Synthesis and Stereoisomerism of [*n*]Cyclo-2,9-phenanthrenylene Congeners Possessing Alternating *E*/*Z*- and *R*/*S*-Biaryl Linkages

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Table of contents

General

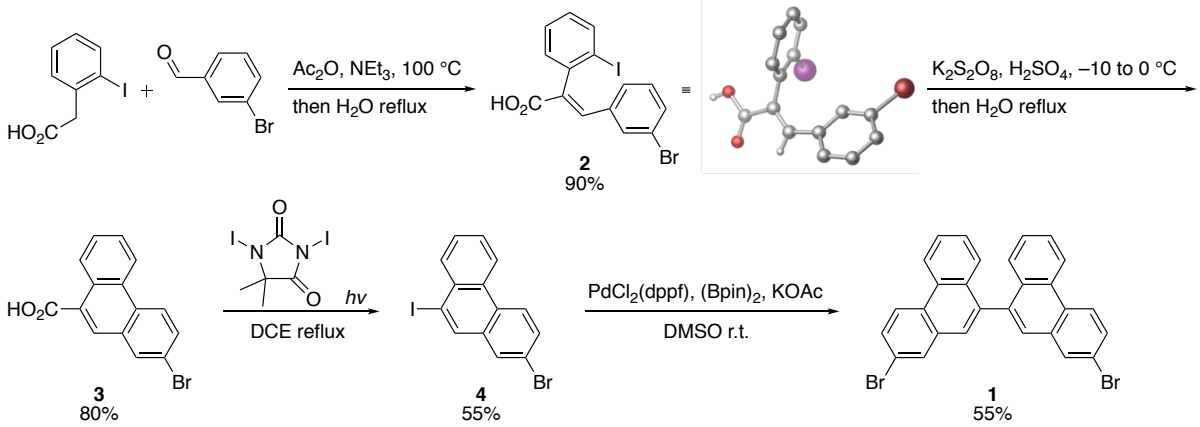
Flash silica gel column chromatography was performed on silica gel 60N (spherical and neutral gel, 40-50 μm, Kanto). High performance column chromatography (HPLC) and gel permeation chromatography (GPC) were performed on JASCO LC-2000 Plus Series Systems equipped with a UV detector. Melting points (mp) were recorded on a Stuart SMP30 instrument. Thermogravimetry differential thermal analysis (TG-DTA) to determine decomposition temperatures (T_d) was performed on a system composed of a NETZSCH TG-DTA2500 instrument, an Agilent Technologies 7980B gas chromatograph and a JEOL JMS-Q1050GC mass spectrometer (initial equilibration at 40 °C, 10 min; heating rate = 10 °C/min in flowing helium). Proton and carbon nuclear magnetic resonance (NMR) spectra were recorded on a JEOL JNM-ECA II 600 (^{1}H: 600 MHz; ^{13}C: 150 MHz) spectrometer. Chemical shift values were given in ppm relative to the solvent resonance: 1,1,2,2-tetrachloroethane-d_2 (for ^{1}H NMR: δ 6.0, for ^{13}C NMR: δ 73.78), and $CDCl_3$ (for ^{1}H NMR: δ 7.26,

for ^{13}C NMR: δ 77.16). High-resolution mass spectra (HRMS) were recorded on a Bruker Daltonics microTOF II spectrometer using a Direct Atmospheric Pressure Chemical Ionization (Direct-APCI) method, on a Bruker Daltonics autoflex speed TOF mass spectrometer using Matrix Assisted Laser Desorption Ionization (MALDI) method or on a Bruker Daltonics FT-ICR solariX 9.4T using a MALDI method. Combustion elemental analysis was performed on a Yanaco JM-10 instrument for CHN and a Yanaco HNS-15/HSU-20 instrument for Cl. Ultraviolet-visible (UV) spectra were recorded on a JASCO V-670 spectrophotometer. Fluorescence spectra were recorded on a JASCO FP-8500 spectrophotometer. Absolute fluorescence quantum yields were determined on a Hamamatsu Quantaurus-QY C11347. X-ray diffraction analyses of single crystals were carried out on a Rigaku CrystaLAB P200 diffractometer equipped with a pixel array detector using multilayer mirror monochromated Cu Kα radiation.

Materials

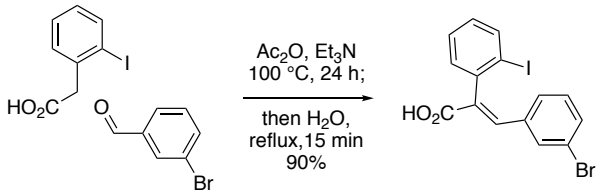
Anhydrous toluene and DMF were purified by a solvent purification system (Glass Contour) equipped with columns of activated alumina and supported copper catalyst (Q-5). All other chemicals were of reagent grade and used without further purification. The reactions were performed under N_2 atmosphere unless otherwise noted.

Synthesis



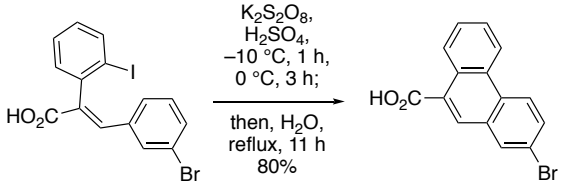
Scheme S1. Synthesis of compound **1**.

Compound **2**



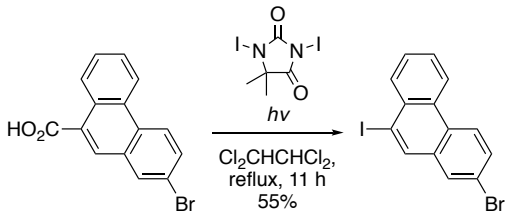
A mixture of 2-iodophenylacetic acid (75.6 g, 286 mmol), 3-bromobenzaldehyde (36.7 ml, 0.315 mol), and NEt_3 (43.7 mL, 315 mmol) in Ac_2O (270 mL, 286 mmol) was stirred at 100 °C for 24 h. After the reaction, water (365 ml) was added and refluxed for 15 min. The reaction mixture was extracted with Et_2O (500 mL) three times. Then the organic layer was extracted with 10% NaOH solution (500 mL) three times, and to the extract conc. HCl was added to pH = 2. The precipitate was separated and washed with water to give compound **2** as a yellow powder in 90% yield (111 g, 0.259 mol). ^{1}H-NMR (600 MHz, $CDCl_3$, 25 °C) δ 7.96 (d, J = 8.0 Hz, 1H), 7.88 (s, 1H), 7.40-7.38 (m, 2H), 7.19 (s, 1H), 7.15 (d, J = 7.8, 1H), 7.10 (t, J = 7.8, 1H), 7.05 (t, J = 7.9 Hz, 1H), 6.92 (d, J = 7.9 Hz, 1H) ppm, ^{13}C-NMR (150 MHz, $CDCl_3$, 25 °C) δ 171.4 (C), 141.4 (C), 140.4 (C), 139.6 (C), 136.0 (C), 135.6 (C), 133.7 (C), 132.8 (C), 130.4 (C), 130.1 (2C), 129.0 (C), 128.9 (C), 122.7 (C), 99.8 (C) ppm. HRMS (direct-APCI-TOF) *m/z* calcd for $C_{15}H_{10}BrIO_2$ $[M+H]^+$ 428.8982, found 428.8987. A single crystal suitable for the X-ray diffraction study was obtained by slow evaporation of $CHCl_3$ solution.

Compound **3**



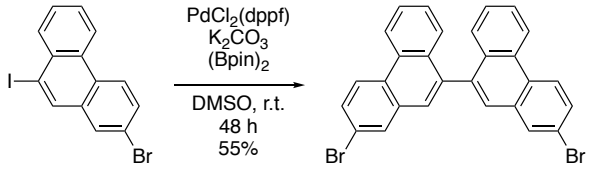
A mixture of compound **2** (10.0 g, 23.3 mmol) and $K_2S_2O_8$ (30.7 g, 113 mmol) in H_2SO_4 (125 mL) was stirred at −10 °C for 1 h, then 0 °C for 3 h. After the reaction, the solution was poured onto ice (620 g), and the resulting mixture was refluxed overnight. After cooling, the precipitate was filtered, dryed under vacuum at 90 °C. Then the precipitate was washed with $CHCl_3$ (80 mL) to give compound **3** as beige powder in 80% yield (5.59 g, 18.5 mmol). ^{1}H-NMR (600 MHz, $CDCl_3$, 25 °C) δ 9.09-9.04 (m, 1H), 8.73-8.68 (m, 1H), 8.58 (d, J = 8.8 Hz, 1H), 8.58 (s, 1H), 8.16 (s, 1H), 7.86 (s, 1H), 7.77-7.72 (m, 2H) ppm, ^{13}C-NMR (150 MHz, $CDCl_3$, 25 °C) δ 169.5 (C), 132.7 (C), 132.5 (C), 132.3 (C), 131.5 (C), 131.4 (C), 130.6 (C), 129.1 (C), 128.1 (C), 127.6 (C), 127.0 (C), 125.9 (C), 124.7 (C), 122.9 (C), 121.2 (C) ppm. HRMS (direct-APCI-TOF) *m/z* calcd for $C_{15}H_9BrO_2$ $[M+H]^+$ 299.9780, found 299.9772.

Compound **4**



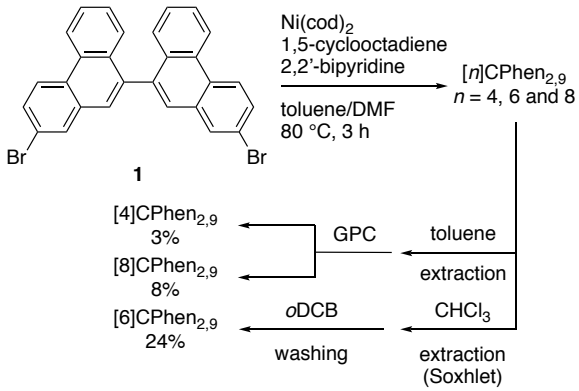
A mixture of compound **3** (1.02 g, 3.32 mmol) and 1,3-diiodo-5,5-dimethylhydantoin (1.90 g, 4.98 mmol) in dichloroethane (111 mL) was irradiated with 100 W tungsten-lamp under reflux condition for 11 h. The reaction was quenched with saturated aqueous $Na_2S_2O_3$, and the insoluble solid was filtered off. The filtrate was extracted with $CHCl_3$ three times, washed with brine, dried over anhydrous Na_2SO_4, concentrated in vacuo to give brown crude material (1.54 g). The crude material was purified by silica gel short pad, and recycling GPC to afford compound **4** in 55% yield (699 mg, 1.83 mmol). ^{1}H-NMR (600 MHz, $CDCl_3$, 25 °C) δ 8.59-8.56 (m, 1H), 8.52 (d, J = 8.8 Hz, 1H), 8.35 (s, 1H), 8.24-8.21 (m, 1H), 7.92 (s, 1H), 7.75 (d, J = 8.8 Hz, 1H), 7.73-7.68 (m, 2H) ppm, ^{13}C-NMR (150 MHz, $CDCl_3$, 25 °C) δ 137.4 (C), 134.3 (C), 133.6 (C), 132.2 (C), 130.5 (C), 130.3 (C), 129.8 (C), 129.2 (C), 128.4 (C), 128.1 (C), 124.7 (C), 122.9 (C), 121.1 (C), 100.4 (C) ppm. HRMS (direct-APCI-TOF) *m/z* calcd for $C_{14}H_8BrI$ $[M+H]^+$ 381.8849, found 381.8840.

Compound **1**



A mixture of compound **4** (5.38 g, 15.7 mmol), $Pd(dppf)Cl_2$•CH_2Cl_2 (1.20 g, 1.57 mmol), K_2CO_3 (6.12 g, 47.1 mmol), bis(pinacolato)diboron (3.81 g, 15.7 mmol) in DMSO (92 mL) was stirred at room temperature for 48 h. After addition of water, crude material was collected by filtration. The crude material was washed with $CHCl_3$ (65 mL) to give compound **1** as a pale grey powder in 55% yield (2.00 g, 3.90 mmol). ^{1}H-NMR (600 MHz, $CDCl_3$, 25 °C) δ 8.76 (d, J = 8.4 Hz, 2H), 8.66 (d, J = 8.9 Hz, 2H), 8.06 (s, 2H), 7.81 (d, J = 8.9 Hz, 2H), 7.74 (s, 2H), 8.76 (d, J = 8.4 Hz, 2H), 7.67 (dd, J = 8.4, 6.8 Hz, 2H), 7.45 (d, J = 8.2 Hz, 2H), 7.40 (dd, J = 8.2, 6.8 Hz, 2H) ppm, ^{13}C-NMR (150 MHz, $CDCl_3$, 25 °C) δ 138.2 (2C), 133.2 (2C), 132.1 (2C), 131.0 (2C), 130.2 (4C), 129.2 (2C), 127.7 (2C), 127.4 (2C), 127.2 (4C), 124.7 (2C), 122.9 (2C), 121.1 (2C) ppm. HRMS (direct-APCI-TOF) *m/z* calcd for $C_{28}H_{16}Br_2$ $[M+H]^+$ 509.9613, found 509.9604.

[*n*]CPhen$_{2,9}$



A mixture of bis(1,5-cyclooctadiene)nickel(0) (2.17 g, 7.82 mmol), 1,5-cyclooctadiene (0.96 mL, 7.82 mmol) and 2,2'-bipyridine (1.22 g, 7.82 mmol) in mixed solvent of toluene (8 mL) and DMF (8 mL) was stirred at 80 °C for 30 min in a 300 mL double-neck flask. To the mixture at 80 °C was added a solution of compound **1** (0.501 g, 0.978 mmol) in hot toluene (73 mL) at 80 °C dropwise over 1 h, and the mixture was stirred at 80 °C for additional 3 hours. After the reaction mixture was cooled down to ambient temperature, 1M aqueous hydrochloric acid (73 mL) was added. The mixture was stirred overnight, and the crude mixture was separated into a toluene solution and precipitates by filtration. The precipitates were washed with hydrochloric acid, water and methanol, then extracted by Soxhlet extraction with $CHCl_3$, washed with *o*DCB (26 mL) to afford [6]CPhen$_{2,9}$ as a white powder in 24% yield (92.9 mg, 0.0879 mmol). On the other hand, the toluene solution was washed with water and brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo. Recycling GPC with JAIGEL 1H-40, 2H-40 and 2.5H-40 columns (40ϕ, 600 mm; eluent = $CHCl_3$) afforded [8]CPhen$_{2,9}$ as a white powder in 8% yield (26.3 mg, 0.0187 mmol), and [4]CPhen$_{2,9}$ as a white powder in 3% yield (11.7 mg, 0.0166 mmol) after washed with *n*-hexane. For kinetic analysis of the isomerization, each stereoisomers were separated by HPLC using COSMOSIL Cholester (20ϕ, 250 mm; eluent = 50% MeOH in $CHCl_3$) for [4]CPhen$_{2,9}$, and DAICEL CHIRALPAK IA (20ϕ, 250 mm; eluent = 50% MeOH in $CHCl_3$) for [6]CPhen$_{2,9}$.

(*Z*,*R*,*Z*,*R*)*-[4]CPhen$_{2,9}$: ^{1}H-NMR (600 MHz, 1,1,2,2-tetrachloroethane-d_2, 25 °C) δ 8.88 (d, J = 8.1 Hz, 4H), 8.69 (d, J = 8.6 Hz, 4H), 8.42 (d, J = 8.1 Hz, 4H), 8.13 (d, J = 8.6 Hz, 4H), 7.80 (dd, J = 8.1, 7.0 Hz, 4H), 7.73 (dd, J = 8.1, 7.0 Hz, 4H), 7.71 (s, 4H), 7.56 (s, 4H) ppm, ^{13}C-NMR (150 MHz, 1,1,2,2-tetrachloroethane-d_2, 25 °C) δ 141.4 (4C), 139.2 (4C), 135.5 (8CH), 132.8 (4C), 132.4 (4C), 130.2 (8C), 127.4 (4CH), 127.1 (4CH), 126.7 (4CH), 125.6 (4CH), 123.6 (4CH), 122.7 (4CH) ppm. (*Z*,*R*,*Z*,*S*)-[4]CPhen$_{2,9}$: ^{1}H-NMR (600 MHz, 1,1,2,2-tetrachloroethane-d_2, 25 °C) δ 8.79 (d, J = 8.1 Hz, 4H), 8.65 (d, J = 8.7 Hz, 4H) , 8.40 (s, 4H), 8.36 (d, J = 8.1 Hz, 4H), 8.11 (d, J = 8.7 Hz, 4H), 7.76 (dd, J = 8.1, 6.9 Hz, 4H), 7.69 (dd, J = 8.1, 6.9 Hz, 4H), 7.62 (s, 4H) ppm, ^{13}C-NMR (150 MHz,

1,1,2,2-tetrachloroethane-d_2, 25 °C) δ 138.8 (4C), 136.9 (4C), 135.4 (4CH), 134.2 (4C), 133.8 (4C), 132.6 (4C), 130.1 (4CH), 129.8 (4C), 127.3 (4CH), 127.0 (4CH), 126.7 (4CH), 124.5 (4CH), 124.3 (4CH), 123.6 (4CH) ppm. HRMS (MALDI-TOF, matrix: TCNQ) *m/z* calcd for $C_{56}H_{32}$ $[M]^+$ 704.2499, found 704.2485. Anal. calcd for $C_{56}H_{32}$•0.072$CHCl_3$•0.13*n*-hexane•0.5H_2O C: 93.07, H: 4.80, Cl: 1.04 found C: 93.15, H: 4.80, Cl: 1.04.

(*Z*,*R*,*Z*,*R*,*Z*,*R*)*-[6]$CPhen_{2,9}$: ^{1}H-NMR (600 MHz, 1,1,2,2-tetrachloroethane-d_2 , 25 °C) δ 8.95 (d, *J* = 8.4 Hz, 6H), 8.91 (d, *J* = 8.3 Hz, 6H), 8.28 (s, 6H), 8.24 (s, 6H), 8.11 (d, *J* = 8.4 Hz, 6H), 7.74 (t, *J* = 8.3 Hz, 6H), 7.68 (d, *J* = 8.3 Hz, 6H), 7.47 (t, *J* = 8.3 Hz, 6H) ppm, ^{13}C-NMR (150 MHz, 1,1,2,2-tetrachloroethane-d_2, 25 °C) δ 140.8 (6C), 138.2 (6C), 132.2 (6C), 131.2 (6C), 130.0 (6C), 129.6 (6C), 129.5 (6C), 129.0 (6C), 128.1 (6C), 126.7 (6C), 126.4 (6C), 123.1 (6C), 122.9 (6C), 120.2 (6C) ppm. (*Z*,*R*,*Z*,*R*,*Z*,*S*)*-[6]$CPhen_{2,9}$: ^{1}H-NMR (600 MHz, 1,1,2,2-tetrachloroethane-d_2 , 25 °C) δ 8.94 (d, *J* = 8.8 Hz, 4H), 8.91–8.85 (m, 8H), 8.71 (s, 2H), 8.69 (s, 2H), 8.43 (d, *J* = 8.8 Hz, 2H), 8.35 (d, *J* = 8.8 Hz, 2H), 8.26 (s, 2H), 8.16 (s, 2H), 8.08 (s, 2H), 8.00 (d, *J* = 8.8 Hz, 2H), 7.93 (s, 2H), 7.79 (d, *J* = 8.8 Hz, 2H), 7.76–7.68 (m, 10H), 7.51–7.45 (m, 6H) ppm, The ^{13}C-NMR spectrum of (*Z*,*R*,*Z*,*R*,*Z*,*S*)*-[6]$CPhen_{2,9}$ was not recorded due to low solubility. HRMS (MALDI-TOF, matrix: TCNQ) *m/z* calcd for $C_{84}H_{48}$ $[M]^+$ 1056.3751, found 1056.3750. Anal. calcd for $C_{84}H_{48}$•0.75*o*DCB•1.75H_2O C: 88.65, H: 4.58, Cl: 4.43 found C: 88.45, H: 4.59, Cl: 4.50.

[8]$CPhen_{2,9}$: ^{1}H-NMR (600 MHz, 1,1,2,2-tetrachloroethane-d_2 , 25 °C) δ 8.98-8.93 (m, 8H), 8.90-8.85 (m, 8H), 8.33 (s, 2H), 8.29 (s, 2H), 8.17 (d, *J* = 8.6 Hz, 2H), 8.15 (s, 2H), 8.14 (d, *J* = 8.6 Hz, 2H), 8.11 (s, 2H), 8.08 (d, *J* = 8.6 Hz, 2H), 8.06 (s, 2H), 8.05 (d, *J* = 8.6 Hz, 2H), 8.01 (s, 2H), 7.97 (s, 2H), 7.94 (s, 2H), 7.77-7.67 (m, 8H), 7.61-7.56 (m, 4H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.49-7.42 (m, 8H), 7.39 (t, *J* = 8.6 Hz, 2H) ppm. ^{13}C-NMR (150 MHz, tetrachloroethane-d_2, 25 °C) δ 140.4 (4C), 139.4 (4C), 138.0 (2C), 137.8 (2C) 137.7 (2C), 137.6 (2C), 132.1 (2C), 132.0 (4C), 131.9 (4C), 131.8 (2C), 131.7 (4C), 129.9 (4C), 129.8 (4C), 129.4 (2C), 129.3 (4C), 129.2 (2C), 128.7 (2CH), 128.6 (2CH), 128.5 (2CH), 128.4 (2CH), 128.3 (2CH), 127.9 (2CH), 127.8 (4CH), 127.5 (4CH), 127.2 (2CH), 126.9 (2CH), 126.7 (20CH), 126.5 (4CH), 123.4 (2CH), 123.3 (6CH), 122.8 (8CH) ppm. HRMS (MALDI-TOF, matrix: TCNQ) *m/z* calcd for $C_{112}H_{64}$ $[M]^+$ 1408.5003, found 1408.5005.

MALDI-TOF spectra of isolated [*n*]CPhen$_{2,9}$

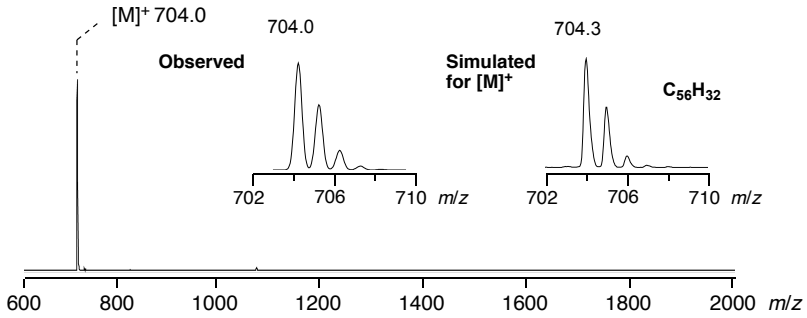


Fig. S1. MALDI-TOF MS of [4]CPhen$_{2,9}$ (ionization: linear positive, matrix: TCNQ).

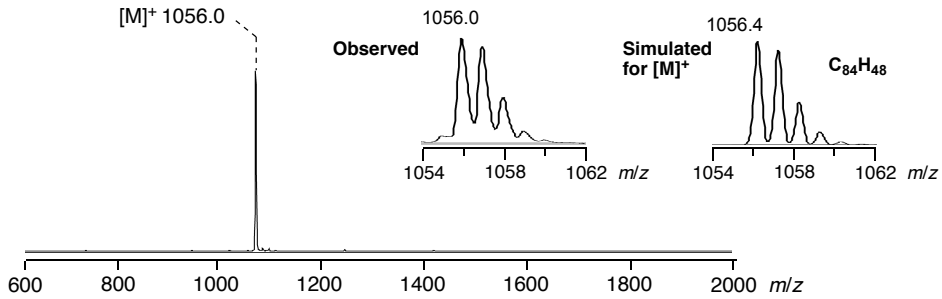


Fig. S2. MALDI-TOF MS of [6]CPhen$_{2,9}$ (ionization: linear positive, matrix: TCNQ).

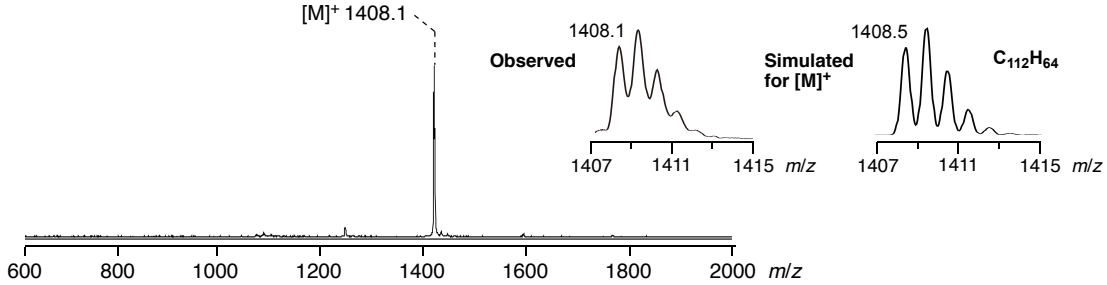


Fig. S3. MALDI-TOF MS of [8]CPhen$_{2,9}$ (ionization: linear positive, matrix: TCNQ).

***J*-resolved NMR of [8]CPhen$_{2,9}$**

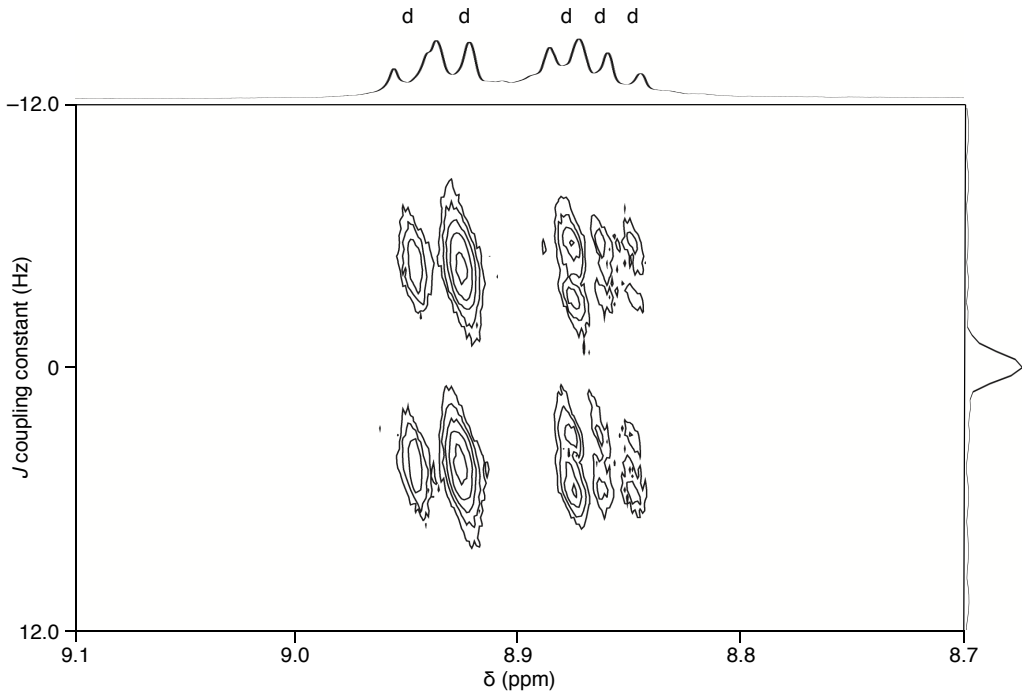


Fig. S4. *J*-resolved NMR spectrum of [8]CPhen$_{2,9}$ in 1,1,2,2-tetrachloroethane-d_2 (9.1−8.7 ppm) (25 °C, 600 MHz).

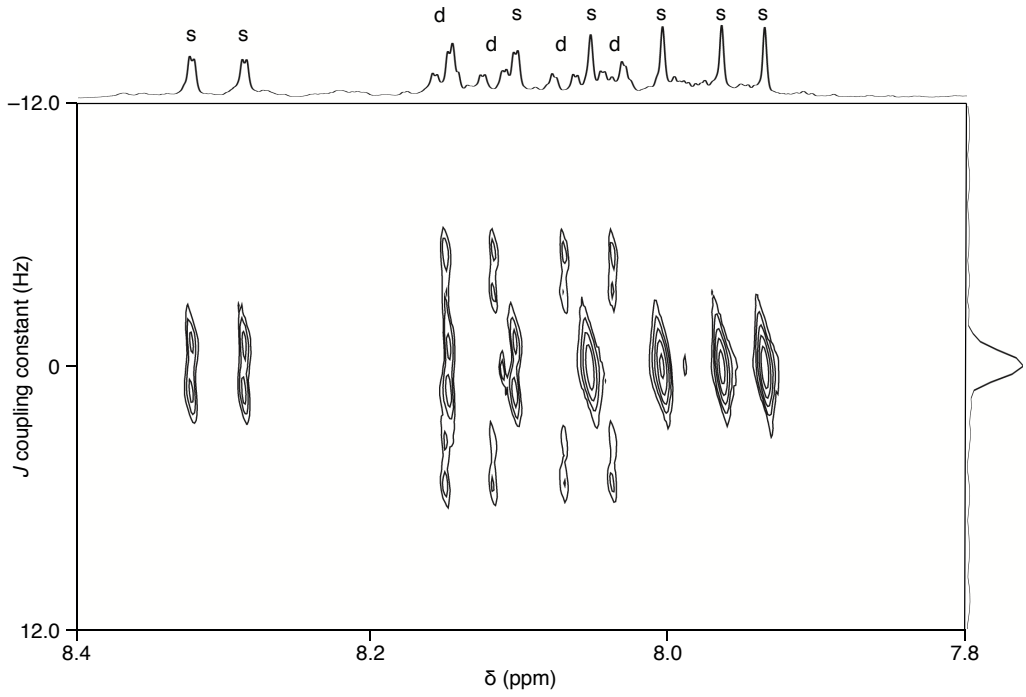


Fig. S5. *J*-resolved NMR spectrum of [8]CPhen$_{2,9}$ in 1,1,2,2-tetrachloroethane-d_2 (8.4−7.8 ppm) (25 °C, 600 MHz).

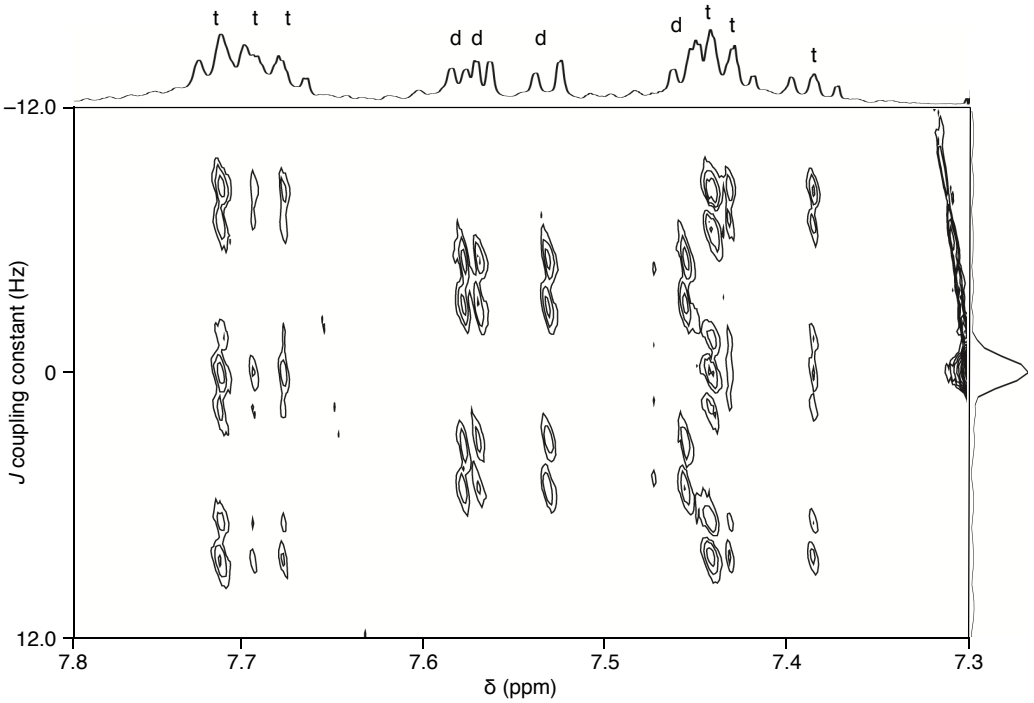
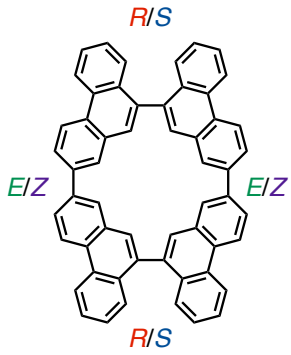


Fig. S6. *J*-resolved NMR spectrum of [8]CPhen$_{2,9}$ in 1,1,2,2-tetrachloroethane-d_2 (7.8−7.3 ppm) (25 °C, 600 MHz).

Stereoisomers

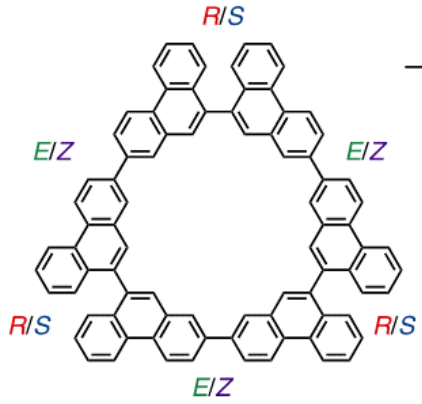
Table S1. Possible stereoisomers of [4]CPhen$_{2,9}$.



	xRxR	xRxS	xSxS
EyEy	ERER*	ERES	ESES*
EyZy	ERZR*	ERZS	ESZS*
ZyZy	ZRZR*	ZRZS	ZSZS*

* indicates the presence of enantiomeric pair.

Table S2. Possible stereoisomers of [6]CPhen$_{2,9}$.



	xRxRxR	xRxRxS	xSxSxR	xSxSxS
EyEyEy	ERERER*	ERERES*	ESESES*	ESESES*
EyEyZy	ERERZR*	ERERZS* ERZRES*	ESESZR* ESZSER*	ESESZS*
ZyZyEy	ZRZRER*	ZRZRES* ZRERZS*	ZSZSER* ZSESZR*	ZSZSES*
ZyZyZy	ZRZRZR*	ZRZRZS*	ZSZSZR*	ZSZSZS*

* indicates the presence of enantiomeric pair.

Table S3. Possible stereoisomers of [8]CPhen$_{2,9}$.

	xRxRxRxR	xRxRxRxS	xRxRxSxS	xRxSxRxS	xSxSxSxR	xSxSxSxS
EyEyEyEy	ERERERER*	ERERERES*	ERERESES	ERESERES	ESESESER*	ESESESES*
EyEyEyZy	ERERERZR*	ERERERZS* ZRERERES*	ERERESZS* ERZRESES* ZRERESES	ERESERZS	ESESESZR* ZSESESER*	ESESESZS*
EyEyZyZy	ERERZRZR*	ERERZRZS* ZRERERZS* ZRZRERES*	ERERZSZS* ZRERESZS*	ERESZRZS* ZRESERZS*	ESESZSZR* ZSESESZR* ESZSZSER*	ESESZSZS*
EyZyEyZy	ERZRERZR*	ERZRERZS*	ERZRESZS ZRERZSES*	ERZSERZS	ESZSESZR*	ESZSESZS*
ZyZyZyEy	ZRZRZRER*	ZRZRZRES* ZRERZRZS*	ZRZRZSES* ERZRZSZS ZRERZSZS*	ZRZSZRES	ZSZSZSER* ZSESZSZR*	ZSZSZSES*
ZyZyZyZy	ZRZRZRZR*	ZRZRZRZS*	ZRZRZSZS	ZRZSZRZS	ZSZSZSZR*	ZSZSZSZS*

Separation of stereoisomers

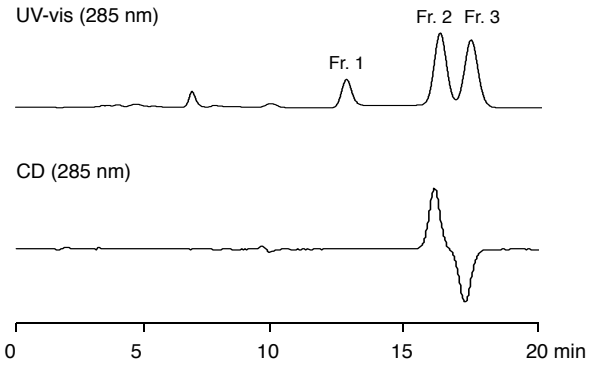


Fig. S7. HPLC analysis of [4]CPhen$_{2,9}$ with COSMOSIL Cholester (4.6ϕ × 250 mm). Conditions: eluent 50% MeOH in $CHCl_3$, flow rate = 1.0 mL/min, column temperature = 25 °C.

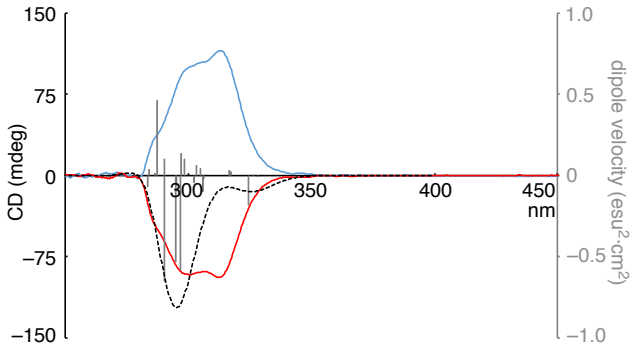


Fig. S8. CD spectra of (*Z*,*S*,*Z*,*S*)/(*Z*,*R*,*Z*,*R*)-[4]CPhen$_{2,9}$. The dotted line and gray bars show the simulated CD spectrum and the rotatory velocity of (*Z*,*R*,*Z*,*R*)-[4]CPhen$_{2,9}$, respectively, as calculated by TD DFT at the B3LYP/6-31G(d,p) level of theory.

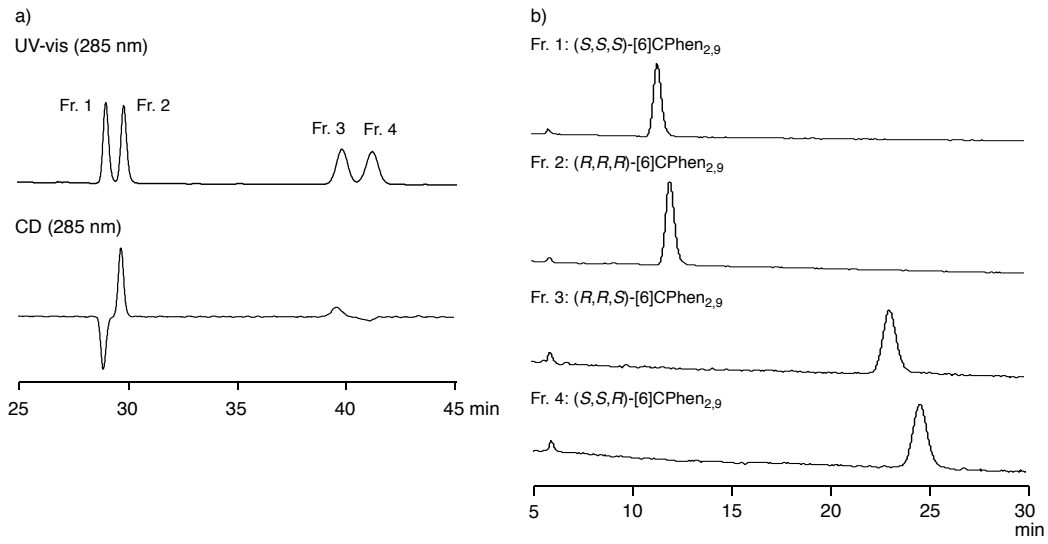


Fig. S9. Separation of stereoisomers of [6]CPhen$_{2,9}$. (a) HPLC analysis with DAICEL CHIRALPAK IA (4.6ϕ × 250 mm). Conditions: eluent 50% MeOH in $CHCl_3$, flow rate = 1.0 mL/min, column temperature = 40 °C. (b) HPLC analysis of the isolated stereoisomers.

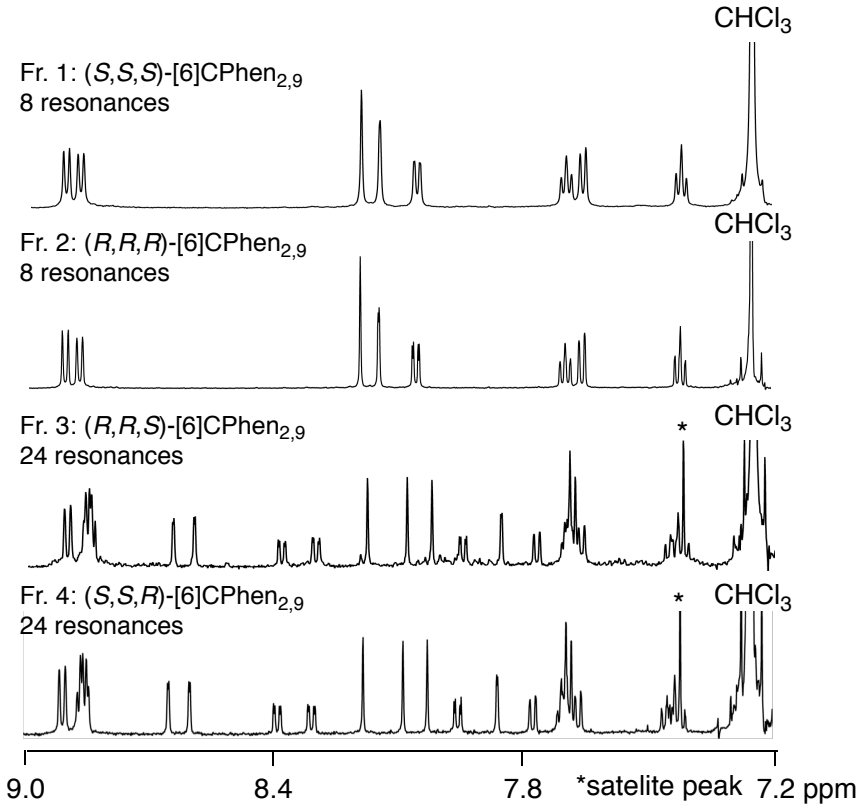


Fig. S10. ^{1}H NMR spectra (600 MHz, $CDCl_3$) of isolated stereoisomers of [6]CPhen$_{2,9}$.

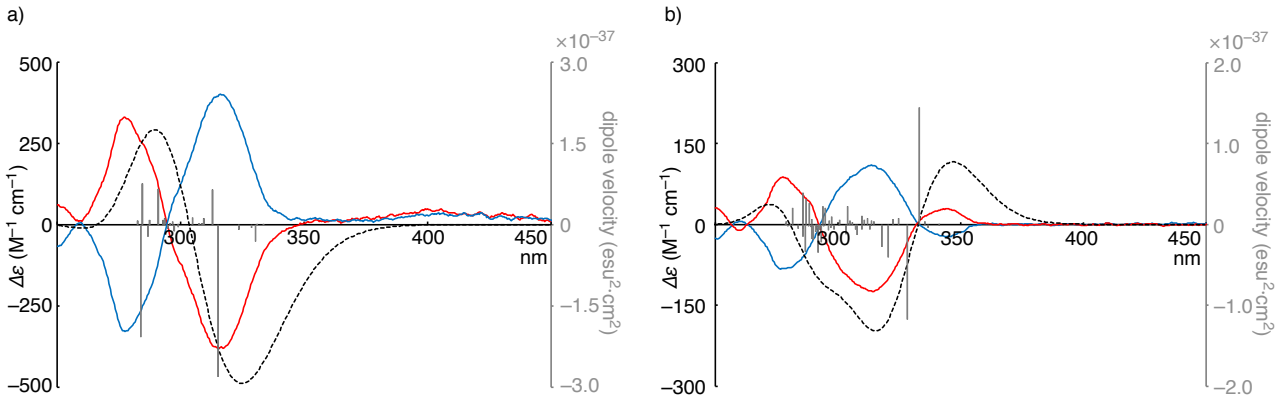


Fig. S11. CD spectra of (a) (*Z*,*S*,*Z*,*S*,*Z*,*S*)/(*Z*,*R*,*Z*,*R*,*Z*,*R*)-[6]CPhen$_{2,9}$, and (b) (*Z*,*S*,*Z*,*S*,*Z*,*R*)/(*Z*,*R*,*Z*,*R*,*Z*,*S*)-[6]CPhen$_{2,9}$. The dotted line and gray bars show the simulated CD spectrum and the rotatory velocity of (a) (*Z*,*R*,*Z*,*R*,*Z*,*R*)-[6]CPhen$_{2,9}$ and (b) (*Z*,*R*,*Z*,*R*,*Z*,*S*)-[6]CPhen$_{2,9}$, respectively, as calculated by TD DFT at the B3LYP/6-31G(d,p) level of theory.

Scan calculations

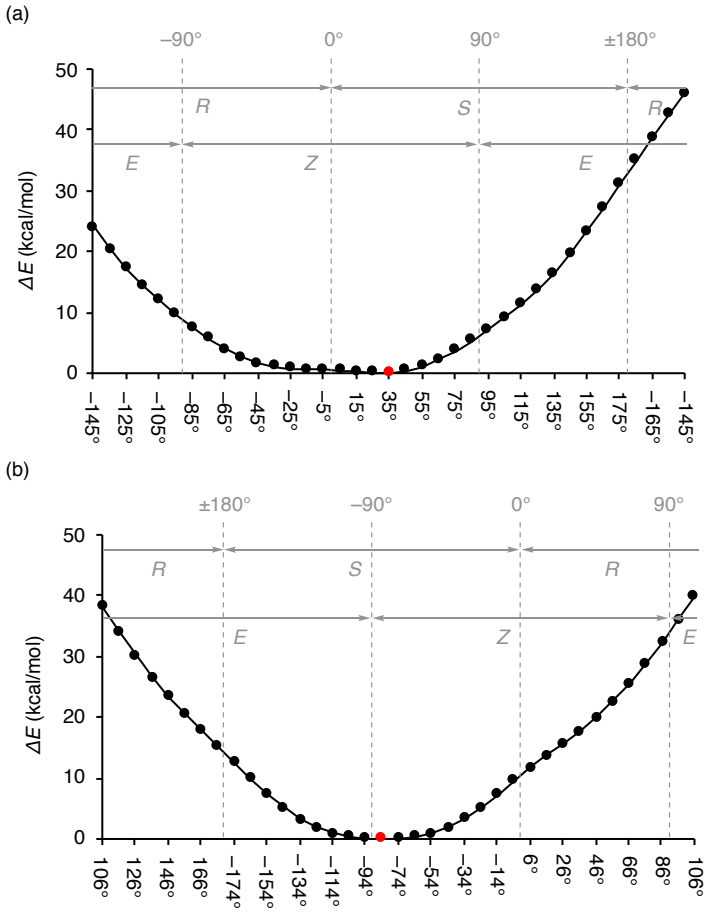


Fig. S12. Energy profile of 2,2′-biaryl linkage (1-2-2′-1′) in (a) (*E*/*Z*,*S*,*Z*,*S*,*Z*,*R*)-[6]CPhen$_{2,9}$, and (b) (*Z*,*S*,*E*/*Z*,*S*,*Z*,*R*)-[6]CPhen$_{2,9}$ from scan calculations at the semiempirical PM6 level of theory. Red dots show stationary points.

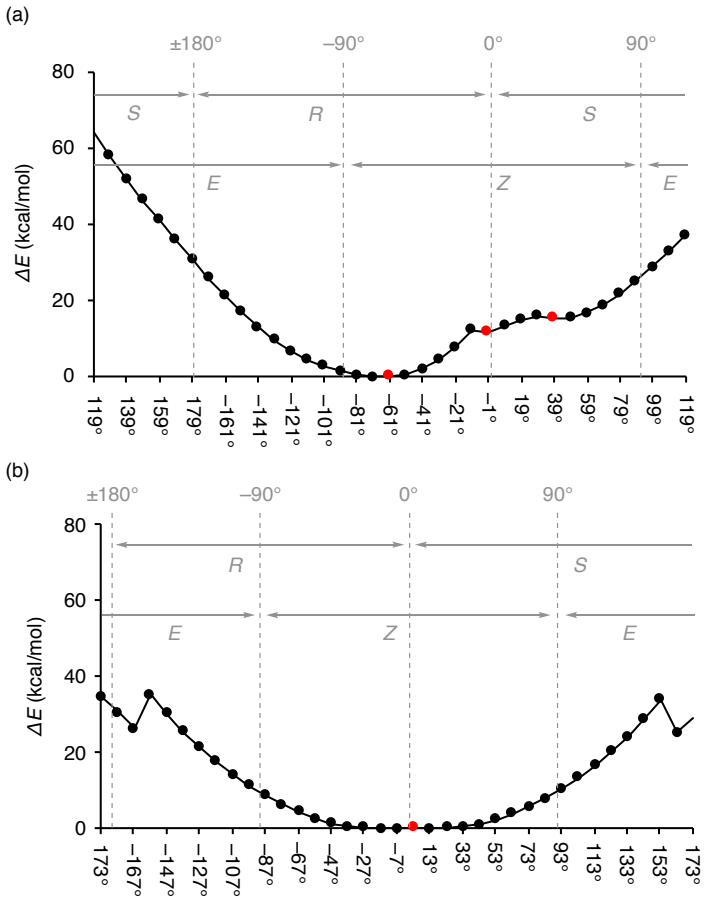


Fig. S13. Energy profile of 2,2′-biaryl linkage (1-2-2′-1′) in (a) (*E*/*Z*,*S*,*Z*,*S*)-[4]CPhen$_{2,9}$, and (b) (*E*/*Z*,*S*,*Z*,*R*)-[4]CPhen$_{2,9}$ from scan calculations at the semiempirical PM6 level of theory. Red dots show stationary points. The relaxations at (b) −167° and 173° are derived from rotations at neighboring 1,1′-binaphthyl linkages.

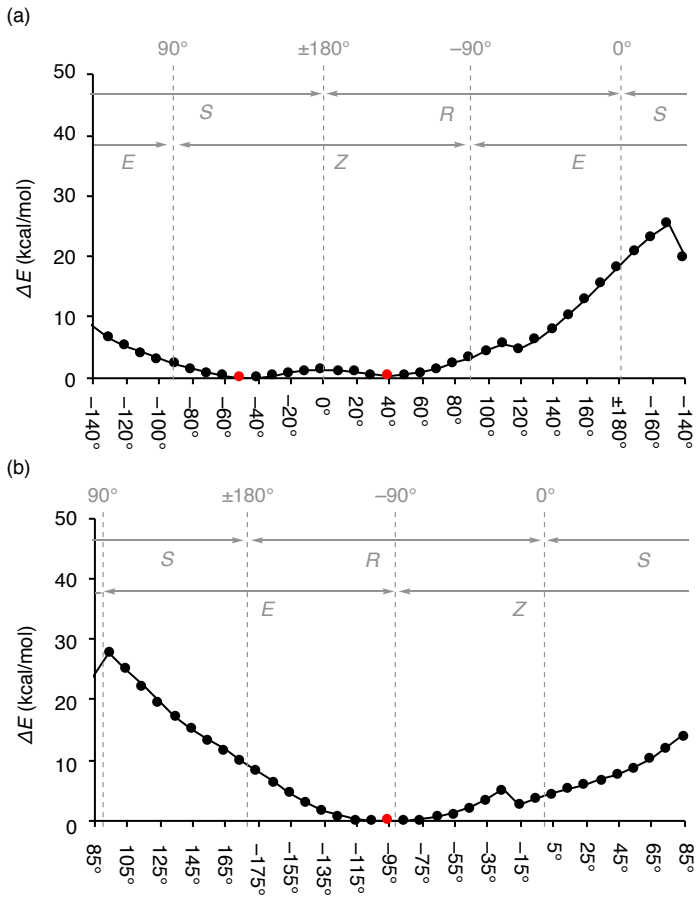


Fig. S14. Energy profile of 2,2′-biaryl linkage (1-2-2′-1′) in (a) (*E*/*Z*,*S*,*E*,*S*,*E*,*S*,*Z*,*R*)-[8]CPhen$_{2,9}$, and (b) (*Z*,*S*,*E*/*Z*,*S*,*E*,*S*,*Z*,*R*)-[8]CPhen$_{2,9}$ from scan calculations at the semiempirical PM6 level of theory. Red dots show stationary points. The relaxations at (a) −150° and (b) 95° are derived from rotations at neighboring 1,1′-binaphthyl linkages. The relaxations at (a) 120° and (b) –15° are derived from rotations at 2,2′-binaphthyl linkages next to the neighboring 1,1′-binaphthyl linkages.

Conformational search calculations

Table S4. The result of conformational search calculations of [8]CPhen$_{2,9}$.

No.	Structure	Energy[a]	Note	Symmetry	No. of ^{1}H NMR resonance
1,2	(*Z*,*S*,*E*,*S*,*Z*,*S*,*E*,*S*)*	0.4 kcal/mol	enantiomer pair	D_2	16
3	(*Z*,*R*,*Z*,*S*,*Z*,*R*,*Z*,*S*)	0		S_4	16
4,5	(*Z*,*S*,*Z*,*S*,*E*,*S*,*Z*,*R*)*	2.3 kcal/mol	enantiomer pair	C_1	64
6,7	(*Z*,*R*,*E*,*R*,*Z*,*S*,*E*,*S*)	2.1 kcal/mol		C_{2h}	16
8,9	(*Z*,*S*,*E*,*S*,*E*,*S*,*Z*,*R*)*	4.3 kcal/mol	enantiomer pair	C_2	32
10	(*Z*,*R*,*E*,*R*,*Z*,*S*,*E*,*S*)	2.1 kcal/mol	same as 6,7	C_{2h}	16
11	(*Z*,*R*,*Z*,*R*,*Z*,*R*,*Z*,*R*)	0	changed to 1,2	D_2	8
12	(*Z*,*R*,*Z*,*S*,*Z*,*R*,*Z*,*S*)	0	same as 3	S_4	16
13	(*Z*,*R*,*Z*,*S*,*Z*,*R*,*Z*,*S*)	0	same as 3,12	S_4	16

[a]The energy values were obtained by DFT calculations at B3LYP/6-31G(d,p) level of theory.

Crystal structures

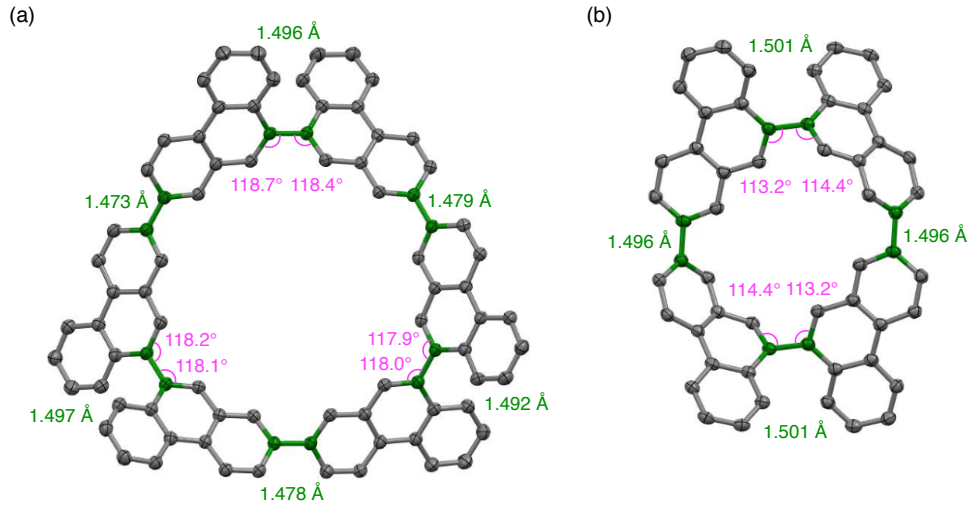


Fig. S15. Crystal structure of (a) (*Z*,*S*,*Z*,*S*,*Z*,*S*)*-[6]CPhen$_{2,9}$ racemate, and (b) (*Z*,*S*,*Z*,*R*)-[4]CPhen$_{2,9}$. Hydrogen atoms and solvent molecules were omitted for clarity.

Thermal isomerization of [6]CPhen$_{2,9}$

Kinetics of the isomerization of [6]CPhen$_{2,9}$ was studied by following the molar ratio of (*Z*,*R*,*Z*,*R*,*Z*,*R*)-[6]CPhen$_{2,9}$ with HPLC equipped with DAICEL CHIRALPAK IA (4.6ϕ × 250 mm) (conditions: eluent: $CHCl_3$/MeOH = 20/80 to 50/50, flow rate: 1.0 mL/min, detector: UV 285 nm.) after heated in 1,2,4-trichrolobenzene at 149 °C, 181 °C, 191 °C and 201°C. A solution of (*Z*,*R*,*Z*,*R*,*Z*,*R*)-[6]CPhen$_{2,9}$ in 1,2,4-trichrolobenzene (2 mL) in a sealed tube was heated in an oil bath.

After certain time, the reaction mixture was immediately cooled to 0 °C, and an aliquot (100 μL) of the reaction mixture was sampled. The sample solution was diluted with 1,2,4-trichrolobenzene (200 μL) and eluent (500 μL), then subjected to HPLC analysis.

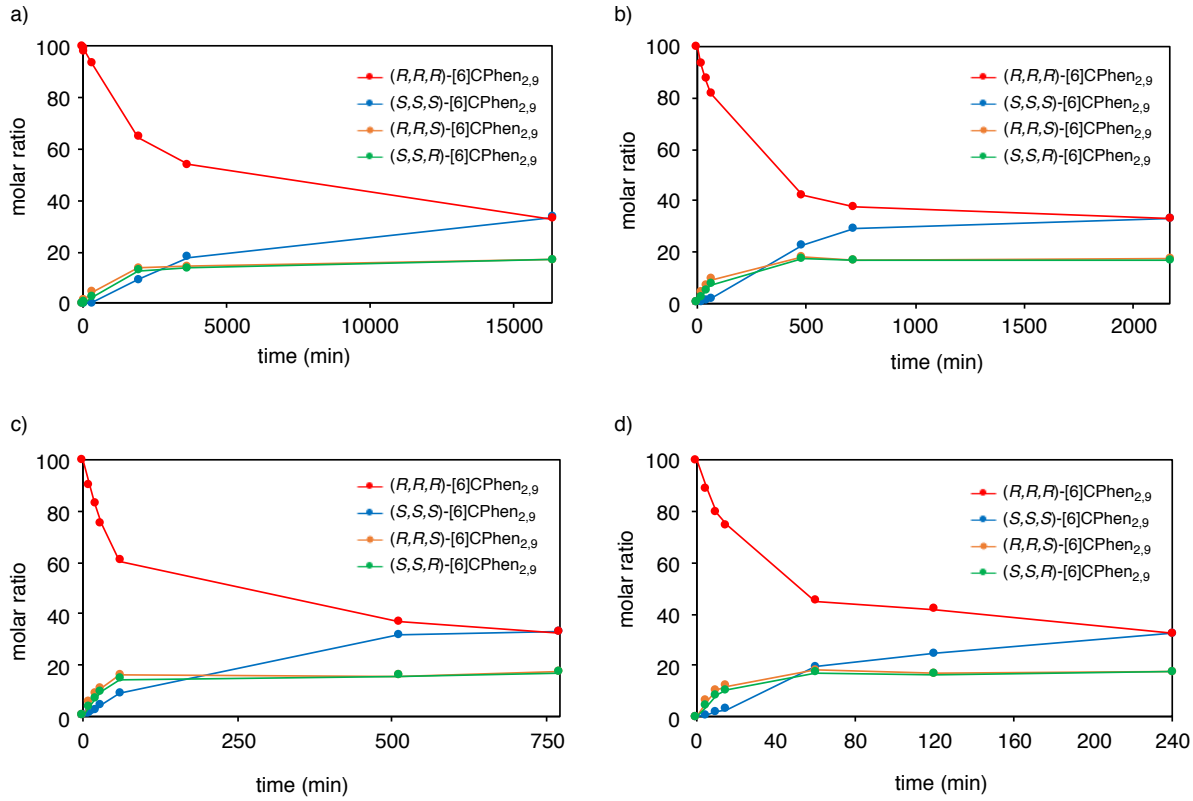
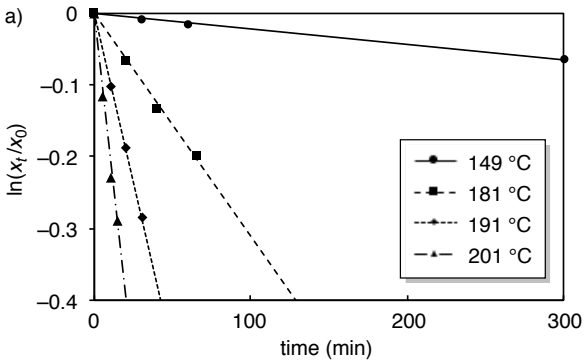


Fig. S16. Time-course analysis of isomerization of (*Z*,*R*,*Z*,*R*,*Z*,*R*)-[6]CPhen$_{2,9}$ in 1,2,4-trichlorobenzene at (a) 149 °C, (b) 181 °C, (c) 191 °C, and (d) 201 °C.



T (°C)	k (s^{-1})	R^2
149	3.5838×10^{-6}	0.9958
181	5.1905×10^{-5}	0.9959
191	1.5751×10^{-4}	0.9985
201	3.2791×10^{-4}	0.9809

Fig. S17. Plots for the decreasing integration of (*Z*,*R*,*Z*,*R*,*Z*,*R*)-[6]CPhen$_{2,9}$ and rate constant at varied temperatures.

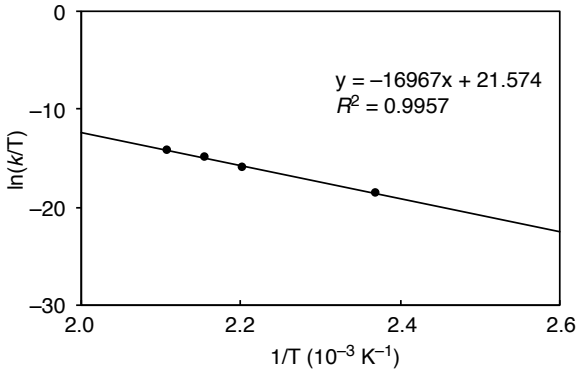


Fig. S18. Eyring plot for the isomerization of (*Z*,*R*,*Z*,*R*,*Z*,*R*)-[6]CPhen$_{2,9}$ to reveal the activation energy with $\Delta H^{\ddagger} = +33.7$ kcal/mol, $\Delta S^{\ddagger} = -4.4$ kcal/mol·K, and $\Delta G^{\ddagger} = +35.0$ kcal/mol at 25 °C.

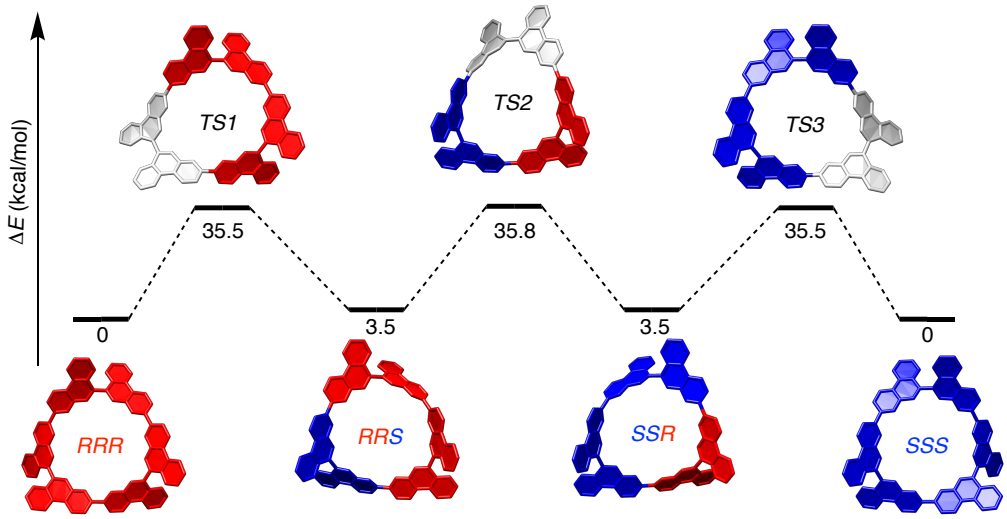


Fig. S19. Plausible isomerization pathway of [6]CPhen$_{2,9}$ by DFT calculation at the B3LYP/6-31G(d,p) level of theory.

Racemization of [4]CPhen$_{2,9}$

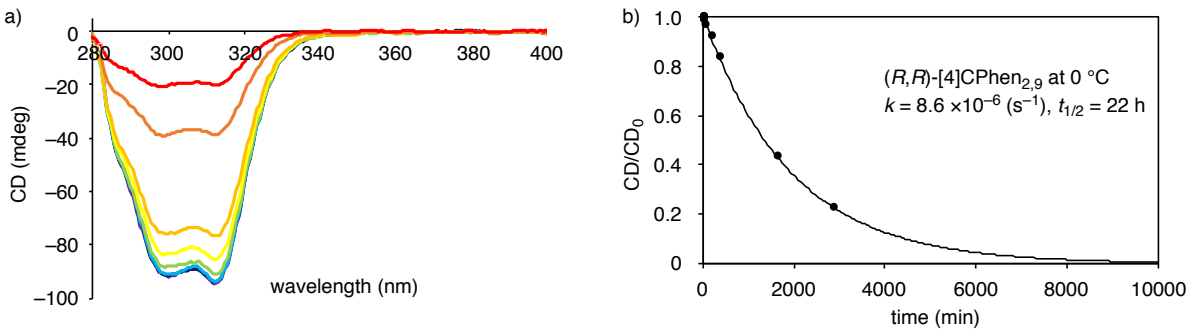


Fig. S20. Racemization of (*Z*,*R*,*Z*,*R*)-[4]CPhen$_{2,9}$ in toluene at 0 °C. (a) VT CD spectra. (b) Decay of the CD signal at 298 nm. The coefficient of (R^2) was 0.99998 and confirmed the sufficient of fit for analysis.

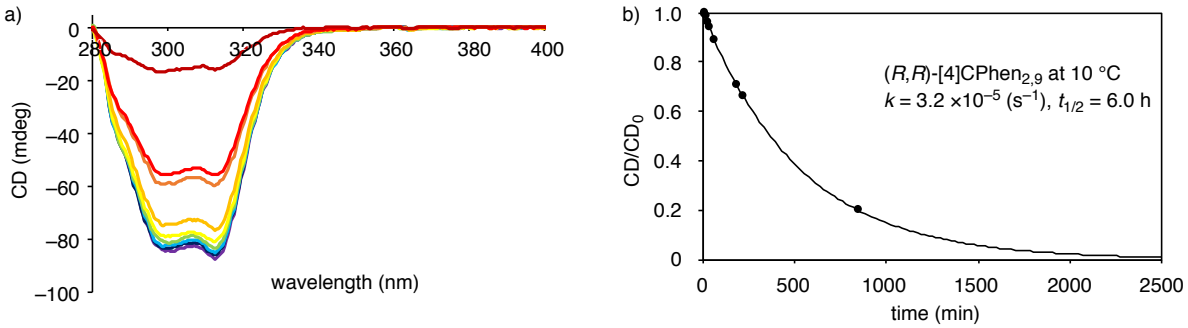


Fig. S21. Racemization of (*Z*,*R*,*Z*,*R*)-[4]CPhen$_{2,9}$ in toluene at 10 °C. (a) VT CD spectra. (b) Decay of the CD signal at 298 nm. The coefficient of (R^2) was 0.99994 and confirmed the sufficient of fit for analysis.

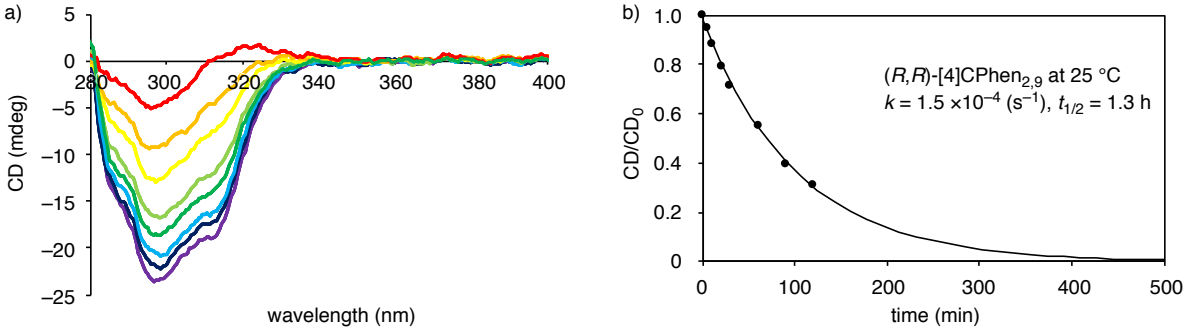


Fig. S22. Racemization of (*Z*,*R*,*Z*,*R*)-[4]CPhen$_{2,9}$ in toluene at 25 °C. (a) VT CD spectra. (b) Decay of the CD signal at 298 nm. The coefficient of (R^2) was 0.99333 and confirmed the sufficient of fit for analysis.

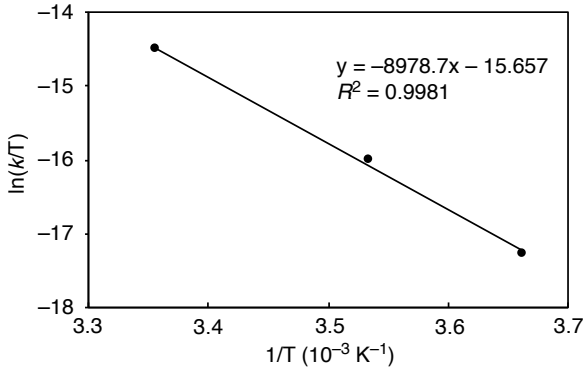


Fig. S23. Eyring plot for racemization of (*Z*,*R*,*Z*,*R*)-[4]CPhen$_{2,9}$ to reveal the activation energy with $\Delta H^{\ddagger} = +17.8$ kcal/mol, $\Delta S^{\ddagger} = -16.2$ kcal/mol·K, and $\Delta G^{\ddagger} = +22.7$ kcal/mol at 25 °C.

X-ray crystallographic analysis

The data collections were performed at BL38B1 beamline in SPring-8, and the data processing was performed on the XDS software.[1] The structures were solved by the direct method with SUPERFLIP program[2] for [4]CPhen$_{2,9}$ and SHELXT[3] for [4]CPhen$_{2,9}$, and refined by full-matrix least-squares methods using the SHELXL program suite[3] running on the Yadokari-XG 2009 software program.[4] Crystallographic data were deposited in the Cambridge Crystallographic Data Centre (CCDC 1976911 and 1976912). The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

[1] W. Kabsch, *J. Appl. Cryst.* **1993**, *26*, 795−800.
[2] L. Palatinus, G. Chapuis, *J. Appl. Crystallogr.* **2007**, *40*, 786−790.
[3] G. M. Sheldrick, *Acta Crystallogr.* **2008**, *A64*, 112−122.
[4] C. Kabuto, S. Akine, T. Nemoto, E. Kwon, *Nippon Kessho Gakkaishi* **2009**, *51*, 218−224.

Table S5. Crystal data and structure refinement for compound **1**. (CCDC 1977015)

Empirical formula	$C_{15}H_{10}BrIO_2$	
Formula weight	429.04	
Temperature	93(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 7.9349(2) Å	α = 108.099(2)°
	b = 8.1555(2) Å	β = 92.664(2)°
	c = 11.7247(3) Å	γ = 92.600(2)°
Volume	718.99(3) Å^3	
Z	2	
Density (calculated)	1.982 mg/m^3	
Absorption coefficient	20.713 mm^{-1}	
F(000)	408	
Crystal size	0.130 × 0.070 × 0.070 mm^3	
Theta range for data collection	3.975 to 68.246°	
Index ranges	−9<=h<=9, −9<=k<=9, −14<=l<=14	
Reflections collected	18739	
Independent reflections	2616 (R_{int} = 0.0555)	
Completeness to theta = 67.684°	99.2 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2616 / 38 / 225	
Goodness-of-fit on F^2	1.075	
Final R indices [I>2σ(I)]	R_1 = 0.0407, wR_2 = 0.1090	
R indices (all data)	R_1 = 0.0415, wR_2 = 0.1095	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.154 and −0.721 e•Å^{-3}	

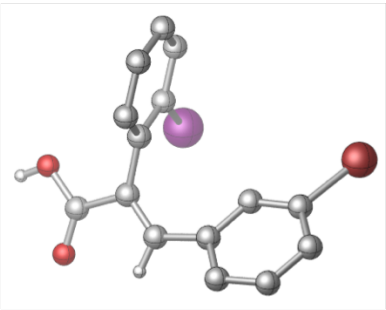


Fig. S24. Crystal structure of compound **1**.

Table S6. Crystal data and structure refinement of [4]CPhen$_{2,9}$ (CCDC 1976912)

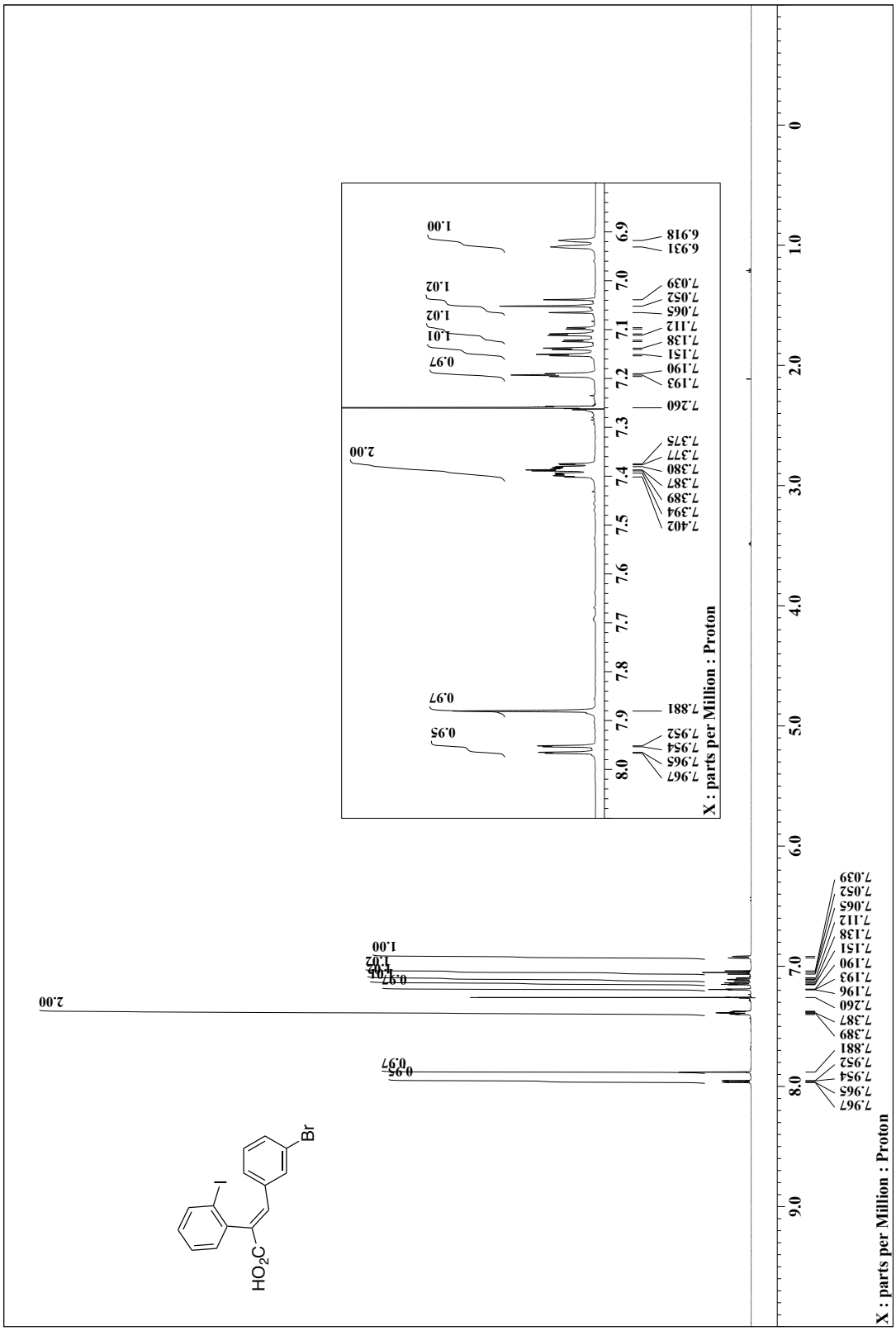
Empirical formula	$C_{56}H_{32}$	
Formula weight	704.81	
Temperature	100(2) K	
Wavelength	0.760 Å	
Crystal system	Monoclinic	
Space group	$P\,2_1/c$	
Unit cell dimensions	a = 7.6620(16) Å	α = 90°
	b = 15.9490(11) Å	β = 99.232(4)°
	c = 14.374(2) Å	γ = 90°
Volume	1733.8(5) Å^3	
Z	2	
Density (calculated)	1.350 mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	736	
Crystal size	0.060 × 0.030 × 0.020 mm^3	
Theta range for data collection	2.054 to 27.210°	
Index ranges	−9<=h<=9, −19<=k<=19, −17<=l<=17	
Reflections collected	40355	
Independent reflections	3157 (R_{int} = 0.0215)	
Completeness to theta = 27.129°	99.7%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.900	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3157 / 0 / 253	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2σ(I)]	R_1 = 0.0436, wR_2 = 0.1187	
R indices (all data)	R_1 = 0.0454, wR_2 = 0.1205	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.591 and −0.212 e•Å^{-3}	

Table S7. Crystal data and structure refinement of [6]CPhen$_{2,9}$ (CCDC 1976911)

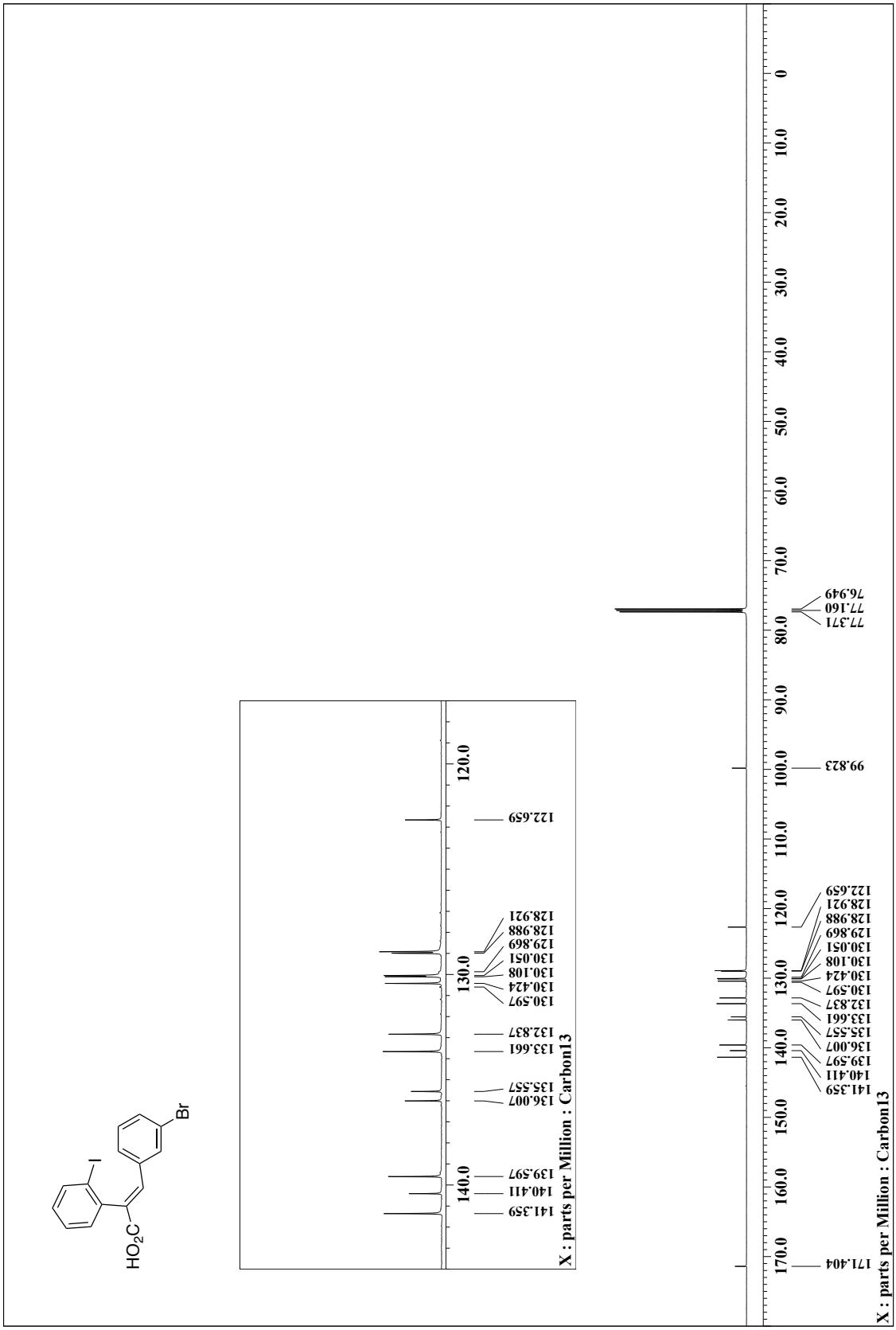
Empirical formula	$C_{90}H_{51}Cl_3$	
Formula weight	1238.65	
Temperature	100(2) K	
Wavelength	0.76000 Å	
Crystal system	Monoclinic	
Space group	$P\,2_1/n$	
Unit cell dimensions	a = 7.6200(15) Å	α = 90°
	b = 43.657(16) Å	β = 90.53(3)°
	c = 25.190(5) Å	γ = 90°
Volume	8380(4) Å^3	
Z	4	
Density (calculated)	0.982 mg/m^3	
Absorption coefficient	0.174 mm^{-1}	
F(000)	2568	
Crystal size	0.100 × 0.030 × 0.030 mm^3	
Theta range for data collection	1.320 to 27.241°	
Index ranges	−9<=h<=9, −52<=k<=52, −30<=l<=30	
Reflections collected	191760	
Independent reflections	15163 (R_{int} = 0.0350)	
Completeness to theta = 27.129°	98.9%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.852	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15163 / 282 / 920	
Goodness-of-fit on F^2	1.100	
Final R indices [I>2σ(I)]	R_1 = 0.0654, wR_2 = 0.1904	
R indices (all data)	R_1 = 0.0697, wR_2 = 0.1941	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.355 and −0.358 e•Å^{-3}	

Supplementary Data

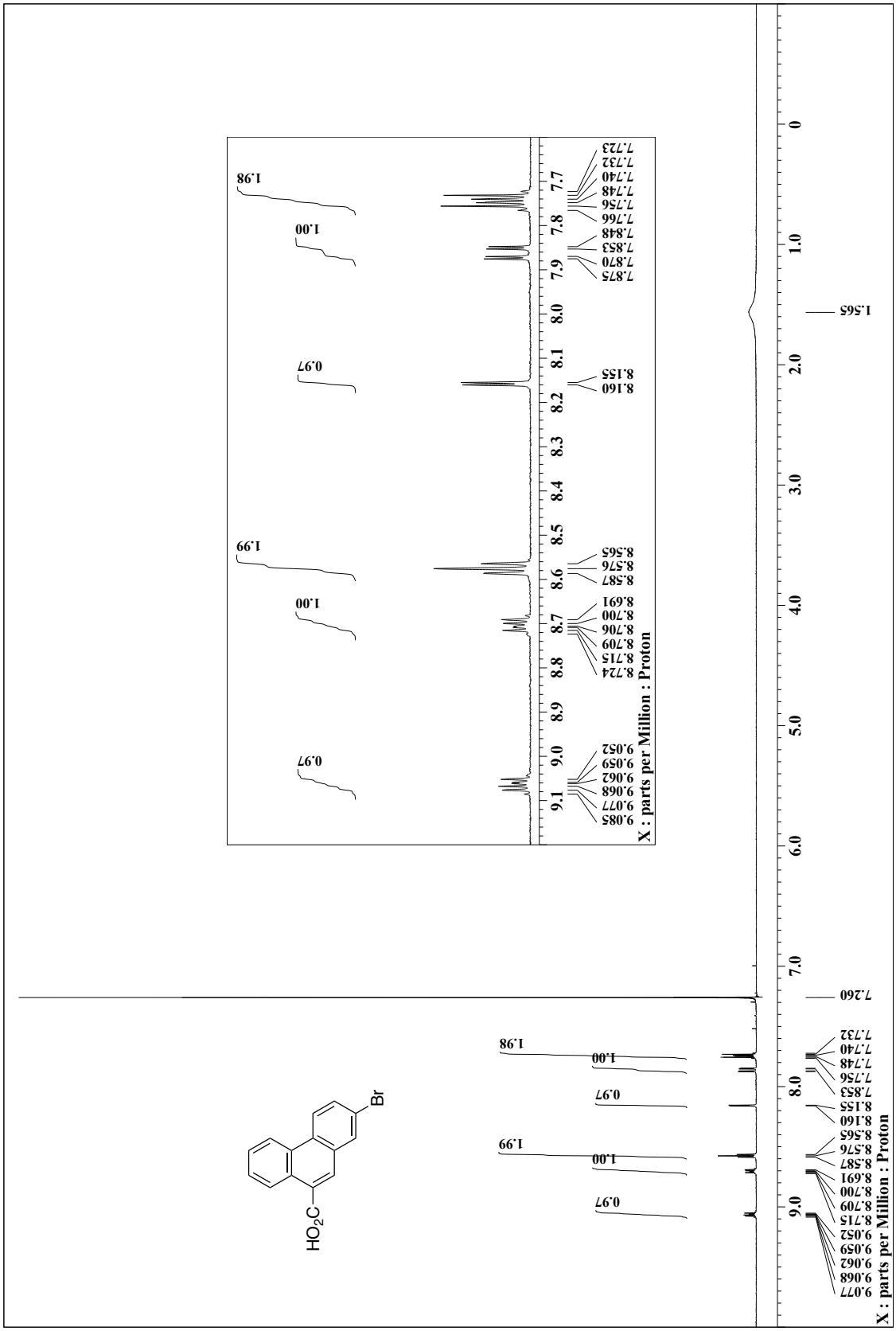
NMR Spectra



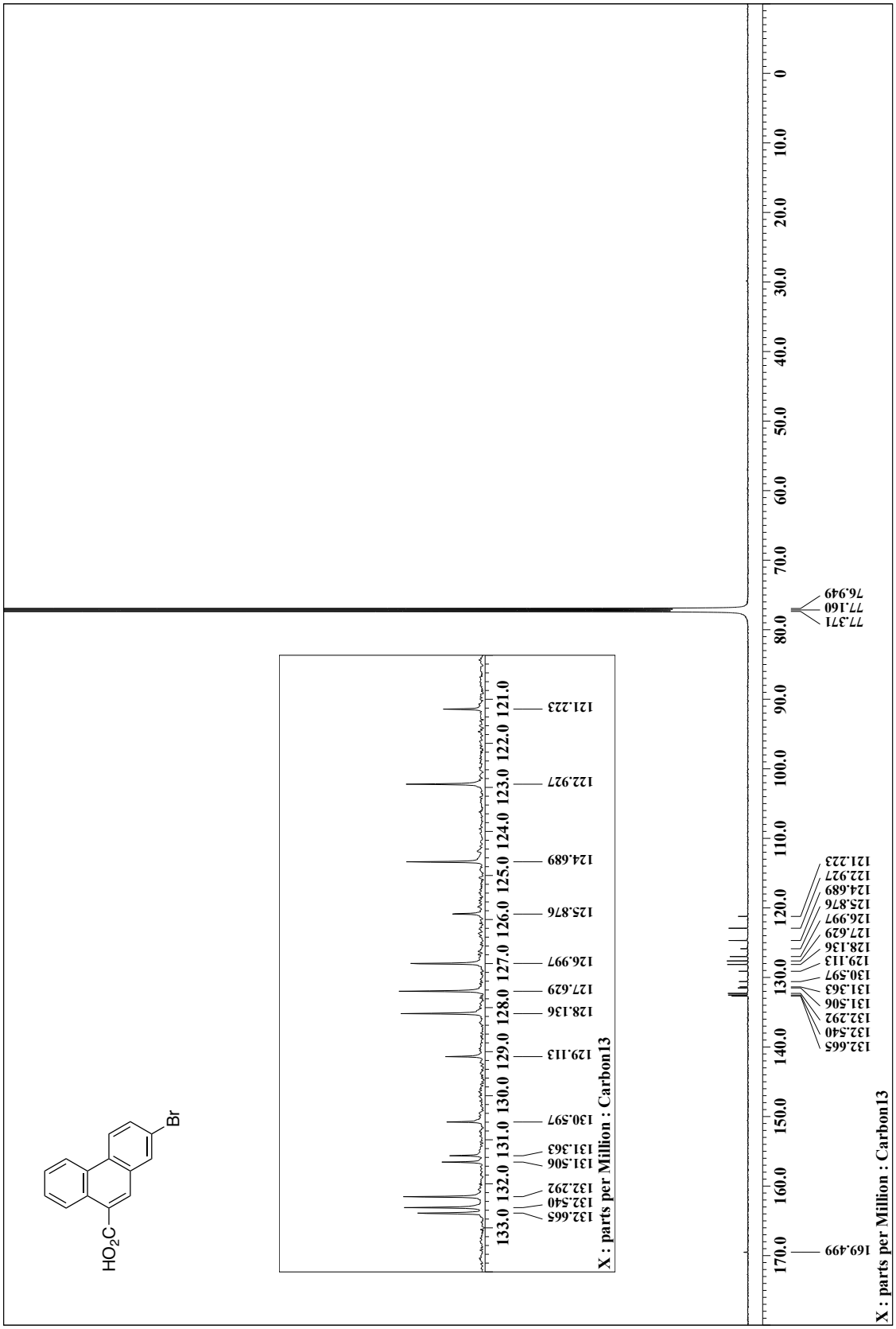
^{1}H NMR spectrum of **2** in $CDCl_3$ (25 °C, 600 MHz).



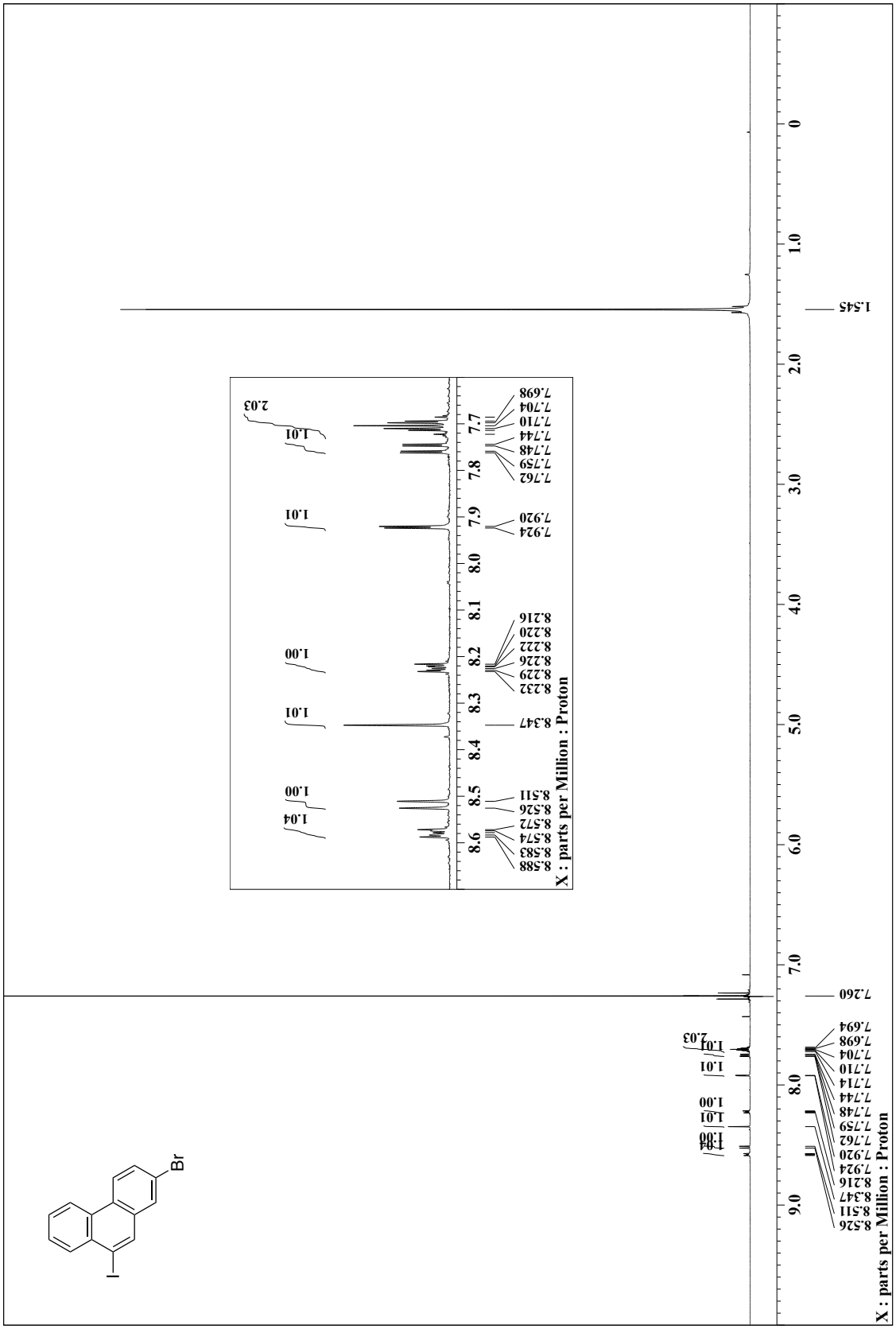
^{13}C NMR spectrum of **2** in $CDCl_3$ (25 °C, 600 MHz).



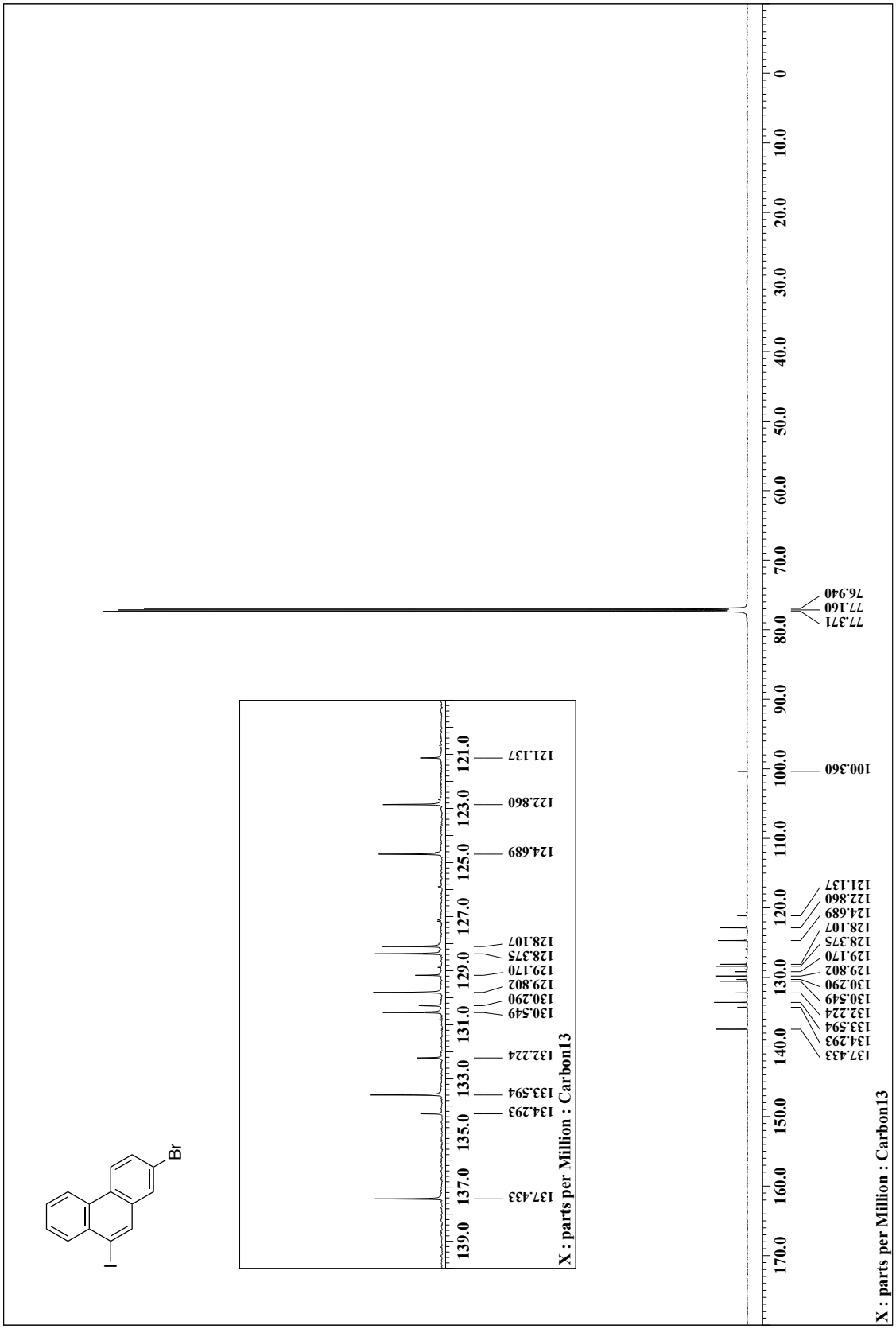
^{1}H NMR spectrum of **3** in $CDCl_3$ (25 °C, 600 MHz).



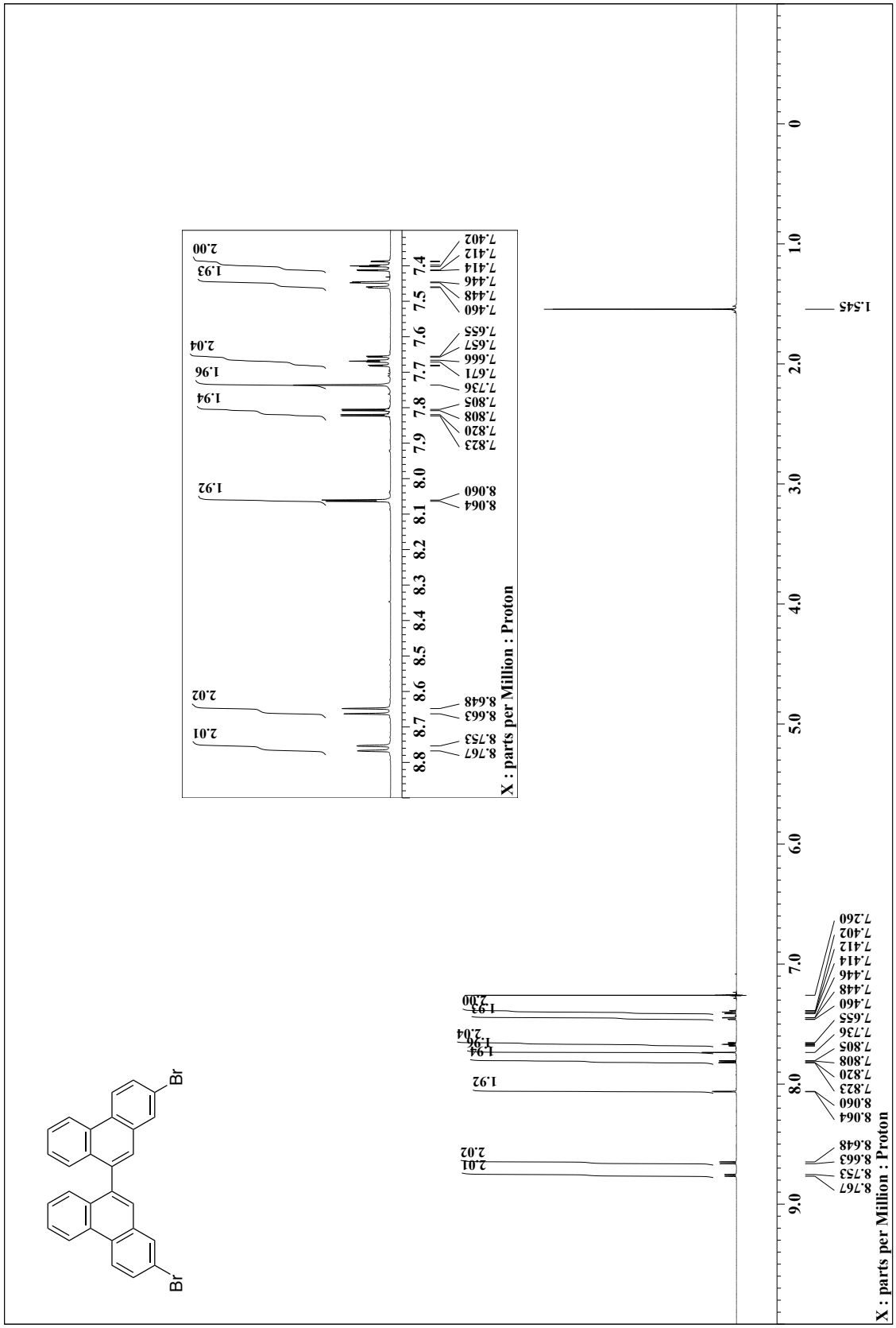
^{13}C NMR spectrum of **3** in $CDCl_3$ (25 °C, 600 MHz).



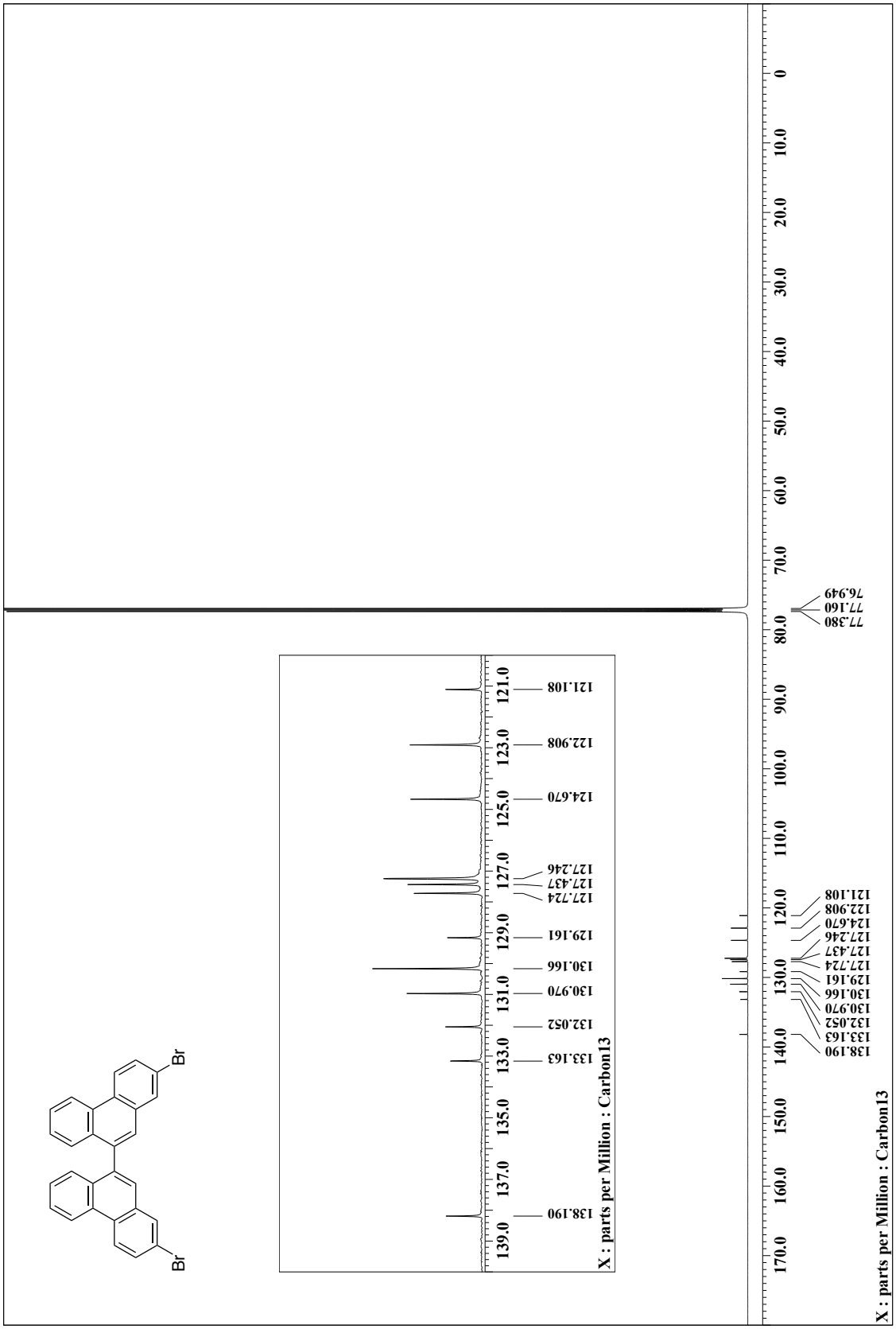
^{1}H NMR spectrum of **4** in $CDCl_3$ (25 °C, 600 MHz).



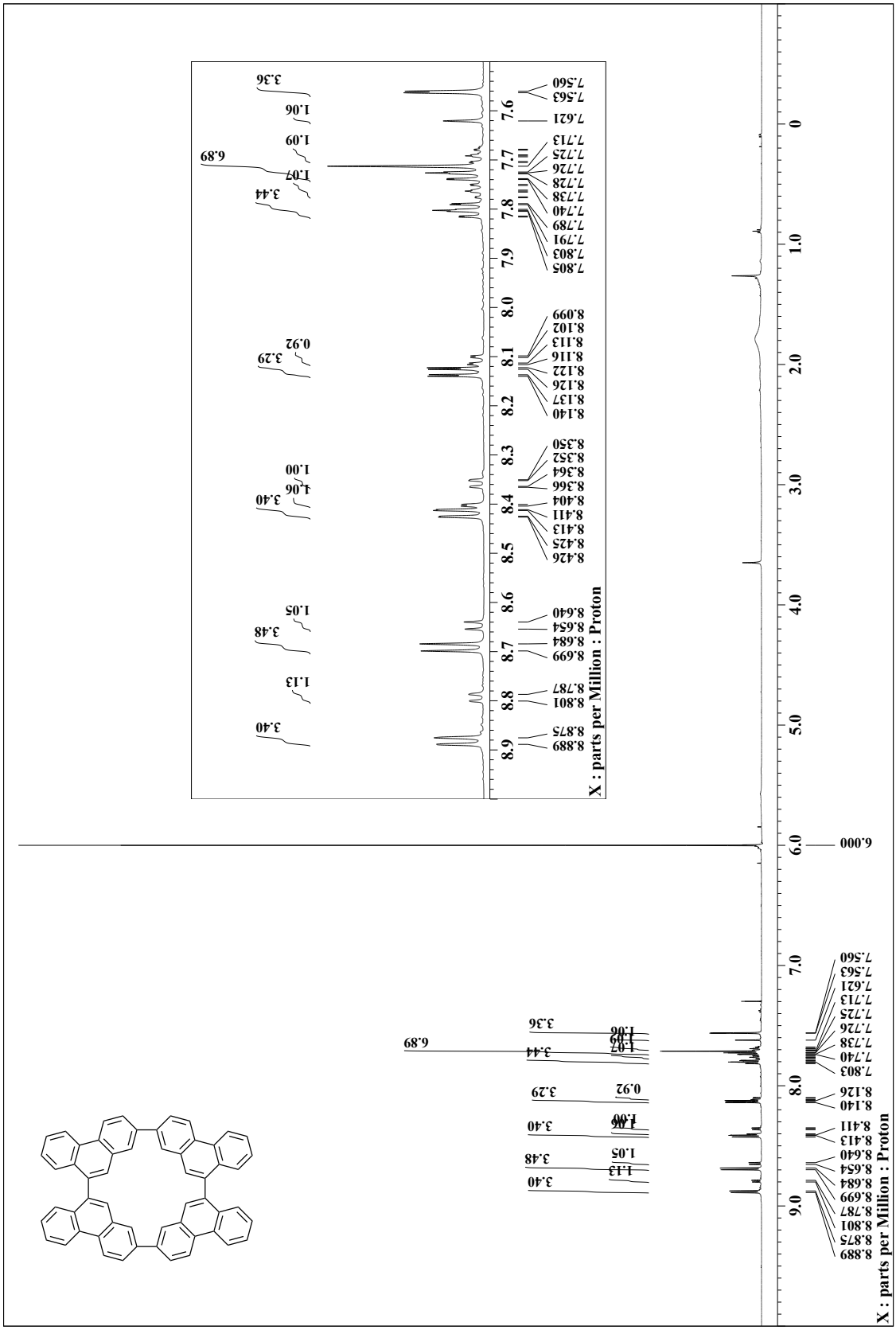
^{13}C NMR spectrum of **4** in $CDCl_3$ (25 °C, 600 MHz).



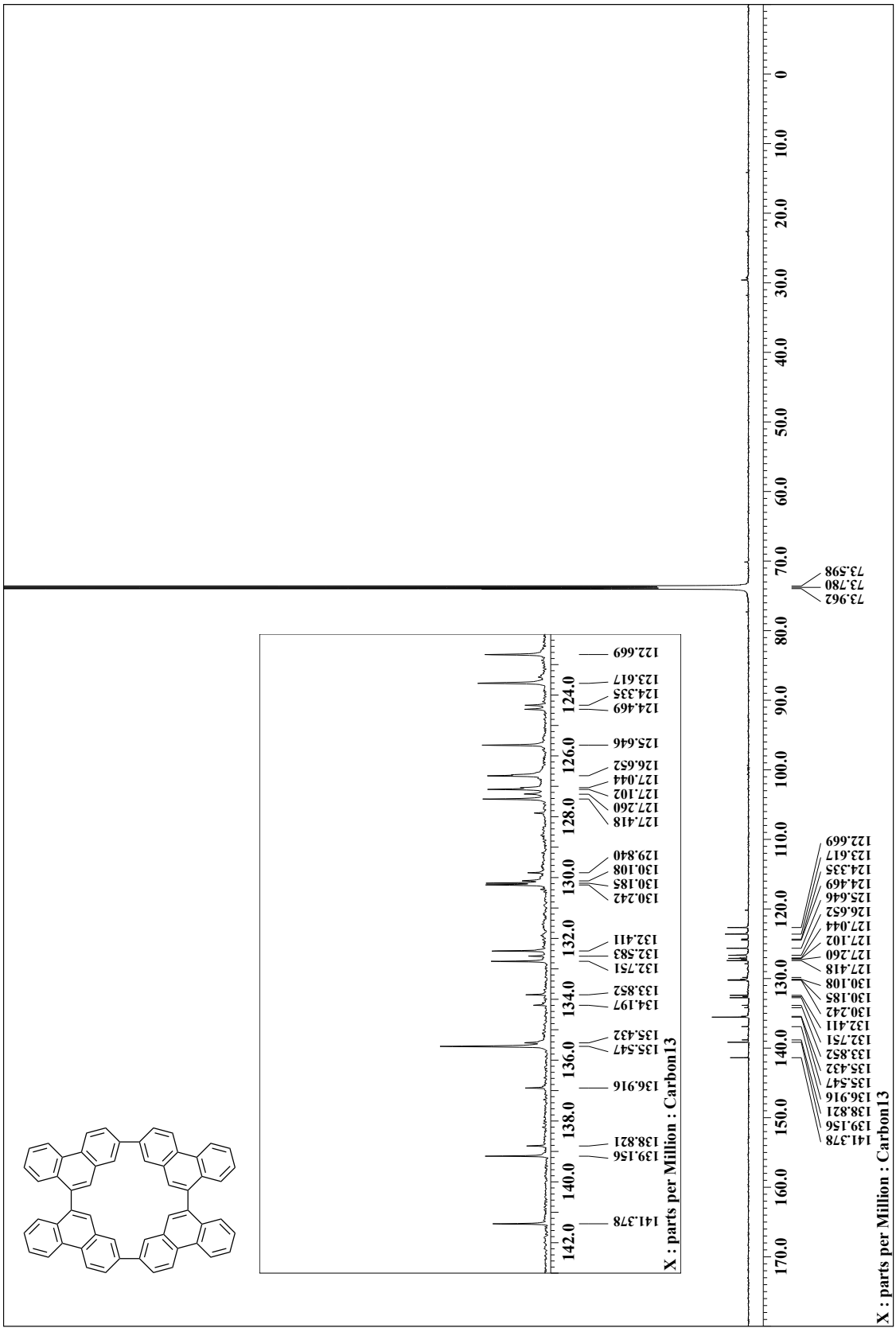
^{1}H NMR spectrum of **1** in $CDCl_3$ (25 °C, 600 MHz).



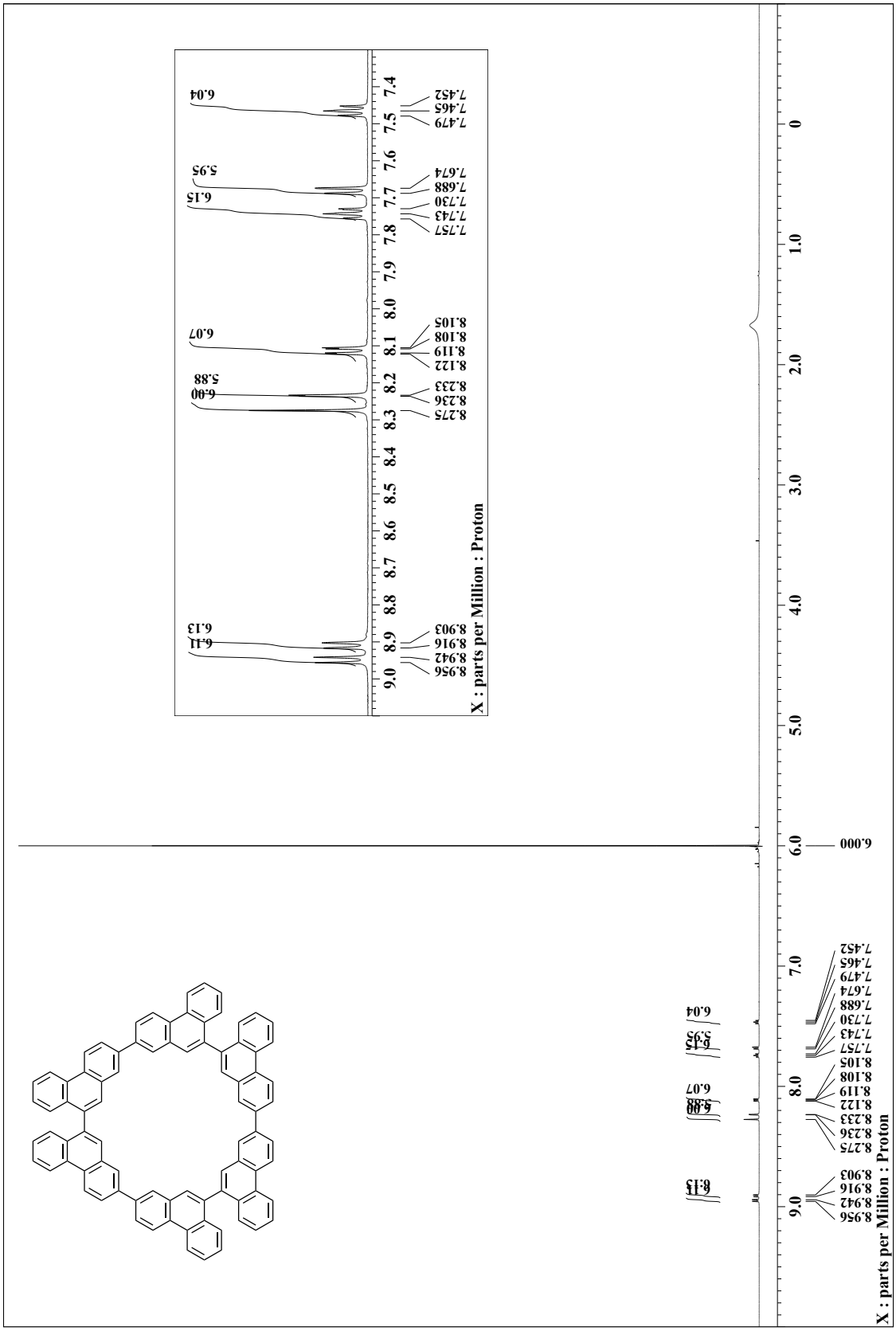
^{13}C NMR spectrum of **1** in $CDCl_3$ (25 °C, 600 MHz).



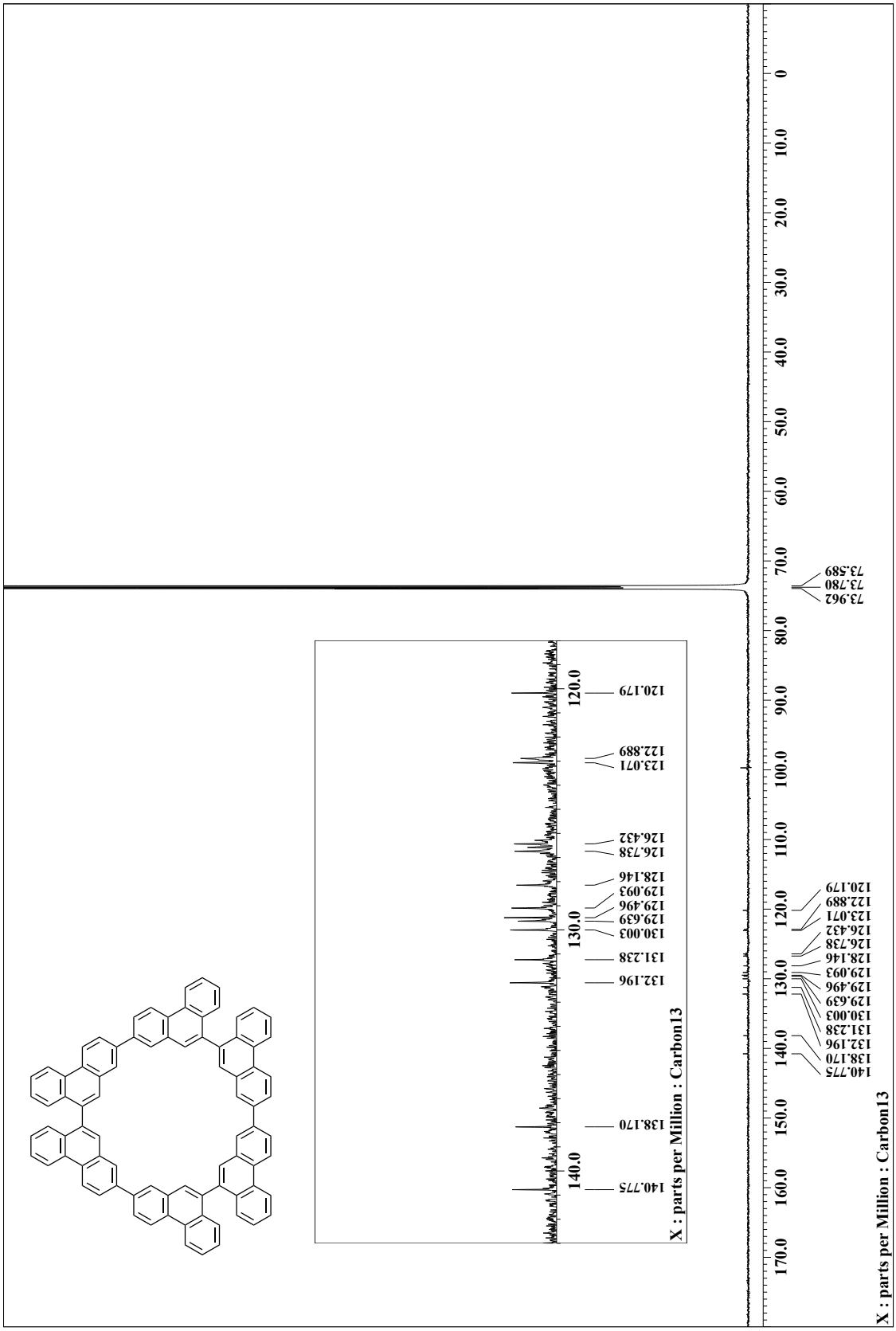
^{1}H NMR spectrum of [4]CPhen$_{2,9}$ in 1,1,2,2-tetrachloroethane-d_2 (25 °C, 600 MHz).



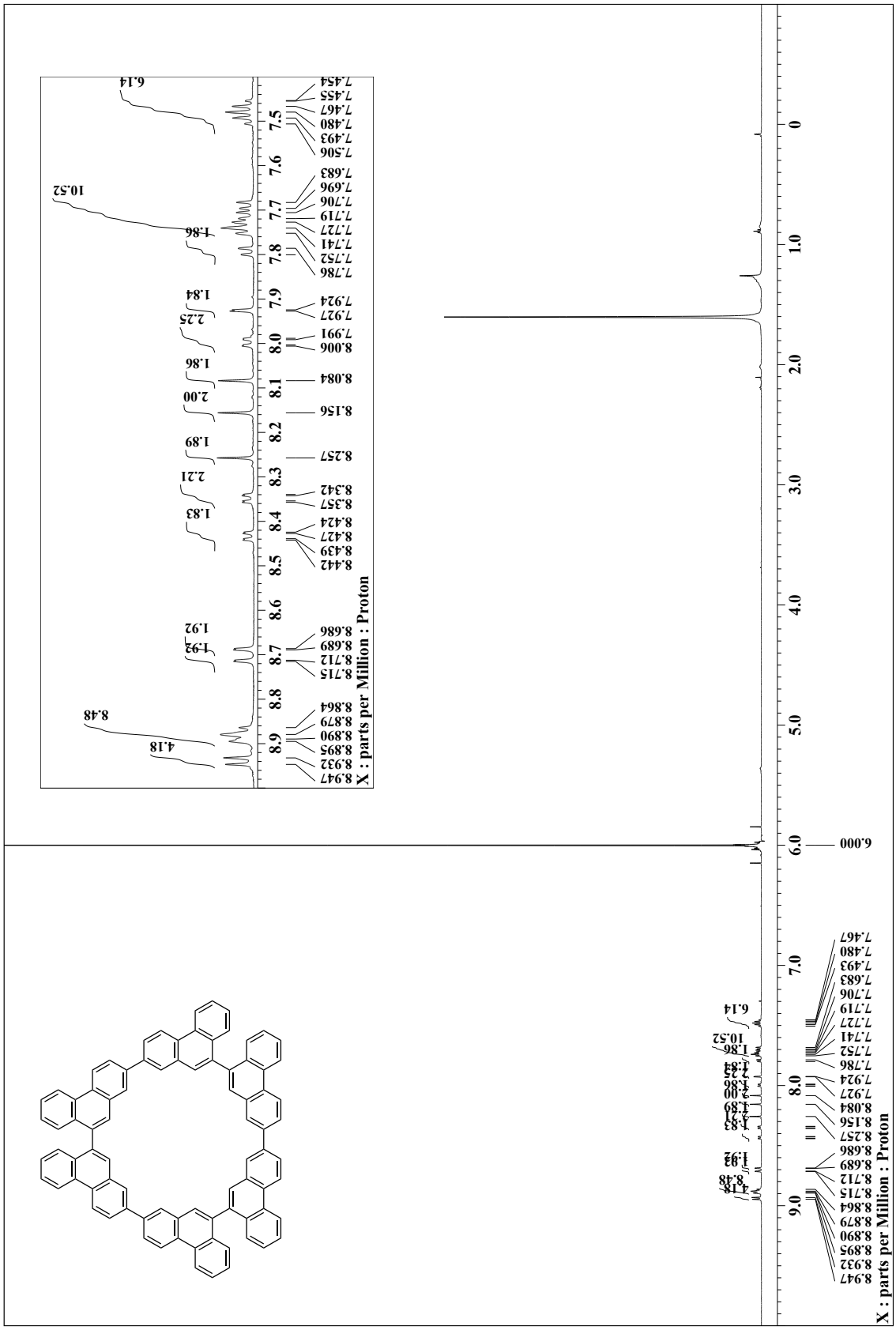
^{13}C NMR spectrum of [4]CPhen$_{2,9}$ in 1,1,2,2-tetrachloroethane-d_2 (25 °C, 600 MHz).



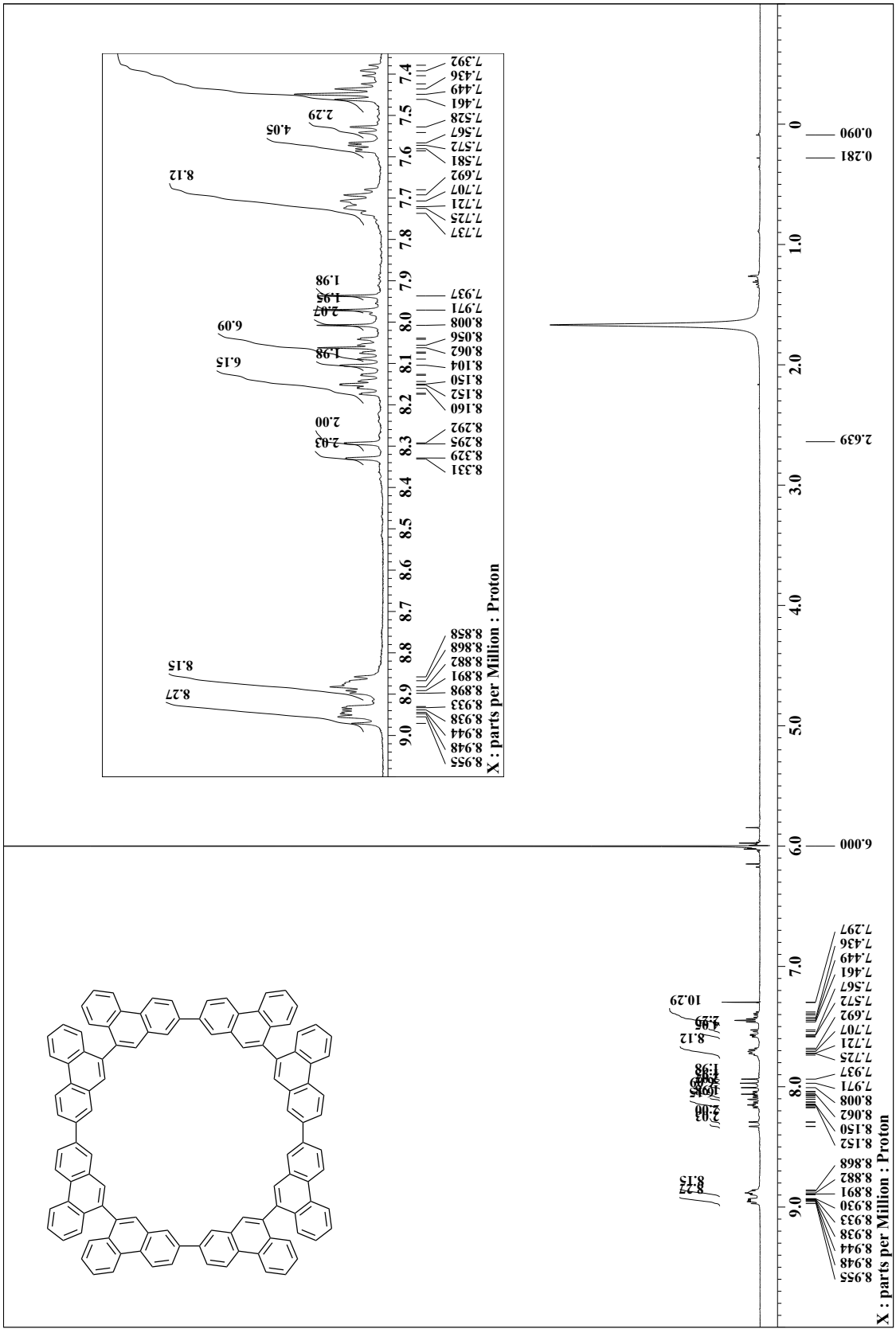
^{1}H NMR spectrum of (*Z*,*R*,*Z*,*R*,*Z*,*R*)*-[6]CPhen$_{2,9}$ in 1,1,2,2-tetrachloroethane-d_2 (25 °C, 600 MHz).



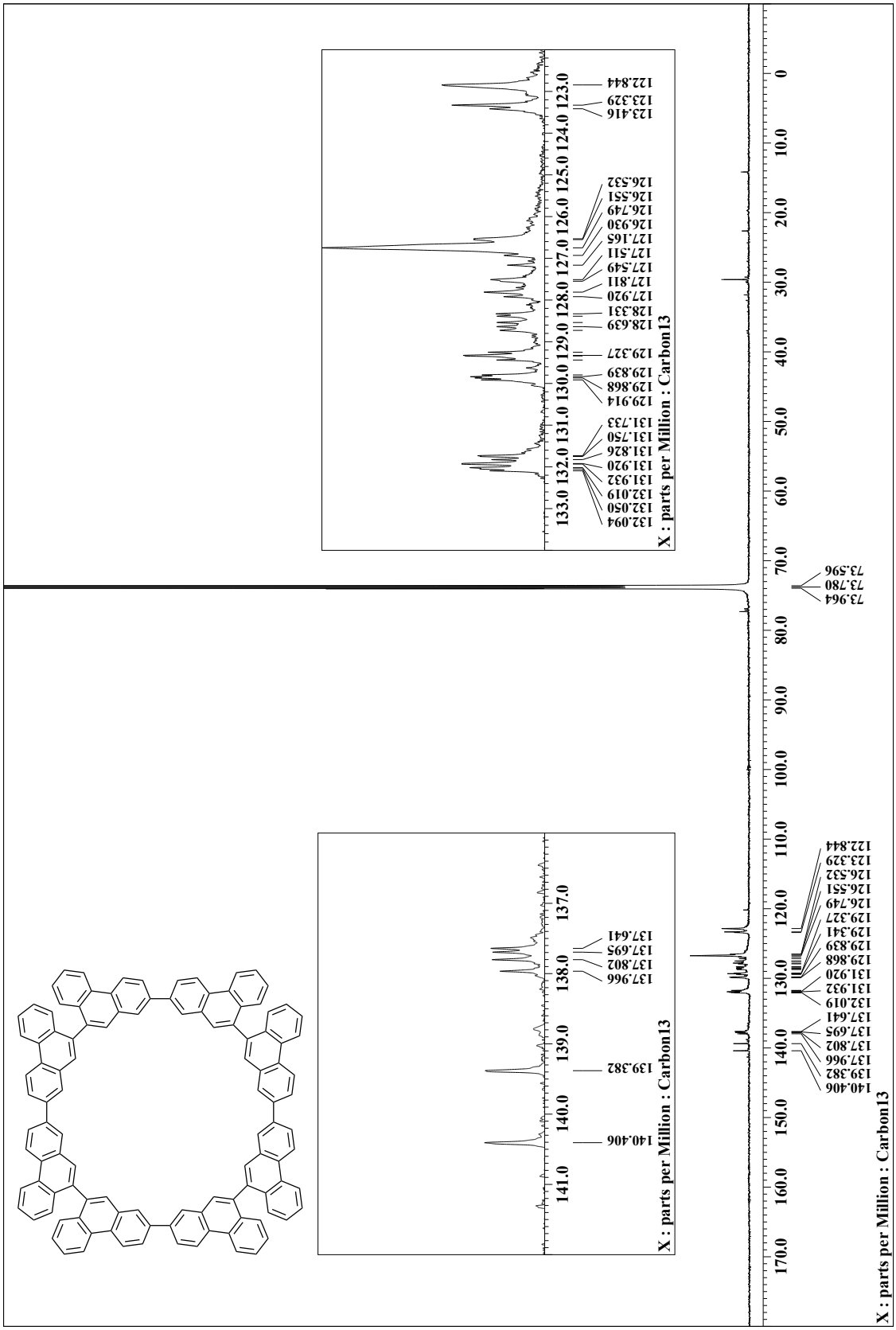
^{13}C NMR spectrum of (*Z*,*R*,*Z*,*R*,*Z*,*R*)*-[6]CPhen$_{2,9}$ in 1,1,2,2-tetrachloroethane-d_2 (25 °C, 600 MHz).



^{1}H NMR spectrum of (*Z*,*R*,*Z*,*R*,*Z*,*S*)*-[6]CPhen$_{2,9}$ in 1,1,2,2-tetrachloroethane-d_2 (25 °C, 600 MHz).



^{1}H NMR spectrum of [8]CPhen$_{2,9}$ in 1,1,2,2-tetrachloroethane-d_2 (25 °C, 600 MHz).



^{13}C NMR spectrum of [8]CPhen$_{2,9}$ in 1,1,2,2-tetrachloroethane-d_2 (25 °C, 600 MHz).

Cartesian coordinates

(*Z*,*S*,*Z*,*S*,*Z*,*S*)-[6]CPhen$_{2,9}$

SCF Done: E(RB3LYP) = −3230.13193158 A.U. after 6 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.228775	-5.267436	0.168204
2	6	0	-1.928938	-4.896009	-0.146878
3	6	0	-0.819055	-5.691554	0.208771
4	6	0	-1.014613	-6.899399	0.933594
5	6	0	-2.347641	-7.286875	1.207392
6	6	0	-3.422218	-6.503057	0.830804
7	6	0	0.504612	-5.292697	-0.160466
8	6	0	0.156272	-7.645059	1.373617
9	6	0	1.466156	-7.176088	1.038579
10	6	0	1.620365	-5.993174	0.206790
11	6	0	2.590016	-7.862390	1.558673
12	1	0	3.581705	-7.487538	1.334587
13	6	0	2.446678	-8.989286	2.344142
14	6	0	1.161762	-9.473107	2.643588
15	6	0	0.046272	-8.808517	2.171209
16	1	0	0.615019	-4.400233	-0.769892
17	1	0	-1.753395	-3.973691	-0.693837
18	1	0	-2.546665	-8.211227	1.737829
19	1	0	-4.430728	-6.819399	1.080842
20	1	0	3.325376	-9.496001	2.731722
21	1	0	1.042462	-10.360920	3.257542
22	1	0	-0.934835	-9.185589	2.436319
23	6	0	5.969608	-1.592922	-0.167927
24	6	0	4.771589	-2.219322	0.147021
25	6	0	4.515320	-3.560577	-0.208735
26	6	0	5.489286	-4.301204	-0.933555
27	6	0	6.722437	-3.663596	-1.207168
28	6	0	6.961204	-2.355165	-0.830460
29	6	0	3.281150	-4.183528	0.160428
30	6	0	5.154388	-5.648290	-1.373778
31	6	0	3.881889	-6.210900	-1.038836
32	6	0	2.955127	-5.459931	-0.206928
33	6	0	3.540134	-7.482527	-1.559144
34	1	0	2.563093	-7.894080	-1.335097
35	6	0	4.420391	-8.200405	-2.344766
36	6	0	5.685025	-7.665766	-2.644139

37	6	0	6.035670	-6.415634	-2.171528
38	1	0	2.586224	-3.612830	0.769902
39	1	0	4.008853	-1.671844	0.693965
40	1	0	7.503608	-4.196393	-1.737545
41	1	0	7.910134	-1.889590	-1.080370
42	1	0	4.132606	-9.172984	-2.732526
43	1	0	6.383139	-8.226933	-3.258233
44	1	0	7.006542	-6.012927	-2.436624
45	6	0	6.176225	-0.162412	0.170150
46	6	0	5.204712	0.777459	-0.145479
47	6	0	7.342706	0.288053	0.833191
48	6	0	5.338514	2.136478	0.209977
49	1	0	4.318459	0.468188	-0.692792
50	6	0	7.484008	1.610658	1.209584
51	1	0	8.120852	-0.427083	1.083703
52	6	0	6.482014	2.571265	0.935139
53	6	0	4.331346	3.083233	-0.159870
54	1	0	8.383799	1.900617	1.740337
55	6	0	6.542107	3.958246	1.374804
56	6	0	4.379970	4.399861	0.206951
57	1	0	3.503427	2.732396	-0.769415
58	6	0	5.481184	4.858055	1.038978
59	6	0	7.604257	4.444957	2.172811
60	6	0	3.250895	5.289014	-0.207396
61	6	0	5.513369	6.174674	1.558613
62	6	0	7.621829	5.743448	2.644792
63	1	0	8.421180	3.783884	2.438622
64	6	0	1.982417	4.933334	0.159863
65	6	0	3.438085	6.466747	-1.039761
66	1	0	4.692991	6.845994	1.333891
67	6	0	6.560561	6.614240	2.344474
68	1	0	8.450013	6.084207	3.259102
69	6	0	0.825926	5.690532	-0.209874
70	1	0	1.835501	4.046444	0.769717
71	6	0	2.314655	7.287253	-1.375410
72	6	0	4.710360	6.806401	-1.559848
73	1	0	6.559864	7.628706	2.731699
74	6	0	-0.463828	5.242048	0.145915
75	6	0	0.980487	6.903941	-0.935294
76	6	0	2.538737	8.433745	-2.173666
77	1	0	5.555256	6.166181	-1.335229
78	6	0	4.892114	7.927287	-2.345972
79	6	0	-1.605243	5.966245	-0.169563
80	1	0	-0.556716	4.308054	0.693338

81	6	0	-0.188218	7.652930	-1.209540
82	6	0	3.796830	8.754959	-2.646083
83	1	0	1.704604	9.073044	-2.439300
84	1	0	5.878389	8.164206	-2.733552
85	6	0	-1.440809	7.205719	-0.832782
86	1	0	-0.117286	8.595549	-1.740424
87	1	0	3.933887	9.639839	-3.260564
88	1	0	-2.318430	7.794604	-1.083141
89	6	0	-2.947430	5.430105	0.168790
90	6	0	-3.275789	4.118819	-0.146680
91	6	0	-3.920518	6.215174	0.832091
92	6	0	-4.519524	3.555249	0.209268
93	1	0	-2.565014	3.505875	-0.694168
94	6	0	-5.136446	5.676292	1.208993
95	1	0	-3.690142	7.246657	1.082404
96	6	0	-5.467472	4.328211	0.934814
97	6	0	-4.836055	2.209625	-0.160371
98	1	0	-5.837243	6.310615	1.739952
99	6	0	-6.698444	3.686776	1.375158
100	6	0	-6.000383	1.593417	0.207125
101	1	0	-4.118596	1.668038	-0.770304
102	6	0	-6.947375	2.318048	1.039610
103	6	0	-7.650629	4.363327	2.173592
104	6	0	-6.206060	0.170993	-0.207003
105	6	0	-8.103383	1.687616	1.559938
106	6	0	-8.783656	3.729300	2.646258
107	1	0	-7.486503	5.401382	2.439194
108	6	0	-5.263575	-0.749646	0.159852
109	6	0	-7.320022	-0.255868	-1.038735
110	1	0	-8.274664	0.641476	1.335365
111	6	0	-9.007248	2.374773	2.346229
112	1	0	-9.492551	4.276190	3.260882
113	6	0	-5.341162	-2.129814	-0.209802
114	1	0	-4.421798	-0.433355	0.769318
115	6	0	-7.468938	-1.639056	-1.374302
116	6	0	-8.250748	0.676018	-1.558240
117	1	0	-9.885219	1.866940	2.733992
118	6	0	-4.307720	-3.022484	0.145646
119	6	0	-6.469549	-2.602729	-0.934770
120	6	0	-8.574336	-2.018371	-2.171852
121	1	0	-8.118779	1.727846	-1.333686
122	6	0	-9.312795	0.272850	-2.343684
123	6	0	-4.364204	-4.373073	-0.169847
124	1	0	-3.452272	-2.635886	0.692816

125	6	0	-6.533801	-3.989335	-1.209112
126	6	0	-9.481978	-1.089549	-2.643683
127	1	0	-8.710988	-3.060419	-2.437365
128	1	0	-10.011455	1.008446	-2.730801
129	6	0	-5.520008	-4.850437	-0.832760
130	1	0	-7.385733	-4.399262	-1.739742
131	1	0	-10.317204	-1.413392	-3.257610
132	1	0	-5.591186	-5.904908	-1.083183

(*Z*,*S*,*Z*,*S*,*Z*,*R*)-[6]CPhen$_{2,9}$

SCF Done: E(RB3LYP) = −3230.12652359 A.U. after 6 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.829836	3.582021	-1.076943
2	6	0	3.645462	3.822232	-0.389626
3	6	0	2.806528	4.914055	-0.696453
4	6	0	3.184161	5.843924	-1.704491
5	6	0	4.412890	5.615703	-2.365755
6	6	0	5.201529	4.520682	-2.072680
7	6	0	1.548273	5.067651	-0.029698
8	6	0	2.281806	6.940242	-2.024280
9	6	0	1.019552	7.035888	-1.358367
10	6	0	0.667075	6.064779	-0.339363
11	6	0	0.125720	8.069998	-1.725585
12	1	0	-0.839188	8.125154	-1.234196
13	6	0	0.461134	9.000358	-2.689705
14	6	0	1.711266	8.924607	-3.327948
15	6	0	2.595268	7.913484	-3.002154
16	1	0	1.282588	4.342105	0.734185
17	1	0	3.332707	3.151999	0.405422
18	1	0	4.741089	6.288214	-3.150231
19	1	0	6.105419	4.358337	-2.650353
20	1	0	-0.239700	9.786727	-2.953428
21	1	0	1.982739	9.656824	-4.082637
22	1	0	3.550482	7.872562	-3.513151
23	6	0	-4.830265	3.581465	1.076974
24	6	0	-3.645908	3.821802	0.389670
25	6	0	-2.807104	4.913725	0.696487
26	6	0	-3.184860	5.843571	1.704498
27	6	0	-4.413579	5.615227	2.365742

28	6	0	-5.202087	4.520108	2.072680
29	6	0	-1.548863	5.067454	0.029741
30	6	0	-2.282635	6.939999	2.024277
31	6	0	-1.020394	7.035791	1.358360
32	6	0	-0.667792	6.064703	0.339380
33	6	0	-0.126689	8.070021	1.725554
34	1	0	0.838207	8.125287	1.234156
35	6	0	-0.462214	9.000354	2.689662
36	6	0	-1.712333	8.924452	3.327917
37	6	0	-2.596210	7.913214	3.002143
38	1	0	-1.283085	4.341919	-0.734120
39	1	0	-3.333070	3.151597	-0.405365
40	1	0	-4.741876	6.287729	3.150185
41	1	0	-6.105975	4.357675	2.650330
42	1	0	0.238520	9.786816	2.953368
43	1	0	-1.983889	9.656644	4.082600
44	1	0	-3.551412	7.872175	3.513153
45	6	0	-5.635756	2.356488	0.841157
46	6	0	-5.047746	1.191280	0.362582
47	6	0	-7.018515	2.301907	1.151260
48	6	0	-5.765082	-0.016686	0.235083
49	1	0	-3.988509	1.175414	0.125316
50	6	0	-7.735714	1.125787	1.051658
51	1	0	-7.531645	3.202809	1.471677
52	6	0	-7.129852	-0.079693	0.626985
53	6	0	-5.116494	-1.193719	-0.255962
54	1	0	-8.786566	1.142228	1.317924
55	6	0	-7.800456	-1.371214	0.616614
56	6	0	-5.725761	-2.418458	-0.297507
57	1	0	-4.094836	-1.098144	-0.612256
58	6	0	-7.088154	-2.540629	0.199114
59	6	0	-9.132840	-1.523759	1.068014
60	6	0	-4.917339	-3.585904	-0.767919
61	6	0	-7.721923	-3.801120	0.318798
62	6	0	-9.736749	-2.764084	1.142258
63	1	0	-9.694981	-0.651590	1.381642
64	6	0	-3.709576	-3.807373	-0.164518
65	6	0	-5.314579	-4.445813	-1.872406
66	1	0	-7.170879	-4.692597	0.044691
67	6	0	-9.019347	-3.916224	0.778295
68	1	0	-10.759612	-2.847386	1.497480
69	6	0	-2.831733	-4.868999	-0.547265
70	1	0	-3.397328	-3.161760	0.651174
71	6	0	-4.505121	-5.572932	-2.225133

72	6	0	-6.473523	-4.173991	-2.639038
73	1	0	-9.480471	-4.895852	0.860648
74	6	0	-1.555410	-4.985006	0.043319
75	6	0	-3.243489	-5.805036	-1.534483
76	6	0	-4.937414	-6.400691	-3.287846
77	1	0	-7.065199	-3.298350	-2.399851
78	6	0	-6.859075	-4.995060	-3.680543
79	6	0	-0.687814	-6.015554	-0.285466
80	1	0	-1.247042	-4.237909	0.769611
81	6	0	-2.372512	-6.885246	-1.812132
82	6	0	-6.090419	-6.127528	-3.998634
83	1	0	-4.343881	-7.262756	-3.570165
84	1	0	-7.751705	-4.761994	-4.253244
85	6	0	-1.135576	-6.995437	-1.201332
86	1	0	-2.658671	-7.642298	-2.533655
87	1	0	-6.391254	-6.780194	-4.812819
88	1	0	-0.480169	-7.822649	-1.458099
89	6	0	0.688539	-6.015499	0.285475
90	6	0	1.556013	-4.984841	-0.043302
91	6	0	1.136432	-6.995348	1.201310
92	6	0	2.832335	-4.868690	0.547268
93	1	0	1.247555	-4.237775	-0.769587
94	6	0	2.373361	-6.885021	1.812094
95	1	0	0.481121	-7.822635	1.458085
96	6	0	3.244203	-5.804696	1.534467
97	6	0	3.710041	-3.806948	0.164536
98	1	0	2.659632	-7.642065	2.533582
99	6	0	4.505794	-5.572448	2.225132
100	6	0	4.917769	-3.585332	0.767955
101	1	0	3.397706	-3.161358	-0.651141
102	6	0	5.315114	-4.445224	1.872424
103	6	0	4.938181	-6.400166	3.287837
104	6	0	5.726058	-2.417792	0.297545
105	6	0	6.474037	-4.173285	2.639058
106	6	0	6.091145	-6.126872	3.998638
107	1	0	4.344750	-7.262307	3.570143
108	6	0	5.116660	-1.193119	0.256036
109	6	0	7.088445	-2.539805	-0.199136
110	1	0	7.065622	-3.297590	2.399862
111	6	0	6.859678	-4.994318	3.680557
112	1	0	6.392045	-6.779510	4.812823
113	6	0	5.765093	-0.016008	-0.235032
114	1	0	4.095003	-1.097659	0.612366
115	6	0	7.800610	-1.370306	-0.616633

116	6	0	7.722348	-3.800223	-0.318850
117	1	0	7.752278	-4.761154	4.253265
118	6	0	5.047608	1.191873	-0.362522
119	6	0	7.129860	-0.078860	-0.626979
120	6	0	9.133003	-1.522699	-1.068054
121	1	0	7.171403	-4.691765	-0.044749
122	6	0	9.019776	-3.915179	-0.778375
123	6	0	5.635469	2.357140	-0.841135
124	1	0	3.988375	1.175886	-0.125238
125	6	0	7.735568	1.126688	-1.051673
126	6	0	9.737048	-2.762957	-1.142328
127	1	0	9.695049	-0.650461	-1.381661
128	1	0	9.481000	-4.894758	-0.860750
129	6	0	7.018227	2.302722	-1.151265
130	1	0	8.786412	1.143258	-1.317965
131	1	0	10.759919	-2.846141	-1.497555
132	1	0	7.531249	3.203683	-1.471687

TS1-[6]CPhen$_{2,9}$

SCF Done: E(RB3LYP) = −3230.07457873 A.U. after 12 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.557904	-4.505002	0.343324
2	6	0	-3.914311	-3.221985	-0.052158
3	6	0	-5.166681	-2.660826	0.305080
4	6	0	-6.066064	-3.402803	1.109587
5	6	0	-5.667140	-4.687125	1.543818
6	6	0	-4.459588	-5.228329	1.158145
7	6	0	-5.540366	-1.345455	-0.119737
8	6	0	-7.399626	-2.866323	1.313796
9	6	0	-7.800226	-1.644546	0.671572
10	6	0	-6.763867	-0.742128	0.119224
11	6	0	-9.198723	-1.460075	0.555345
12	6	0	-10.128796	-2.246943	1.208119
13	6	0	-9.700225	-3.295178	2.031972
14	6	0	-8.358233	-3.610254	2.044713
15	1	0	-4.776377	-0.789770	-0.649643
16	1	0	-3.245749	-2.648477	-0.689189
17	1	0	-6.327282	-5.290996	2.154146
18	1	0	-4.187288	-6.228954	1.482175
19	1	0	-11.187659	-2.054005	1.063730

20	1	0	-10.411143	-3.888969	2.598198
21	1	0	-8.033998	-4.475969	2.609284
22	6	0	-3.534264	4.521705	-0.355029
23	6	0	-3.896026	3.239721	0.039427
24	6	0	-5.152275	2.685161	-0.314594
25	6	0	-6.050067	3.431870	-1.116348
26	6	0	-5.645733	4.713822	-1.551651
27	6	0	-4.435005	5.249227	-1.168012
28	6	0	-5.531985	1.371662	0.110787
29	6	0	-7.387936	2.904282	-1.314316
30	6	0	-7.793160	1.685066	-0.670475
31	6	0	-6.759583	0.775590	-0.124862
32	6	0	-9.191993	1.512464	-0.541747
33	6	0	-10.120826	2.306703	-1.187267
34	6	0	-9.690210	3.351405	-2.014690
35	6	0	-8.345937	3.656183	-2.037503
36	1	0	-4.769557	0.811105	0.637936
37	1	0	-3.229497	2.662750	0.675406
38	1	0	-6.304578	5.320831	-2.160392
39	1	0	-4.159433	6.248310	-1.492954
40	1	0	-11.180040	2.122711	-1.033978
41	1	0	-10.400790	3.951278	-2.574868
42	1	0	-8.019182	4.520413	-2.603014
43	6	0	-2.282298	5.189643	0.090220
44	6	0	-1.019143	4.670507	-0.151437
45	6	0	-2.373516	6.441410	0.747482
46	6	0	0.151806	5.358585	0.248098
47	1	0	-0.914607	3.732693	-0.690927
48	6	0	-1.246264	7.108682	1.180281
49	1	0	-3.355323	6.866819	0.933717
50	6	0	0.047619	6.585918	0.959767
51	6	0	1.447910	4.854675	-0.091831
52	1	0	-1.371024	8.053928	1.696931
53	6	0	1.262018	7.233730	1.428217
54	6	0	2.609316	5.477987	0.279723
55	1	0	1.500611	3.953898	-0.696784
56	6	0	2.536720	6.670902	1.109394
57	6	0	1.222821	8.395922	2.233833
58	6	0	3.905115	4.850148	-0.124655
59	6	0	3.700382	7.274297	1.647082
60	6	0	2.375869	8.975300	2.726527
61	1	0	0.266824	8.838882	2.490089
62	6	0	4.115447	3.549145	0.235750
63	6	0	4.914800	5.528692	-0.926098

64	1	0	4.665534	6.831356	1.434649
65	6	0	3.627075	8.403778	2.438525
66	1	0	2.311561	9.864293	3.346965
67	6	0	5.293045	2.825028	-0.126058
68	1	0	3.364471	3.033487	0.827240
69	6	0	6.139225	4.857823	-1.246596
70	6	0	4.706636	6.836890	-1.427667
71	1	0	4.534039	8.844149	2.841747
72	6	0	5.409030	1.460631	0.201439
73	6	0	6.340265	3.477304	-0.830539
74	6	0	7.105990	5.554416	-2.008879
75	1	0	3.768543	7.335045	-1.216120
76	6	0	5.667772	7.483931	-2.179855
77	6	0	6.528145	0.713187	-0.138977
78	1	0	4.590469	0.984817	0.733441
79	6	0	7.502817	2.720943	-1.113519
80	6	0	6.883965	6.840111	-2.463145
81	1	0	8.042227	5.068000	-2.258721
82	1	0	5.480922	8.486252	-2.553415
83	6	0	7.599331	1.382049	-0.776725
84	1	0	8.338023	3.182816	-1.628343
85	1	0	7.645582	7.345729	-3.049412
86	1	0	8.493085	0.825140	-1.042982
87	6	0	6.523129	-0.745251	0.134068
88	6	0	5.401256	-1.486181	-0.214082
89	6	0	7.586457	-1.420131	0.780054
90	6	0	5.275274	-2.849469	0.113800
91	1	0	4.588769	-1.006344	-0.751703
92	6	0	7.479908	-2.757928	1.117349
93	1	0	8.481703	-0.868979	1.052969
94	6	0	6.314863	-3.504236	0.826449
95	6	0	4.095903	-3.569221	-0.253263
96	1	0	8.307309	-3.227553	1.640144
97	6	0	6.107173	-4.878529	1.245989
98	6	0	3.878438	-4.867347	0.113186
99	1	0	3.348900	-3.051815	-0.848820
100	6	0	4.882300	-5.546229	0.924323
101	6	0	7.071498	-5.569147	2.013857
102	6	0	2.579383	-5.490390	-0.288035
103	6	0	4.672631	-6.853675	1.428899
104	6	0	6.847037	-6.852359	2.473508
105	1	0	8.007672	-5.079144	2.262166
106	6	0	1.422454	-4.858441	0.081838
107	6	0	2.498628	-6.691104	-1.109414

108	1	0	3.736510	-7.353118	1.213082
109	6	0	5.631658	-7.497632	2.187835
110	1	0	7.607126	-7.355406	3.063825
111	6	0	0.123481	-5.356994	-0.256118
112	1	0	1.480933	-3.953990	0.681253
113	6	0	1.219669	-7.247851	-1.420803
114	6	0	3.655897	-7.314001	-1.640706
115	1	0	5.444374	-8.498816	2.564451
116	6	0	-1.044418	-4.661123	0.138052
117	6	0	0.012161	-6.588349	-0.959118
118	6	0	1.165987	-8.417546	-2.212765
119	1	0	4.625723	-6.880420	-1.433038
120	6	0	3.569595	-8.451353	-2.420604
121	6	0	-2.309511	-5.177797	-0.100699
122	1	0	-0.936156	-3.720828	0.672506
123	6	0	-1.282199	-7.108214	-1.177530
124	6	0	2.312256	-9.013255	-2.701312
125	1	0	0.203561	-8.853666	-2.460036
126	1	0	4.471228	-8.905947	-2.820133
127	6	0	-2.406723	-6.433216	-0.749821
128	1	0	-1.408528	-8.057679	-1.687677
129	1	0	2.237754	-9.908713	-3.311158
130	1	0	-3.390530	-6.856717	-0.931465
131	1	0	-9.568756	-0.734953	-0.142345
132	1	0	-9.561966	0.791213	0.160188

TS2-[6]CPhen[2,9]

SCF Done: E(RB3LYP) = −3230.07490519 A.U. after 9 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.089543	-5.000759	0.903422
2	6	0	0.136158	-4.817388	0.281041
3	6	0	1.353882	-4.992207	0.970353
4	6	0	1.352823	-5.429867	2.323457
5	6	0	0.094297	-5.626991	2.940209
6	6	0	-1.090251	-5.402447	2.260499
7	6	0	2.586913	-4.630595	0.343769
8	6	0	2.632072	-5.602233	2.999846
9	6	0	3.841530	-5.210381	2.340812
10	6	0	3.785980	-4.678256	0.995664
11	6	0	5.072609	-5.331288	3.027250

12	6	0	5.130601	-5.845135	4.308134
13	6	0	3.948001	-6.250867	4.951415
14	6	0	2.729641	-6.126282	4.309635
15	1	0	2.546127	-4.233258	-0.666551
16	1	0	0.168425	-4.477756	-0.750737
17	1	0	0.041974	-5.940179	3.977190
18	1	0	-2.038786	-5.554291	2.767295
19	1	0	6.086310	-5.936579	4.815479
20	1	0	3.989087	-6.662157	5.955677
21	1	0	1.832218	-6.450096	4.825118
22	6	0	6.233221	0.352617	-1.466433
23	6	0	5.603072	-0.452022	-0.525515
24	6	0	5.789948	-1.844119	-0.476260
25	6	0	6.727122	-2.474638	-1.336763
26	6	0	7.429749	-1.637638	-2.236894
27	6	0	7.178088	-0.278387	-2.315811
28	6	0	4.933584	-2.635224	0.349747
29	6	0	6.852073	-3.924558	-1.279423
30	6	0	5.942046	-4.683311	-0.472374
31	6	0	4.941081	-3.999091	0.320121
32	6	0	6.029203	-6.094868	-0.477102
33	6	0	6.991802	-6.750698	-1.220386
34	6	0	7.900909	-6.009422	-1.995570
35	6	0	7.825289	-4.628951	-2.024776
36	1	0	4.187419	-2.120205	0.948147
37	1	0	4.903174	-0.022274	0.182135
38	1	0	8.147351	-2.067105	-2.927717
39	1	0	7.691071	0.302574	-3.075665
40	1	0	7.046993	-7.835065	-1.203984
41	1	0	8.663919	-6.520502	-2.575231
42	1	0	8.538523	-4.077679	-2.627931
43	6	0	5.843528	1.780106	-1.601326
44	6	0	4.625185	2.214342	-1.091018
45	6	0	6.643130	2.749410	-2.257756
46	6	0	4.193411	3.548356	-1.187752
47	1	0	3.953116	1.513842	-0.608917
48	6	0	6.218165	4.058632	-2.404002
49	1	0	7.617803	2.470639	-2.645715
50	6	0	4.978867	4.503959	-1.885293
51	6	0	2.979585	3.949154	-0.545993
52	1	0	6.872162	4.755064	-2.917415
53	6	0	4.459670	5.857536	-2.021175
54	6	0	2.516439	5.233036	-0.580252
55	1	0	2.444198	3.206233	0.038215

56	6	0	3.229367	6.214581	-1.380112
57	6	0	5.120562	6.842004	-2.791953
58	6	0	1.299322	5.545651	0.232691
59	6	0	2.715971	7.520268	-1.561659
60	6	0	4.601646	8.114506	-2.941972
61	1	0	6.049183	6.593634	-3.293766
62	6	0	0.127610	4.895736	-0.045429
63	6	0	1.375368	6.409275	1.399987
64	1	0	1.773662	7.779110	-1.091069
65	6	0	3.385468	8.456494	-2.325907
66	1	0	5.130872	8.846024	-3.545447
67	6	0	-1.034896	5.001600	0.786921
68	1	0	0.075453	4.246866	-0.915503
69	6	0	0.224286	6.580301	2.229729
70	6	0	2.578810	7.063066	1.760763
71	1	0	2.969600	9.451343	-2.453978
72	6	0	-2.203166	4.258853	0.495990
73	6	0	-0.995054	5.844117	1.933306
74	6	0	0.325257	7.444344	3.346137
75	1	0	3.463033	6.908472	1.154776
76	6	0	2.646803	7.890123	2.864530
77	6	0	-3.326531	4.305988	1.313440
78	1	0	-2.214629	3.648081	-0.402832
79	6	0	-2.147352	5.888155	2.750386
80	6	0	1.504781	8.092088	3.657973
81	1	0	-0.539312	7.606972	3.979123
82	1	0	3.581634	8.381433	3.117137
83	6	0	-3.269814	5.143377	2.456125
84	1	0	-2.155825	6.496354	3.647440
85	1	0	1.549130	8.748966	4.521645
86	1	0	-4.116636	5.176358	3.133838
87	6	0	-4.557761	3.526479	1.028467
88	6	0	-4.530809	2.255680	0.463316
89	6	0	-5.824949	4.069223	1.357678
90	6	0	-5.718121	1.526371	0.213947
91	1	0	-3.577745	1.785137	0.236796
92	6	0	-6.993114	3.376423	1.118544
93	1	0	-5.881760	5.067609	1.778901
94	6	0	-6.978473	2.093567	0.528099
95	6	0	-5.665956	0.184422	-0.280508
96	1	0	-7.931564	3.852337	1.376747
97	6	0	-8.171077	1.363037	0.135350
98	6	0	-6.766505	-0.619363	-0.520632
99	1	0	-4.674776	-0.222910	-0.440817

100	6	0	-8.068356	0.077215	-0.499519
101	6	0	-9.446848	1.958103	0.283343
102	6	0	-6.399620	-2.092173	-0.679742
103	6	0	-9.239020	-0.387498	-1.141850
104	6	0	-10.587684	1.400936	-0.256375
105	1	0	-9.531588	2.902569	0.806840
106	6	0	-5.312844	-2.474014	0.084067
107	6	0	-6.883506	-3.130224	-1.617621
108	1	0	-9.163362	-1.215521	-1.818772
109	6	0	-10.466005	0.239561	-1.028773
110	1	0	-11.549510	1.888369	-0.129605
111	6	0	-4.450123	-3.576744	-0.224290
112	1	0	-5.011736	-1.850166	0.918312
113	6	0	-5.961502	-4.130164	-2.078509
114	6	0	-8.229262	-3.304713	-2.015110
115	1	0	-11.324557	-0.164520	-1.557083
116	6	0	-3.302994	-3.847645	0.557434
117	6	0	-4.675093	-4.302312	-1.422506
118	6	0	-6.372482	-5.036999	-3.082935
119	1	0	-9.000551	-2.766325	-1.494688
120	6	0	-8.621827	-4.235587	-2.961023
121	6	0	-2.342506	-4.761358	0.139340
122	1	0	-3.147194	-3.283085	1.473278
123	6	0	-3.680790	-5.207971	-1.847317
124	6	0	-7.669870	-5.072928	-3.554230
125	1	0	-5.664645	-5.768151	-3.455217
126	1	0	-9.673447	-4.329393	-3.215350
127	6	0	-2.542041	-5.422335	-1.095125
128	1	0	-3.796437	-5.751796	-2.777893
129	1	0	-7.956878	-5.789699	-4.317461
130	1	0	-1.792279	-6.127357	-1.441123
131	1	0	5.981100	-5.015279	2.524903
132	1	0	5.324578	-6.660883	0.123686

(*Z*,*S*,*Z*,*S*)-[4]CPhen$_{2,9}$

SCF Done: E(RB3LYP) = −2153.35963640 A.U. after 7 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.091631	-1.324178	-0.513663
2	1	0	2.413935	-0.707051	-1.094762
3	6	0	4.206787	-0.752285	0.035620

4	6	0	5.111137	-1.601929	0.789554
5	6	0	6.303564	-1.091040	1.353094
6	1	0	6.527957	-0.037017	1.228285
7	6	0	7.181106	-1.904869	2.044692
8	1	0	8.094882	-1.489561	2.459105
9	6	0	6.888558	-3.269505	2.207733
10	1	0	7.581861	-3.915677	2.737905
11	6	0	5.709989	-3.789592	1.704357
12	1	0	5.496039	-4.843081	1.850396
13	6	0	4.782664	-2.986571	1.003134
14	6	0	3.486165	-3.502733	0.573706
15	6	0	2.920360	-4.741517	0.971868
16	1	0	3.505961	-5.437376	1.563599
17	6	0	1.588541	-5.054408	0.723659
18	1	0	1.173570	-5.970877	1.133653
19	6	0	0.748290	-4.153274	0.026845
20	6	0	1.341025	-3.012555	-0.499144
21	1	0	0.731374	-2.310816	-1.059823
22	6	0	2.669088	-2.652119	-0.211008
23	6	0	-1.340808	-3.012249	0.498518
24	1	0	-0.731045	-2.310451	1.059003
25	6	0	-0.748260	-4.153148	-0.027251
26	6	0	-1.588682	-5.054351	-0.723797
27	1	0	-1.173844	-5.970970	-1.133592
28	6	0	-2.920508	-4.741417	-0.971874
29	1	0	-3.506263	-5.437390	-1.563321
30	6	0	-3.486181	-3.502513	-0.573864
31	6	0	-4.782797	-2.986422	-1.002996
32	6	0	-5.710282	-3.789524	-1.703927
33	1	0	-5.496291	-4.842994	-1.850041
34	6	0	-6.889057	-3.269556	-2.206932
35	1	0	-7.582456	-3.915797	-2.736894
36	6	0	-7.181696	-1.904945	-2.043801
37	1	0	-8.095668	-1.489741	-2.457886
38	6	0	-6.303992	-1.091024	-1.352527
39	1	0	-6.528431	-0.037018	-1.227641
40	6	0	-5.111313	-1.601785	-0.789398
41	6	0	-4.206722	-0.751989	-0.035934
42	6	0	-3.091310	-1.323772	0.512972
43	1	0	-2.413392	-0.706504	1.093663
44	6	0	-2.668890	-2.651763	0.210486
45	6	0	-3.091580	1.324182	-0.513646
46	1	0	-2.413863	0.707056	-1.094723
47	6	0	-4.206752	0.752288	0.035603

48	6	0	-5.111140	1.601931	0.789483
49	6	0	-6.303624	1.091048	1.352904
50	1	0	-6.528029	0.037033	1.228034
51	6	0	-7.181205	1.904874	2.044456
52	1	0	-8.095022	1.489573	2.458782
53	6	0	-6.888642	3.269501	2.207557
54	1	0	-7.581978	3.915672	2.737689
55	6	0	-5.710029	3.789583	1.704280
56	1	0	-5.496081	4.843068	1.850349
57	6	0	-4.782663	2.986564	1.003108
58	6	0	-3.486139	3.502721	0.573748
59	6	0	-2.920336	4.741494	0.971950
60	1	0	-3.505953	5.437350	1.563671
61	6	0	-1.588510	5.054386	0.723778
62	1	0	-1.173548	5.970852	1.133788
63	6	0	-0.748249	4.153267	0.026957
64	6	0	-1.340974	3.012557	-0.499061
65	1	0	-0.731313	2.310830	-1.059746
66	6	0	-2.669044	2.652118	-0.210962
67	6	0	1.340865	3.012255	0.498606
68	1	0	0.731116	2.310450	1.059099
69	6	0	0.748302	4.153155	-0.027143
70	6	0	1.588706	5.054366	-0.723699
71	1	0	1.173854	5.970982	-1.133487
72	6	0	2.920524	4.741432	-0.971820
73	1	0	3.506258	5.437402	-1.563290
74	6	0	3.486203	3.502522	-0.573839
75	6	0	4.782794	2.986425	-1.003038
76	6	0	5.710239	3.789526	-1.704021
77	1	0	5.496244	4.842998	-1.850115
78	6	0	6.888976	3.269555	-2.207111
79	1	0	7.582344	3.915794	-2.737115
80	6	0	7.181609	1.904939	-2.044020
81	1	0	8.095545	1.489729	-2.458178
82	6	0	6.303944	1.091018	-1.352694
83	1	0	6.528377	0.037007	-1.227853
84	6	0	5.111313	1.601783	-0.789466
85	6	0	4.206760	0.751992	-0.035945
86	6	0	3.091369	1.323778	0.513001
87	1	0	2.413475	0.706513	1.093721
88	6	0	2.668938	2.651770	0.210533

(*Z*,*R*,*Z*,*S*)-[4]CPhen$_{2,9}$

SCF Done: E(RB3LYP) = −2153.35576591 A.U. after 7 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.297373	1.322651	1.274985
2	1	0	2.689264	0.624315	1.842029
3	6	0	4.305572	0.832499	0.487278
4	6	0	5.132283	1.780763	-0.242173
5	6	0	6.264643	1.368839	-0.982547
6	1	0	6.509708	0.313428	-1.020881
7	6	0	7.068484	2.282678	-1.638995
8	1	0	7.940909	1.940611	-2.187727
9	6	0	6.758705	3.652165	-1.589646
10	1	0	7.398799	4.374304	-2.087736
11	6	0	5.629187	4.080274	-0.916083
12	1	0	5.396037	5.139844	-0.894467
13	6	0	4.778616	3.173141	-0.245856
14	6	0	3.510302	3.592059	0.337404
15	6	0	2.834184	4.793835	0.010847
16	1	0	3.327684	5.541851	-0.600867
17	6	0	1.492167	4.972166	0.312008
18	1	0	0.973237	5.835556	-0.094034
19	6	0	0.761953	3.990159	1.029676
20	6	0	1.490681	2.929156	1.557653
21	1	0	0.991207	2.178675	2.161573
22	6	0	2.814167	2.664600	1.152749
23	6	0	-1.252899	2.597985	0.878710
24	1	0	-0.600372	1.737291	0.960991
25	6	0	-0.723745	3.879923	0.958902
26	6	0	-1.635485	4.950629	0.764930
27	1	0	-1.286191	5.976060	0.847439
28	6	0	-2.967548	4.720714	0.445397
29	1	0	-3.607205	5.581587	0.280856
30	6	0	-3.487072	3.410072	0.282161
31	6	0	-4.819045	3.068526	-0.207811
32	6	0	-5.789089	4.059427	-0.481220
33	1	0	-5.563594	5.098035	-0.264204
34	6	0	-7.021235	3.742966	-1.023919
35	1	0	-7.743239	4.529979	-1.220339
36	6	0	-7.332597	2.408197	-1.334182
37	1	0	-8.290886	2.161093	-1.781102
38	6	0	-6.413437	1.409925	-1.071281
39	1	0	-6.646290	0.378788	-1.317054

40	6	0	-5.159183	1.696847	-0.484457
41	6	0	-4.206369	0.641718	-0.195228
42	6	0	-2.997691	0.995370	0.338702
43	1	0	-2.277406	0.219466	0.575650
44	6	0	-2.592407	2.344717	0.545633
45	6	0	-3.297157	-1.322521	-1.275058
46	1	0	-2.688945	-0.624135	-1.841930
47	6	0	-4.305450	-0.832438	-0.487428
48	6	0	-5.132301	-1.780759	0.241772
49	6	0	-6.264801	-1.368881	0.981953
50	1	0	-6.509861	-0.313468	1.020317
51	6	0	-7.068781	-2.282767	1.638165
52	1	0	-7.941308	-1.940738	2.186759
53	6	0	-6.759011	-3.652254	1.588752
54	1	0	-7.399212	-4.374430	2.086651
55	6	0	-5.629377	-4.080323	0.915353
56	1	0	-5.396251	-5.139897	0.893669
57	6	0	-4.778667	-3.173143	0.245367
58	6	0	-3.510272	-3.592024	-0.337744
59	6	0	-2.834226	-4.793842	-0.011199
60	1	0	-3.327826	-5.541904	0.600377
61	6	0	-1.492171	-4.972175	-0.312189
62	1	0	-0.973316	-5.835613	0.093843
63	6	0	-0.761845	-3.990134	-1.029696
64	6	0	-1.490471	-2.929055	-1.557662
65	1	0	-0.990885	-2.178526	-2.161433
66	6	0	-2.814003	-2.664499	-1.152903
67	6	0	1.253017	-2.598009	-0.878622
68	1	0	0.600518	-1.737309	-0.961079
69	6	0	0.723844	-3.879941	-0.958739
70	6	0	1.635535	-4.950655	-0.764583
71	1	0	1.286223	-5.976085	-0.847041
72	6	0	2.967570	-4.720743	-0.444929
73	1	0	3.607190	-5.581616	-0.280243
74	6	0	3.487112	-3.410097	-0.281780
75	6	0	4.819049	-3.068537	0.208282
76	6	0	5.789020	-4.059445	0.481921
77	1	0	5.563505	-5.098070	0.265008
78	6	0	7.021115	-3.742972	1.024728
79	1	0	7.743061	-4.529992	1.221332
80	6	0	7.332489	-2.408181	1.334880
81	1	0	8.290729	-2.161065	1.781899
82	6	0	6.413404	-1.409902	1.071747
83	1	0	6.646266	-0.378751	1.317449

84	6	0	5.159215	-1.696833	0.484783
85	6	0	4.206472	-0.641702	0.195309
86	6	0	2.997818	-0.995387	-0.338656
87	1	0	2.277585	-0.219488	-0.575782
88	6	0	2.592504	-2.344745	-0.545452

(*Z*,*S*,*E*,*S*,*E*,*S*,*Z*,*R*)-[8]CPhen$_{2,9}$

SCF Done: E(RB3LYP) = −4306.84610453 A.U. after 6 cycles

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.038441	5.902541	0.072105
2	6	0	-3.814150	6.276206	0.607029
3	6	0	-2.942876	7.154343	-0.073346
4	6	0	-3.336925	7.726813	-1.315278
5	6	0	-4.601317	7.358339	-1.831861
6	6	0	-5.420319	6.462947	-1.170209
7	6	0	-1.625550	7.394707	0.431100
8	6	0	-2.413163	8.621643	-1.997427
9	6	0	-1.097789	8.816990	-1.469698
10	6	0	-0.706785	8.146230	-0.245592
11	6	0	-0.205035	9.680016	-2.149089
12	6	0	-0.581004	10.335633	-3.305092
13	6	0	-1.873236	10.147280	-3.825676
14	6	0	-2.764347	9.308657	-3.182952
15	6	0	0.708192	8.146128	0.245524
16	6	0	1.626836	7.394431	-0.431139
17	6	0	1.099305	8.816865	1.469610
18	6	0	2.944128	7.153890	0.073303
19	6	0	2.414655	8.621346	1.997330
20	6	0	0.206672	9.680029	2.148987
21	6	0	3.815261	6.275589	-0.607046
22	6	0	3.338286	7.726365	1.315197
23	6	0	2.765939	9.308341	3.182841
24	6	0	0.582737	10.335622	3.304970
25	6	0	5.039511	5.901784	-0.072136
26	6	0	4.602642	7.357739	1.831767
27	6	0	1.874948	10.147101	3.825550
28	6	0	5.421505	6.462202	1.170137
29	6	0	-5.877010	4.888385	0.761029
30	6	0	-6.302753	3.747836	0.094738
31	6	0	-6.201468	5.017893	2.132271

32	6	0	-7.004047	2.717794	0.759308
33	6	0	-6.920501	4.040125	2.791874
34	6	0	-7.336137	2.857982	2.136133
35	6	0	-7.330980	1.503610	0.072309
36	6	0	-8.046443	1.775201	2.801752
37	6	0	-7.952197	0.455559	0.689306
38	6	0	-8.337126	0.573620	2.083904
39	6	0	-8.446795	1.856639	4.156252
40	6	0	-8.151666	-0.820602	-0.068262
41	6	0	-8.981251	-0.491026	2.758856
42	6	0	-9.089659	0.808133	4.786482
43	6	0	-7.065046	-1.611720	-0.311760
44	6	0	-9.452559	-1.220483	-0.569419
45	6	0	-9.354342	-0.380126	4.083904
46	6	0	-7.157828	-2.850947	-1.024715
47	6	0	-9.590833	-2.449869	-1.286182
48	6	0	-10.591683	-0.402539	-0.378410
49	6	0	-6.005778	-3.637121	-1.243694
50	6	0	-8.421669	-3.287095	-1.512377
51	6	0	-10.875528	-2.801540	-1.763425
52	6	0	-11.831657	-0.776038	-0.858210
53	6	0	-6.059006	-4.847872	-1.922841
54	6	0	-8.461574	-4.522106	-2.200243
55	6	0	-11.973750	-1.988836	-1.554761
56	6	0	-7.322771	-5.276717	-2.399743
57	6	0	5.877919	4.887473	-0.761037
58	6	0	6.303415	3.746837	-0.094738
59	6	0	6.202451	5.016934	-2.132265
60	6	0	7.004539	2.716667	-0.759292
61	6	0	6.921316	4.039030	-2.791851
62	6	0	7.336701	2.856804	-2.136104
63	6	0	7.331232	1.502422	-0.072287
64	6	0	8.046806	1.773886	-2.801714
65	6	0	7.952286	0.454264	-0.689266
66	6	0	8.337247	0.572248	-2.083866
67	6	0	8.447170	1.855247	-4.156214
68	6	0	8.151519	-0.821925	0.068319
69	6	0	8.981148	-0.492530	-2.758826
70	6	0	9.089824	0.806615	-4.786447
71	6	0	7.064762	-1.612868	0.311774
72	6	0	9.452322	-1.221992	0.569572
73	6	0	9.354265	-0.381700	-4.083873
74	6	0	7.157313	-2.852102	1.024746
75	6	0	9.590364	-2.451396	1.286349

76	6	0	10.591578	-0.404209	0.378661
77	6	0	6.005129	-3.638092	1.243679
78	6	0	8.421061	-3.288443	1.512477
79	6	0	10.874972	-2.803254	1.763690
80	6	0	11.831463	-0.777889	0.858552
81	6	0	6.058134	-4.848842	1.922847
82	6	0	8.460739	-4.523449	2.200364
83	6	0	11.973328	-1.990711	1.555109
84	6	0	7.321809	-5.277880	2.399816
85	6	0	-4.842730	-5.667910	-2.145109
86	6	0	-3.832126	-5.745667	-1.194534
87	6	0	-4.674090	-6.404508	-3.343838
88	6	0	-2.672147	-6.525756	-1.397032
89	6	0	-3.549778	-7.174374	-3.562537
90	6	0	-2.515330	-7.266404	-2.602503
91	6	0	-1.651236	-6.586725	-0.392702
92	6	0	-1.320131	-8.076382	-2.782246
93	6	0	-0.519230	-7.336905	-0.541064
94	6	0	-0.330022	-8.115012	-1.751258
95	6	0	-1.098512	-8.844654	-3.949586
96	6	0	0.517988	-7.336998	0.540954
97	6	0	0.816157	-8.926636	-1.930380
98	6	0	0.033047	-9.623074	-4.101302
99	6	0	1.650121	-6.587006	0.392608
100	6	0	0.328635	-8.115075	1.751145
101	6	0	0.998575	-9.668409	-3.080845
102	6	0	2.671024	-6.526199	1.396957
103	6	0	1.318737	-8.076612	2.782146
104	6	0	-0.817683	-8.926506	1.930249
105	6	0	3.831130	-5.746293	1.194483
106	6	0	2.514062	-7.266816	2.602429
107	6	0	1.096981	-8.844861	3.949475
108	6	0	-1.000235	-9.668258	3.080706
109	6	0	4.841720	-5.668684	2.145085
110	6	0	3.548492	-7.174928	3.562496
111	6	0	-0.034707	-9.623096	4.101171
112	6	0	4.672929	-6.405238	3.343821
113	1	0	0.788893	9.825587	-1.740424
114	1	0	-1.333973	6.896919	1.352048
115	1	0	-3.480781	5.836466	1.543266
116	1	0	-4.938403	7.761716	-2.780197
117	1	0	-6.378998	6.189663	-1.601110
118	1	0	0.117872	10.998611	-3.806331
119	1	0	-2.175889	10.664180	-4.731577

120	1	0	-3.759295	9.189636	-3.596937
121	1	0	1.335175	6.896649	-1.352064
122	1	0	-0.787239	9.825724	1.740320
123	1	0	3.481808	5.835852	-1.543255
124	1	0	3.760869	9.189189	3.596827
125	1	0	-0.116042	10.998708	3.806201
126	1	0	4.939809	7.761115	2.780074
127	1	0	2.177675	10.663981	4.731438
128	1	0	6.380156	6.188801	1.601023
129	1	0	-6.043855	3.608753	-0.951638
130	1	0	-5.886950	5.908966	2.667422
131	1	0	-7.147972	4.188036	3.841455
132	1	0	-7.046302	1.414308	-0.972538
133	1	0	-8.251580	2.761456	4.720429
134	1	0	-9.183042	-1.407776	2.216550
135	1	0	-9.385934	0.903450	5.826943
136	1	0	-6.090623	-1.306973	0.060027
137	1	0	-9.850371	-1.208894	4.580111
138	1	0	-10.476533	0.535309	0.153718
139	1	0	-5.051337	-3.260542	-0.886539
140	1	0	-11.010274	-3.727047	-2.311527
141	1	0	-12.692379	-0.133119	-0.700326
142	1	0	-9.403510	-4.904058	-2.577336
143	1	0	-12.946173	-2.287517	-1.935049
144	1	0	-7.402573	-6.231914	-2.909298
145	1	0	6.044458	3.607802	0.951629
146	1	0	5.888116	5.908070	-2.667419
147	1	0	7.148849	4.186901	-3.841425
148	1	0	7.046513	1.413172	0.972553
149	1	0	8.252127	2.760102	-4.720392
150	1	0	9.182748	-1.409325	-2.216528
151	1	0	9.386114	0.901873	-5.826909
152	1	0	6.090406	-1.307973	-0.060068
153	1	0	9.850123	-1.210568	-4.580084
154	1	0	10.476606	0.533660	-0.153467
155	1	0	5.050765	-3.261367	0.886476
156	1	0	11.009541	-3.728779	2.311806
157	1	0	12.692289	-0.135094	0.700736
158	1	0	9.402596	-4.905538	2.577516
159	1	0	12.945679	-2.289533	1.935471
160	1	0	7.401434	-6.233080	2.909393
161	1	0	-3.938029	-5.217943	-0.250764
162	1	0	-5.432671	-6.341700	-4.117784
163	1	0	-3.468905	-7.710067	-4.501455

164	1	0	-1.792703	-6.006847	0.515606
165	1	0	-1.830285	-8.830457	-4.749116
166	1	0	1.560097	-8.958720	-1.142693
167	1	0	0.172670	-10.201539	-5.009772
168	1	0	1.791697	-6.007151	-0.515697
169	1	0	1.885282	-10.284708	-3.195244
170	1	0	-1.561620	-8.958460	1.142555
171	1	0	3.937140	-5.218591	0.250712
172	1	0	1.828754	-8.830801	4.749007
173	1	0	-1.887047	-10.284408	3.195093
174	1	0	3.467502	-7.710584	4.501425
175	1	0	-0.174432	-10.201552	5.009632
176	1	0	5.431494	-6.342530	4.117791