88536600
C	1.42154500	1.69036500	4.00047700
C	0.64038300	0.72585900	3.36571800
H	4.91056600	1.89792300	-1.18752600
H	5.26633300	4.09212800	-0.55293100
H	3.90435700	5.49242500	0.73202900
H	1.77097000	5.04927500	1.61255700
H	0.40902600	3.19830600	1.24337400
H	-1.83467300	-2.81789400	-2.91410200
H	-0.38477900	-4.81042000	-2.64090000
H	1.96755100	-4.51636200	-2.04964400
H	3.82078900	-4.25075500	-1.72528500
H	6.21303400	-3.90789500	-1.42536300
H	7.08354100	-1.63105200	-0.85619500
H	5.53653000	0.23295500	-0.60285700
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H	-3.82094800	-4.25040700	1.72563200
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H	0.38451900	-4.81004800	2.64178200
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H	-0.94134500	2.45895500	-4.60060300
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H	-0.43839500	0.73924100	3.48841800

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C	-2.84486200	1.81755700	0.81333000
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C	-3.98774900	-0.52131800	0.42820400
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C	-0.94562000	-4.11095700	1.82612400
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C	3.69907700	-1.91898800	-0.46453900
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C	3.91201000	3.99880100	-1.54515100
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C	2.86209000	-0.63584900	-1.17644000
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C	5.09353000	-0.31217500	-0.31373100
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C	-4.80018500	-1.16887800	-0.74912700
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4

C	-1.21190600	4.49339100	0.33246500
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C	1.21006900	4.49391800	-0.33239700
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C	2.46568500	-0.00933000	0.01555100
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C	4.94085200	-1.38244400	0.02498300
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C	-3.74869500	-2.08712600	0.05429100
C	-4.94032900	-1.38406800	-0.02511800
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C	-3.69444800	0.67411900	-0.15566200
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H	-5.83295500	0.57181300	-0.26297300
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