Supporting Information

Synthesis and Properties of [9]Cyclo-1,4-naphthylene: A π-Extended Carbon Nanoring

Akiko Yagi, Yasutomo Segawa, and Kenichiro Itami*

Department of Chemistry, Graduate School of Science, Nagoya University, Chikusa, Nagoya 464-8602, Japan

E-mail: itami.kenichiro@a.mbox.nagoya-u.ac.jp

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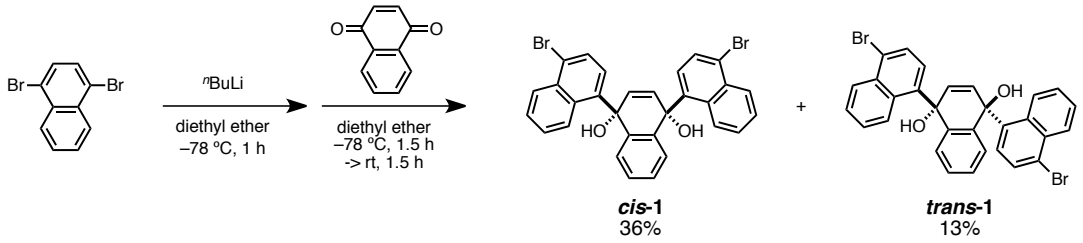
1. Experimental Section

General

Unless otherwise noted, all materials including dry solvents (dimethylformamide (DMF)) were obtained from commercial suppliers and used without further purification. Tetrahydrofuran (THF) and diethyl ether were purified by passing through a solvent purification system (Glass Contour). All reactions were performed using standard vacuum-line and Schlenk techniques. Work-up and purification procedures were carried out with reagent-grade solvents under air. 1,4-Dibromonaphthalene[S1] and $Ni(cod)_2$[S2] were prepared according to procedures reported in the literatures.

Analytical thin-layer chromatography (TLC) was performed using E. Merck silica gel 60 F254 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). Preparative thin-layer chromatography (PTLC) was performed using Wako-gel® B5-F silica coated plates (0.75 mm) prepared in our laboratory. 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. High-resolution mass spectra (HRMS) were obtained from a JEOL JMS700 (fast atom bombardment mass spectrometry, FAB MS) or a Bruker Daltonics Ultraflex III TOF/TOF (MALDI-TOF MS) with 9-nitroanthracene as matrix. Melting points were measured on a MPA100 Optimelt automated melting point system. Nuclear magnetic resonance (NMR) spectra were recorded on a JEOL JNM-ECA-600 (^{1}H 600 MHz, ^{13}C 150 MHz) spectrometer. Chemical shifts for ^{1}H NMR are expressed in parts per million (ppm) relative to $CHCl_3$ (δ 7.26 ppm), $CHDCl_2$ (δ 5.32 ppm), DMSO-d_5 (δ 2.50 ppm) and THF-d_7 (δ 1.72 ppm). Chemical shifts for ^{13}C NMR are expressed in ppm relative to $CDCl_3$ (δ 77.0 ppm), CD_2Cl_2 (δ 53.8 ppm), DMSO-d_6 (δ 39.5 ppm) and THF-d_8 (δ 67.2 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, ddd = doublet of doublets of doublets, t = triplet, m = multiplet), coupling constant (Hz), and integration.

Synthesis of *cis*-1 and *trans*-1

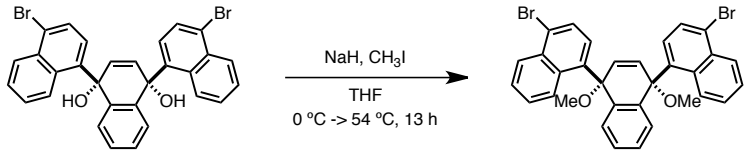


A three-necked 1-L glass round bottom flask containing a magnetic stirring bar was dried under vacuum and filled with argon after cooling to room temperature. A hexane solution *n*-butyllithium (1.6 M, 18.0 mL, 28.9 mmol) was added slowly to a solution of 1,4-dibromonaphthalene (7.50 g, 26.3 mmol) in dry diethyl ether (450 mL) at –78 °C under argon atmosphere. The reaction mixture was stirred at –78 °C for 1 h. The solution of 1,4-naphthoquinone (1.66 g, 10.5 mmol) in dry diethyl ether (120 mL) was added and the mixture was stirred for 1.5 h at –78 °C and for 1 h at room temperature. The reaction mixture was quenched with water, extracted with EtOAc (100 mL × 3), dried over Na_2SO_4, and concentrated under reduced pressure. ^{1}H NMR of the residue was taken to determine *cis*/*trans* ratio. The crude product was purified by silica gel column chromatography ($CHCl_3$/hexane = 3:1) and by reprecipitation (THF/hexane) to obtain *cis*-**1** (2.15 g, 36%) and *trans*-**1** (736 mg, 13%) as white solids.

cis-**1**: ^{1}H NMR (600 MHz, 150 °C, DMSO-d_6) δ 5.67 (s, 2H), 6.39 (s, 2H), 7.13 (dd, J = 6, 4 Hz, 2H), 7.17 (dd, J = 6, 4 Hz, 2H), 7.44 (ddd, J = 9, 7, 1 Hz, 2H), 7.62 (ddd, J = 9, 7, 1 Hz, 2H), 7.79 (d, J = 8 Hz, 2H), 7.93 (d, J = 8 Hz, 2H), 8.26 (dd, J = 8, 1 Hz, 2H), 8.42 (d, J = 9 Hz, 2H); ^{13}C NMR (150 MHz, 120 °C, DMSO-d_6) δ 71.1 (4°), 121.6 (4°), 125.4 (CH), 125.6 (CH), 126.3 (CH), 126.4 (CH), 126.7 (CH), 127.1 (CH), 127.6 (CH), 128.5 (CH), 131.3 (4°), 131.5 (4°), 132.8 (CH), 140.4 (4°), 140.9 (4°); HRMS (FAB) *m*/*z* calcd for $C_{30}H_{20}NaO_2Br_2$ $[M{\cdot}Na]^+$: 594.9702, found: 594.9719; mp: 175.3–177.3 °C.

trans-**1**: ^{1}H NMR (600 MHz, 100 °C, DMSO-d_6) δ 6.12 (s, 2H), 6.19 (s, 2H), 7.09 (dd, J = 6, 3 Hz, 2H), 7.13 (dd, J = 6, 3 Hz, 2H), 7.40 (t, J = 8 Hz, 2H), 7.57 (t, J = 7 Hz, 2H), 7.94 (d, J = 8 Hz, 2H), 7.99 (d, J = 8 Hz, 2H), 8.19 (d, J = 8 Hz, 2H), 8.65 (d, J = 9 Hz, 2H); ^{13}C NMR (150 MHz, 100 °C, DMSO-d_6) δ 71.1 (4°), 121.5 (4°), 125.1 (CH), 125.5 (CH), 126.2 (CH), 126.3 (CH), 126.9 (CH), 127.1 (CH), 127.2 (CH), 128.6 (CH), 131.1 (4°), 131.2 (4°), 131.3 (CH), 139.6 (4°), 143.0 (4°); HRMS (FAB) *m*/*z* calcd for $C_{30}H_{20}NaO_2Br_2$ $[M{\cdot}Na]^+$: 594.9702, found: 594.9766; mp: 158.0–160.0 °C.

Synthesis of L-shaped unit 2

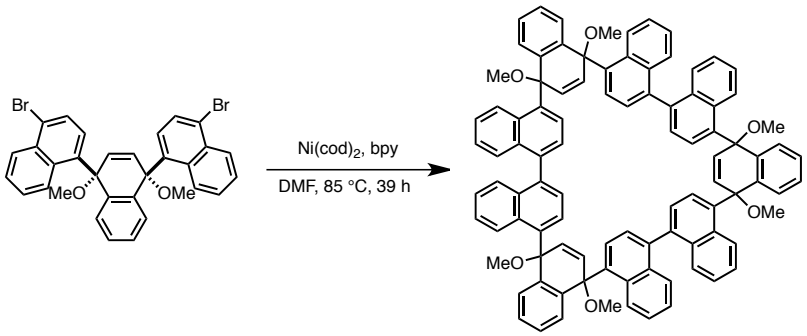


***cis*-1** **2** 99%

A two-necked 200-mL glass round bottom flask containing a magnetic stirring bar was dried under vacuum and filled with argon after cooling to room temperature. A solution of *cis*-**1** (1.00 g, 1.74 mmol) in dry THF (15 mL) was added slowly to a suspension of sodium hydride (60% oil suspension, 367 mg, 8.74 mmol) in dry THF (30 mL) at 0 °C. Methyl iodide (800 μL, 12.9 mmol) was added dropwise at 0 °C and the reaction mixture was stirred at 54 °C for 13 h. The reaction mixture was quenched with water and extracted with EtOAc (30 mL × 3), and the combined organic phase was dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by short column chromatography (hexane/EtOAc = 3:1) and follow-up reprecipitation (THF/hexane). The product **2** (1.06 g, 99%) was obtained as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 3.35 (s, 6H), 6.74 (s, 2H), 6.94 (d, *J* = 8 Hz, 2H), 7.44 (t, *J* = 8 Hz, 2H), 7.47 (dd, *J* = 6, 3 Hz, 2H), 7.54 (t, *J* = 8 Hz, 2H), 7.57 (d, *J* = 8 Hz, 2H), 7.63 (dd, *J* = 6, 3 Hz, 2H) 8.28 (d, *J* = 8 Hz, 2H), 8.85 (d, *J* = 9 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 51.6 (CH_3), 79.3 (4°), 124.2 (4°), 126.4 (CH), 126.9 (CH), 127.2 (CH), 127.5 (CH), 128.4 (CH), 128.8 (CH), 128.9 (CH), 129.2 (CH), 132.8 (CH), 132.9 (4°), 133.1 (4°), 138.9 (4°), 140.1 (4°); HRMS (FAB) *m/z* calcd for $C_{32}H_{24}NaO_2Br_2$ $[M{\cdot}Na]^+$: 623.0015, found: 623.0018; mp: 190.6–192.6 °C.

Synthesis of cyclic trimer 3 by Ni-mediated "shortgun" macrocyclization of 2

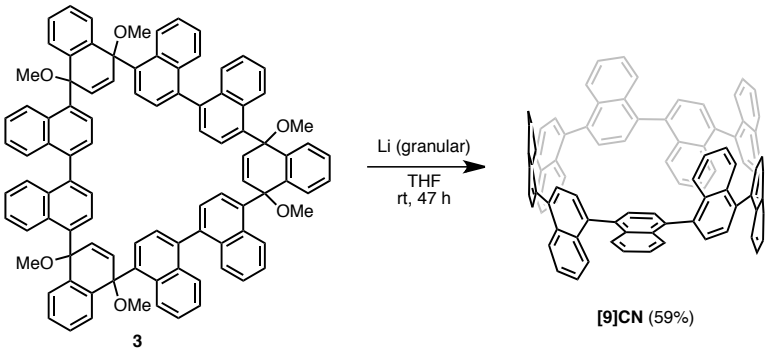


2 **3** 2%

To a Schlenk tube containing a magnetic stirring bar were added **2** (100 mg, 166 μmol), $Ni(cod)_2$ (101 mg, 367 μmol) and 2,2'-bipyridyl (57.2 mg, 366 μmol). After dry DMF (20 mL) was added via syringe through septum, the septum was replaced with oven-dried and argon-balloon-equipped condenser. The resultant mixture was stirred at 85 °C for 39 h. After the reaction mixture was cooled to room temperature, brine (ca. 100 mL) was added to the mixture. The mixture was extracted with EtOAc (50 mL × 3). The combined organic phase was subjected to preparative recycling gel permeation chromatography ($CHCl_3$) and then purified by PTLC (CH_2Cl_2/hexane = 4:1) to afford compound **3** (3.8 mg, 2%) as a white solid.

^{1}H NMR (600 MHz, CD_2Cl_2) δ 3.34 (s, 3H), 3.35 (s, 3H), 3.37 (s, 3H), 3.40 (s, 3H), 3.40 (s, 3H), 3.46 (s, 3H), 6.52 (d, *J* = 10 Hz, 1H), 6.72 (d, *J* = 8 Hz, 1H), 6.86 (s, 1H), 6.87 (d, *J* = 3 Hz, 1H), 6.96 (d, *J* = 8 Hz, 1H), 6.97–7.01 (m, 3H), 7.02–7.10 (m, 7H), 7.10–7.33 (m, 16H), 7.37 (t, *J* = 7 Hz, 1H), 7.41 (t, *J* = 7 Hz, 1H), 7.45–7.58 (m, 7H), 7.60 (dd, *J* = 6, 3 Hz, 2H), 7.63 (d, *J* = 8 Hz, 1H), 7.69 (d, *J* = 8 Hz, 1H), 7.76 (dd, *J* = 6, 3 Hz, 2H), 7.78 (d, *J* = 7Hz, 1H), 8.08 (d, *J* = 8 Hz, 1H), 8.76 (d, *J* = 9 Hz, 1H), 9.10 (d, *J* = 9 Hz, 1H), 9.13 (d, *J* = 9 Hz, 1H), 9.19 (t, *J* = 9 Hz, 2H), 9.78 (d, *J* = 9 Hz, 1H); ^{13}C NMR (150 MHz, CD_2Cl_2) δ 51.4 (CH_3), 51.5 (CH_3), 51.6 (CH_3), 51.7 (CH_3), 51.8 (CH_3), 79.3 (4°), 80.5 (4°), 80.5 (4°), 80.7 (4°), 81.1 (4°), 81.8 (4°), 125.4 (CH), 125.4 (CH), 125.6 (CH), 125.6 (CH), 125.7 (CH), 125.7 (CH), 125.9 (CH), 126.1 (CH), 126.1 (CH), 126.4 (CH), 126.5 (CH), 126.5 (CH), 126.6 (CH), 126.8 (CH), 126.9 (CH), 127.6 (CH), 127.9 (CH), 127.9 (CH), 128.1 (CH), 128.6 (CH), 128.8 (CH), 128.9 (CH), 129.0 (CH), 129.8 (CH), 129.9 (CH), 130.0 (CH), 130.5 (CH), 131.6 (4°), 132.0 (4°), 132.1 (CH), 132.1 (4°), 132.2 (4°), 132.2 (CH), 132.3 (4°), 132.5 (CH), 132.9 (CH), 134.6 (CH), 134.9 (4°), 135.0 (4°), 135.0 (4°), 135.1 (4°), 138.4 (4°), 139.1 (4°), 139.4 (4°), 139.5 (4°), 139.5 (4°), 139.8 (4°), 139.9 (4°), 140.2 (4°), 140.3 (4°), 140.8 (4°), 140.9 (4°), 140.9 (4°), 141.3 (4°), 141.7 (4°); HRMS (FAB) *m/z* calcd. for $C_{96}H_{72}NaO_6$ $[M{\cdot}Na]^+$: 1344.5255, found: 1344.5240; mp: 235.5–245.5 °C (dec.).

Synthesis of [9]cyclo-1,4-naphthylene ([9]CN)



A 50-mL flask containing glass-coated magnetic stirring bar was dried under vacuum and filled with argon after cooling to room temperature. In a glovebox, the compound **3** (8.0 mg, 3.7 μmol), lithium granular (20 mg, 2.9 mmol), and dry THF (10 mL) were added to this flask. The reaction mixture was stirred at room temperature for 47 h. The residue was diluted with hexane and quenched with methanol. After evaporated, the reaction mixture was passed through a short silica gel pad ($CHCl_3$). The filtrate was evaporated and purified by PTLC (CH_2Cl_2/hexane = 1:1) to obtain **[9]CN** (4.0 mg, 59%) as a yellow solid.

^{1}H NMR (600 MHz, THF-d_8) δ 6.28 (s, 2H), 6.95 (d, *J* = 8 Hz, 2H), 6.97 (d, *J* = 8 Hz, 2H), 6.99 (d, *J* = 8 Hz, 2H), 7.01 (d, *J* = 8 Hz, 2H), 7.06 (d, *J* = 8 Hz, 2H), 7.12 (d, *J* = 8 Hz, 2H), 7.24 (d, *J* = 8 Hz, 2H), 7.31 (ddd, *J* = 8, 7, 1 Hz, 2H), 7.40 (d, *J* = 8 Hz, 2H), 7.48 (ddd, *J* = 8, 7, 1 Hz, 2H), 7.51–7.61 (m, 8H), 7.61–7.73 (m, 8H), 8.32 (dd, *J* = 6, 3 Hz, 2H), 8.40 (dd, *J* = 8, 1 Hz, 2H), 8.45 (dd, *J* = 7, 2 Hz, 2H), 8.51 (dd, *J* = 7, 2 Hz, 2H), 8.55 (d, *J* = 8, 1 Hz, 2H), 8.58 (d, *J* = 8 Hz, 2H), 8.74 (d, *J* = 8 Hz, 2H); ^{13}C NMR (150 MHz, THF-d_8) δ 126.1 (CH), 126.5 (CH), 126.7 (CH), 126.9 (CH), 127.0 (CH), 127.0 (CH), 127.0 (CH), 127.1 (CH), 127.2 (CH), 127.4 (CH), 127.5 (CH), 127.5 (CH), 127.6 (CH), 127.7 (CH), 128.1 (CH), 128.3 (CH), 129.3 (CH), 129.3 (CH), 129.4 (CH), 129.5 (CH), 129.8 (CH), 130.0 (CH), 130.3 (CH), 130.3 (CH), 132.3 (CH), 132.6 (4°), 132.6 (4°), 133.9 (4°), 134.1(4°), 134.5 (4°), 134.8 (4°), 135.2 (4°), 136.5 (4°), 138.7 (4°), 138.9 (4°), 139.0 (4°), 139.1 (4°), 139.3 (4°), 139.5 (4°), 140.6 (4°), 140.9 (4°); HRMS (MALDI-TOF MS) *m/z* calcd. for $C_{90}H_{54}$ $[M]^+$: 1134.4226, found: 1134.4233; mp: partial decomposition at 300 °C.

2. X-ray Crystallography

Details of the crystal data and a summary of the intensity data collection parameters for *trans*-**1**·EtOAc and **2** are listed in Table S1. In each case, a suitable crystal was mounted with mineral oil on a glass fiber and transferred to the goniometer of a Rigaku Saturn CCD diffractometer. Graphite-monochromated Mo Kα radiation (λ = 0.71070 Å) was used. The structures were solved by direct methods with (SIR-97)[S3] and refined by full-matrix least-squares techniques against F^2 (SHELXL-97).[S4] 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 for *trans*-**1** and **2**.

	trans-**1**·EtOAc	**2**
formula	$C_{34}H_{28}Br_2O_4$	$C_{32}H_{24}Br_2O_2$
fw	660.38	600.33
T (K)	103(2)	103(2)
λ (Å)	0.71070	0.71070
cryst syst	Monoclinic	Triclinic
space group	$P2_1/c$	P-1
a, (Å)	6.9781(14)	7.5571(11)
b, (Å)	18.955(4)	12.8797(16)
c, (Å)	21.355(4)	14.111(2)
α, (deg)	90	68.140(5)
β, (deg)	96.569(3)	83.629(6)
γ, (deg)	90	76.933(6)
V, (Å^3)	2806.1(9)	1241.2(3)
Z	4	2
D_{calc}, (g / cm^3)	1.563	1.606
μ (mm^{-1})	2.928	3.295
F(000)	1336	604
cryst size (mm)	0.15 × 0.03 × 0.01	0.15 × 0.15 × 0.10
2θ range, (deg)	3.07–25.00	3.11-25.00
reflns collected	18674	8344
indep reflns/R_{int}	4935/0.0425	4263/0.0239
params	365	327
GOF on F^2	1.066	1.031
R_1, wR_2 [I>2σ(I)]	0.0408, 0.0903	0.0244, 0.0561
R_1, wR_2 (all data)	0.0527, 0.0976	0.0322, 0.0588

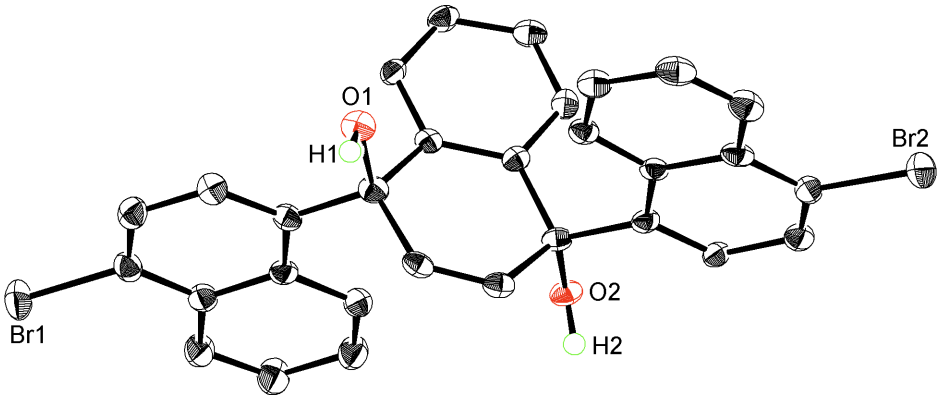


Figure S1. ORTEP drawing of *trans*-**1**·EtOAc with 50% thermal ellipsoid. All hydrogen atoms (except OH) and EtOAc molecule are omitted for clarity.

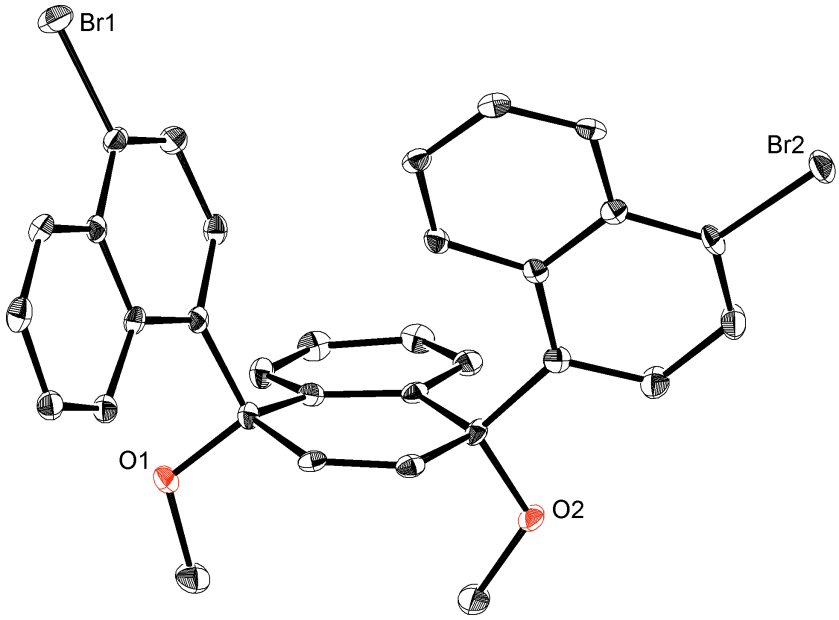


Figure S2. ORTEP drawing of **2** with 50% thermal ellipsoid. All hydrogen atoms are omitted for clarity.

3. VT NMR Study

Variable temperature ^{1}H NMR studies were carried out on a JEOL JNM-ECA-600 at 600 MHz from 30 °C to 150 °C as shown in Figure S1.

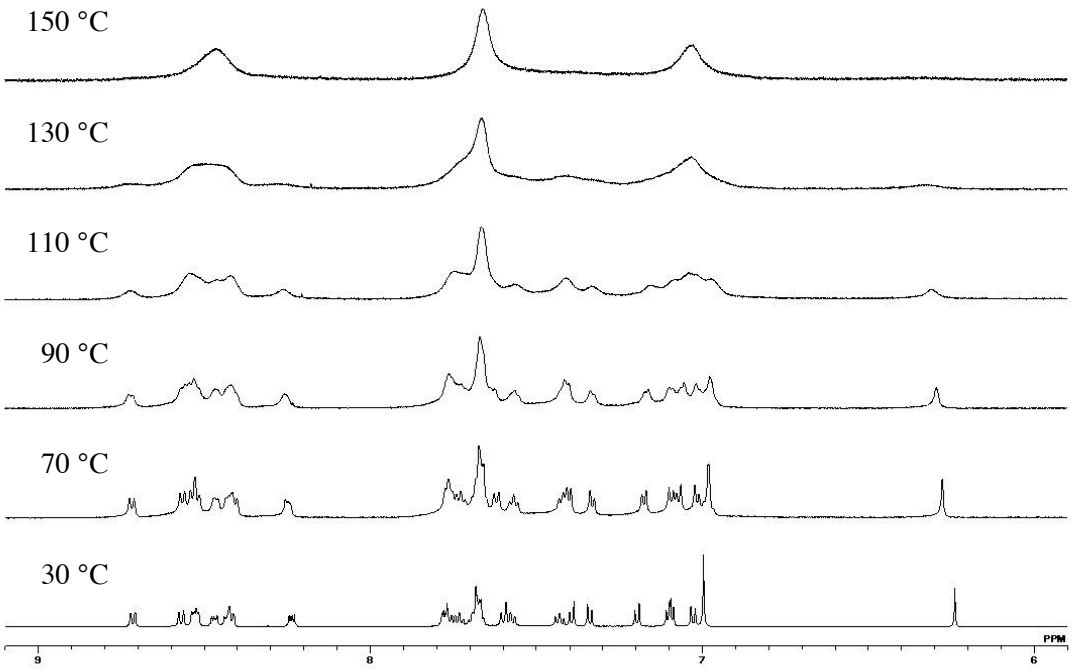


Figure S1. VT NMR of [**9**]**CN** in DMSO-d_6.

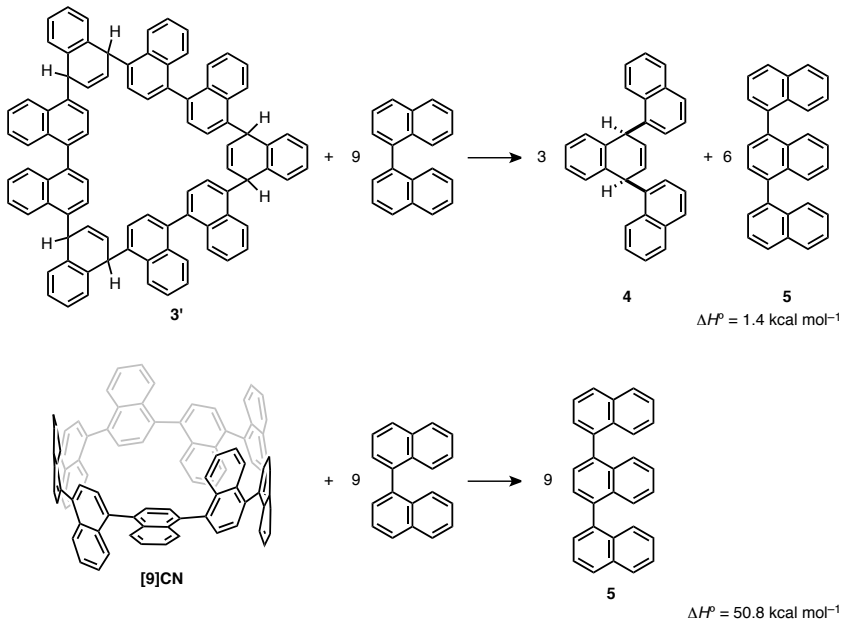
4. Photophysical Properties

UV/Vis absorption spectrum of [9]CN was recorded on a Shimadzu UV-3510 spectrometer with a resolution of 0.5 nm. Emission spectrum of [9]CN was measured with an F-4500 Hitachi spectrometer with a resolution of 0.4 nm upon excitation at 390 nm. Dilute solution in degassed spectral grade chloroform in a 1 cm square quartz cell was used for measurements. Absolute fluorescence quantum yield was determined with a Hamamatsu C9920-02 calibrated integrating sphere system upon excitation at 390 nm.

5. Computational Study

The Gaussian 09 program[S5] running on a SGI Altix4700 system was used for optimization (B3LYP/6-31G(d)).[S6] All 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 unless otherwise noted. Harmonic vibration frequency calculations at the same level were performed to verify all stationary points as local minima (with no imaginary frequency) or transition states (with one imaginary frequency). IRC calculations[S7] were also performed to check transition states. Visualization of the results was performed by use of POV-Ray for Windows v3.5 software.

Scheme S1. Hypothetic homodesmotic reactions for estimation of strain energies.[a]



a) Most stable structure of **3'** out of six isomers was used.

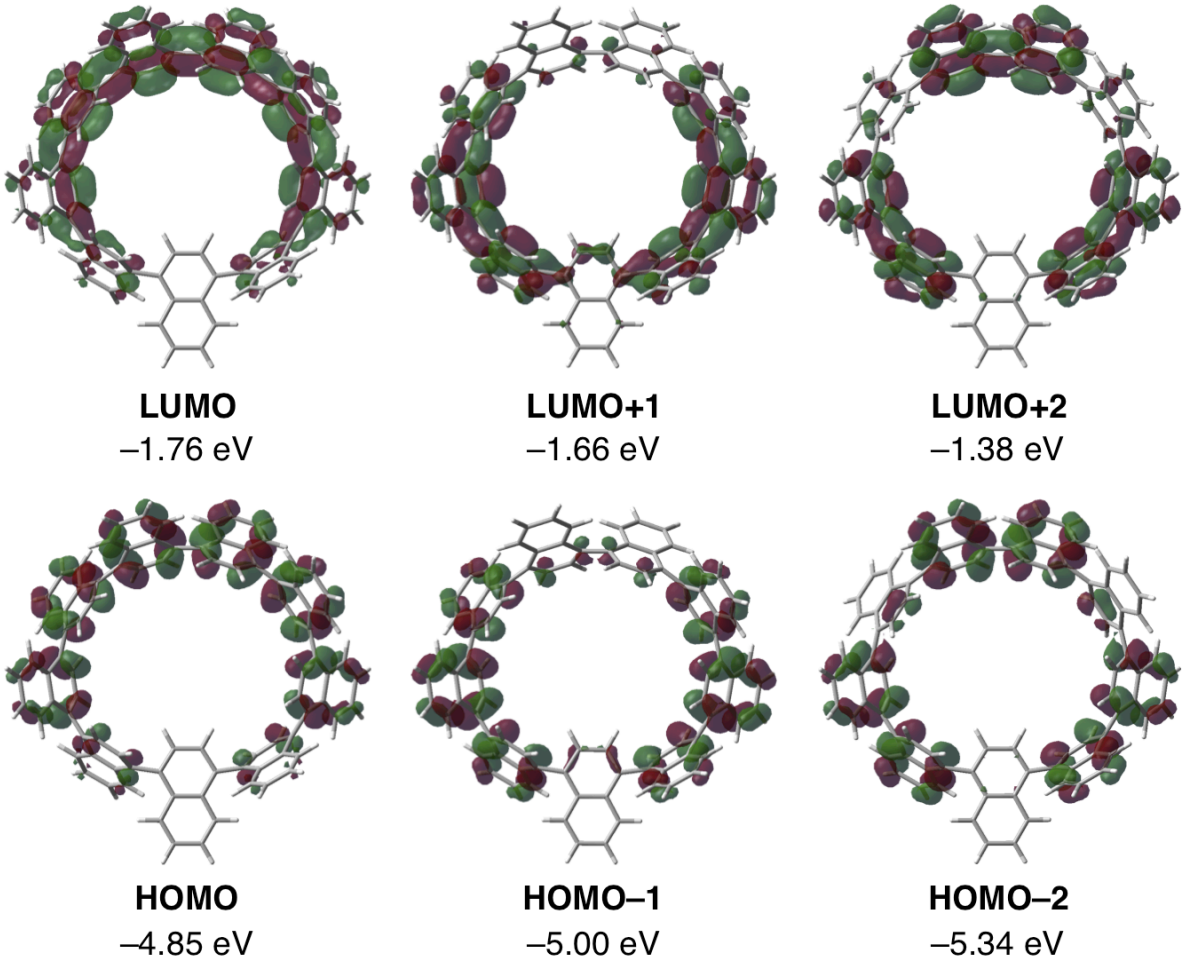


Figure S2. Frontier molecular orbitals of [9]CN.

Table S2. TD-DFT vertical one-electron excitations (6 states) calculated for the conformation A of [9]CN.

energy	wavelength	Oscillator strength (*f*)	Description
2.6281 eV	471.77 nm	0.1653	HOMO -> LUMO (0.65816) HOMO–1 -> LUMO+1 (0.23881)
2.8763 eV	431.05 nm	0.8226	HOMO–1 -> LUMO (0.19078) HOMO -> LUMO+1 (0.67369)
2.9299 eV	423.17 nm	0.2564	HOMO–1 -> LUMO (0.67223) HOMO -> LUMO+1 (-0.18410)
3.0127 eV	411.53 nm	0.2202	HOMO–1 -> LUMO+1 (0.65159) HOMO -> LUMO (-0.23999)

3.1337 eV	395.64 nm	0.1271	HOMO -> LUMO+2 (0.65639) HOMO–2 -> LUMO (-0.18011)
3.2484 eV	381.68 nm	0.3391	HOMO–2 -> LUMO (0.66426) HOMO -> LUMO+2 (0.19699)

Table S3. Uncorrected and thermal-corrected (298K) energies of stationary points (Hartree).[a]

compound	E	E + ZPE	H	G
[9]CN (A)	-3462.16886695	-3461.019367	-3460.954276	-3461.117841
[9]CN (B)	-3462.15892837	-3461.009337	-3460.944387	-3461.108107
[9]CN (TS_{AB})	-3462.13578458	-3460.986469	-3460.922092	-3461.084452
[9]CN (TS_{rac})	-3462.13793163	-3460.988718	-3460.924328	-3461.086813
1,1'-binaphtyl (C)	-770.587625051	-770.311952	-770.296834	-770.354150
1,1'-binaphtyl (TS1)	-770.536568946	-770.260617	-770.246495	-770.299540
1,1'-binaphtyl (TS2)	-770.538606528	-770.263546	-770.249675	-770.302349
3'	-3465.75905328	-3464.538853	-3464.472620	-3464.640161
4	-1156.45242376	-1156.025758	-1156.002836	-1156.078479
ternaphtyl (5)	-1155.28226017	-1154.878843	-1154.856237	-1154.931792

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

Table S4. Cartesian coordinates of optimized species.

[9]CN (A)

C	-1.117604	6.047021	0.294994	C	0.052216	0.720936	6.741010	C	-1.040149	-6.875981	1.883539
C	-1.123824	5.818672	1.681658	C	-0.052216	-0.720936	6.741010	C	-1.053268	-7.096122	0.460138
C	-0.019246	6.101691	2.474288	C	-0.093596	-1.429430	5.498102	C	0.002843	-6.557819	-0.353447
C	1.040149	6.875981	1.883539	C	-0.047280	-0.699540	4.322968	C	1.117604	-6.047021	0.294994
C	1.053268	7.096122	0.460138	C	0.047280	0.699540	4.322968	C	1.123824	-5.818672	1.681658
C	0.140000	5.311464	3.728884	C	-0.186240	-2.911785	5.279538	C	-0.151395	-6.237239	-1.800498
C	-0.964654	5.003840	4.599584	C	-1.319650	-3.384784	4.641704	C	-1.259569	-5.493298	-2.179983
C	-0.954207	3.781129	5.361123	C	-1.301264	-4.566510	3.875650	C	-1.259569	-4.715511	-3.352112
C	0.186240	2.911785	5.279538	C	-0.140000	-5.311464	3.728884	C	-0.153408	-4.656794	-4.187522
C	1.319650	3.384784	4.641704	C	0.964654	-5.003840	4.599584	C	0.911281	-5.594962	-3.955787
C	1.301264	4.566510	3.875650	C	0.954207	-3.781129	5.361123	C	0.912247	-6.389581	-2.755599
C	0.093596	1.429430	5.498102	C	0.019246	-6.101691	2.474288	C	-0.009106	-3.466969	-5.074176

C	-1.067562	-2.969510	-5.909695	C	-3.151880	-3.313679	-7.132830	H	3.911216	8.967736	0.239765
C	-1.040468	-1.600595	-6.356845	C	1.973784	-5.768885	-4.883637	H	3.880835	8.599526	2.708329
C	0.045667	-0.744170	-5.965442	C	1.975569	-7.309972	-2.551570	H	-2.091848	6.792630	4.152941
C	1.133507	-1.325998	-5.331402	C	2.983799	-6.677871	-4.656067	H	-2.116859	2.515161	6.675476
C	1.106551	-2.661983	-4.893960	C	2.985257	-7.456335	-3.477463	H	-4.047874	4.033558	6.804211
C	-0.045667	0.744170	-5.965442	C	-2.119161	-7.850023	-0.100053	H	-4.022335	6.202510	5.567710
C	-1.133507	1.325998	-5.331402	C	-2.089150	-7.431574	2.663680	H	-1.967595	7.919957	-1.653540
C	-1.106551	2.661983	-4.893960	C	-3.117143	-8.378124	0.689966	H	-1.965247	5.183501	-5.797750
C	0.009106	3.466969	-5.074176	C	-3.100558	-8.168879	2.086568	H	-3.777570	8.180243	-3.306924
C	1.067562	2.969510	-5.909695	C	2.096988	-5.855897	4.702044	H	-3.774861	6.804908	-5.390245
C	1.040468	1.600595	-6.356845	C	2.106785	-3.449763	6.124629	H	2.159001	4.832873	-6.001499
C	0.153408	4.656794	-4.187522	C	3.176818	-5.524244	5.490866	H	2.067733	0.112739	-7.541195
C	-0.911281	5.594962	-3.955787	C	3.187096	-4.301125	6.197191	H	3.958230	3.970821	-7.447272
C	-0.912247	6.389581	-2.755599	C	-0.123129	-1.395458	7.990803	H	3.912491	1.597643	-8.220910
C	1.259569	5.493298	-2.179983	C	0.123129	1.395458	7.990803	H	-2.067733	-0.112739	-7.541195
C	1.259569	4.715511	-3.352112	C	-0.066142	-0.704326	9.180283	H	-2.159001	-4.832873	-6.001499
C	0.151395	6.237239	-1.800498	C	0.066142	0.704326	9.180283	H	-3.912491	-1.597643	-8.220910
C	-0.002843	6.557819	-0.353447	H	-1.941774	5.655771	-0.293294	H	-3.958230	-3.970821	-7.447272
C	2.089150	7.431574	2.663680	H	-1.949366	5.253219	2.100748	H	1.965247	-5.183501	-5.797750
C	2.119161	7.850023	-0.100053	H	2.201893	2.752016	4.596459	H	1.967595	-7.919957	-1.653540
C	3.117143	8.378124	0.689966	H	2.161626	4.788282	3.252460	H	3.774861	-6.804908	-5.390245
C	3.100558	8.168879	2.086568	H	-0.073161	-1.224952	3.373338	H	3.777570	-8.180243	-3.306924
C	-2.096988	5.855897	4.702044	H	0.073161	1.224952	3.373338	H	-2.120963	-8.026720	-1.171304
C	-2.106785	3.449763	6.124629	H	-2.201893	-2.752016	4.596459	H	-2.068664	-7.284179	3.739199
C	-3.187096	4.301125	6.197191	H	-2.161626	-4.788282	3.252460	H	-3.911216	-8.967736	0.239765
C	-3.176818	5.524244	5.490866	H	1.941774	-5.655771	-0.293294	H	-3.880835	-8.599526	2.708329
C	-1.975569	7.309972	-2.551570	H	1.949366	-5.253219	2.100748	H	2.091848	-6.792630	4.152941
C	-1.973784	5.768885	-4.883637	H	-2.085509	-5.378469	-1.484681	H	2.116859	-2.515161	6.675476
C	-2.985257	7.456335	-3.477463	H	-2.086948	-4.032097	-3.516943	H	4.022335	-6.202510	5.567710
C	-2.983799	6.677871	-4.656067	H	1.973752	-0.703289	-5.039712	H	4.047874	-4.033558	6.804211
C	2.148383	3.795721	-6.321596	H	1.926331	-3.021132	-4.279561	H	-0.226074	-2.476960	7.988690
C	2.096765	1.138860	-7.188524	H	-1.973752	0.703289	-5.039712	H	0.226074	2.476960	7.988690
C	3.151880	3.313679	-7.132830	H	-1.926331	3.021132	-4.279561	H	-0.121650	-1.241251	10.123418
C	3.125894	1.970935	-7.570654	H	2.085509	5.378469	-1.484681	H	0.121650	1.241251	10.123418
C	-2.096765	-1.138860	-7.188524	H	2.086948	4.032097	-3.516943				
C	-2.148383	-3.795721	-6.321596	H	2.068664	7.284179	3.739199				
C	-3.125894	-1.970935	-7.570654	H	2.120963	8.026720	-1.171304				

[9]CN (B)

C	-6.173537	-0.593415	-1.118273	C	-6.227726	-2.798199	-0.068222	C	-7.210562	-0.803565	1.052958
C	-5.949155	-1.979525	-1.156062	C	-7.003680	-2.228770	1.003010	C	-5.419761	-4.044683	0.064383

C	-5.026901	-4.828187	-1.080568	C	-1.579874	5.930409	1.069441	C	1.391089	-3.025602	0.073730
C	-3.749550	-5.491370	-1.079534	C	-4.689702	3.817760	0.215281	C	-1.391047	-3.025687	-0.074011
C	-2.923015	-5.424864	0.092190	C	-5.647398	3.626216	-0.839975	C	0.703473	-1.834643	0.049945
C	-3.488962	-4.938855	1.256386	C	-6.472131	2.446852	-0.847639	C	-0.703504	-1.834686	-0.050261
C	-4.718788	-4.248498	1.245670	C	-5.564323	1.816623	1.304225	H	-5.784140	0.010539	-1.931835
C	-1.429848	-5.533129	0.024459	C	-4.757579	2.969674	1.311216	H	-5.385231	-2.377242	-1.992538
C	-0.716026	-4.280000	-0.011673	C	-6.328149	1.471021	0.198397	H	-2.891908	-4.913322	2.164135
C	0.716146	-4.279959	0.011427	C	-6.670643	0.032422	0.015206	H	-5.003789	-3.703095	2.139285
C	1.430036	-5.533054	-0.024650	C	-7.571467	-3.029885	2.028914	H	1.236212	-7.660428	-0.057241
C	0.709982	-6.709991	-0.021943	C	-7.956286	-0.263280	2.134343	H	-1.235915	-7.660493	0.057129
C	-0.709735	-6.710029	0.021794	C	-8.493879	-1.073527	3.111030	H	2.892153	-4.913048	-2.164235
C	2.923199	-5.424731	-0.092325	C	-8.303377	-2.471513	3.055142	H	5.003992	-3.702766	-2.139233
C	3.489177	-4.938630	-1.256468	C	-5.841908	-4.931721	-2.238666	H	5.783858	0.010750	1.931923
C	4.718985	-4.248244	-1.245666	C	-3.331109	-6.161056	-2.260852	H	5.385032	-2.377039	1.992579
C	5.419912	-4.044488	-0.064340	C	-4.149595	-6.240144	-3.366072	H	5.455886	1.106094	-2.117857
C	5.027038	-4.828096	1.080537	C	-5.424591	-5.632757	-3.349806	H	4.060793	3.106020	-2.132788
C	3.749701	-5.491308	1.079418	C	-7.411485	2.281826	-1.900955	H	0.743909	4.602402	1.957666
C	6.227825	-2.797981	0.068388	C	-5.811114	4.573598	-1.886751	H	3.071999	3.874615	1.877029
C	7.003917	-2.228524	-1.002731	C	-7.547901	3.226157	-2.894858	H	-0.744123	4.602219	-1.957786
C	7.210737	-0.803309	-1.052662	C	-6.739269	4.384248	-2.887198	H	-3.072189	3.874363	-1.877069
C	6.670631	0.032660	-0.014995	C	-3.757945	5.918994	2.212094	H	-5.455798	1.105954	2.117960
C	6.173400	-0.593192	1.118421	C	-1.092338	6.755303	2.119610	H	-4.060794	3.105941	2.132755
C	5.949070	-1.979311	1.156186	C	-3.250539	6.722045	3.209511	H	-7.440141	-4.106573	1.978380
C	6.328091	1.471241	-0.198242	C	-1.903480	7.144701	3.162565	H	-8.120175	0.809660	2.164500
C	5.564325	1.816787	-1.304130	C	1.092083	6.755149	-2.119912	H	-9.077542	-0.637907	3.917506
C	4.757529	2.969801	-1.311200	C	3.757720	5.918923	-2.212302	H	-8.743893	-3.109331	3.816707
C	4.689546	3.817911	-0.215291	C	1.903221	7.144484	-3.162894	H	-6.818864	-4.457719	-2.229558
C	5.647182	3.626433	0.840033	C	3.250295	6.721869	-3.209793	H	-2.354045	-6.633523	-2.270204
C	6.471960	2.447101	0.847782	C	5.810787	4.573846	1.886797	H	-3.817061	-6.776955	-4.250518
C	3.479259	4.675839	-0.064165	C	7.411246	2.282137	1.901167	H	-6.076200	-5.716188	-4.215418
C	2.953610	5.499936	-1.117511	C	6.738881	4.384557	2.887312	H	-8.043630	1.399199	-1.897851
C	1.579639	5.930362	-1.069668	C	7.547558	3.226498	2.895056	H	-5.201939	5.471961	-1.873334
C	0.744987	5.531517	0.030852	C	7.956598	-0.262997	-2.133939	H	-8.286572	3.085936	-3.679438
C	1.350126	4.900719	1.107695	C	7.571916	-3.029621	-2.028533	H	-6.857776	5.132924	-3.665895
C	2.691478	4.481695	1.061394	C	8.494386	-1.073225	-3.110534	H	-4.798537	5.611281	2.238305
C	-0.745217	5.531496	-0.031050	C	8.303955	-2.471221	-3.054654	H	-0.063073	7.096785	2.075069
C	-1.350344	4.900591	-1.107837	C	5.842031	-4.931728	2.238637	H	-3.890867	7.042082	4.027103
C	-2.691683	4.481527	-1.061491	C	3.331250	-6.161097	2.260674	H	-1.510248	7.789150	3.944210
C	-3.479459	4.675734	0.064063	C	5.424706	-5.632866	3.349710	H	0.062806	7.096599	-2.075409
C	-2.953830	5.499939	1.117333	C	4.149715	-6.240266	3.365902	H	4.798322	5.611241	-2.238478

H	1.509973	7.788851	-3.944599	H	8.120438	0.809952	-2.164080	H	6.076303	-5.716368	4.215323
H	3.890618	7.041857	-4.027408	H	7.440653	-4.106315	-1.978002	H	3.817171	-6.777157	4.250296
H	5.201576	5.472183	1.873318	H	9.078152	-0.637584	-3.916924	H	2.470854	-3.007522	0.140125
H	8.043426	1.399533	1.898129	H	8.744630	-3.109025	-3.816140	H	-2.470815	-3.007677	-0.140399
H	6.857305	5.133257	3.665999	H	6.818983	-4.457719	2.229582	H	1.247112	-0.895038	0.100016
H	8.286179	3.086324	3.679691	H	2.354194	-6.633581	2.269971	H	-1.247200	-0.895115	-0.100356

[9]CN (TS_{AB})

C	-6.573733	-2.122137	-0.981934	C	4.348802	5.231502	0.717013	C	-5.128174	4.928415	2.205559
C	-6.066886	-3.423720	-1.174932	C	5.388155	4.241073	0.808864	C	-2.906673	6.608099	1.958727
C	-5.459795	-4.163140	-0.162675	C	2.018863	5.734513	-0.240193	C	-4.860610	5.866764	3.177267
C	-5.927233	-3.773914	1.174082	C	1.311815	6.337720	-1.336232	C	-3.742052	6.720326	3.048582
C	-6.404838	-2.427360	1.381688	C	-0.125791	6.430734	-1.295254	C	-0.794082	7.049455	-2.386290
C	-4.233435	-5.013052	-0.401231	C	-0.841825	5.909126	-0.162328	C	1.993505	6.861253	-2.467936
C	-3.302157	-4.788439	-1.518100	C	-0.101483	5.522006	0.945849	C	-0.098128	7.551876	-3.464005
C	-1.909427	-5.157219	-1.366587	C	1.300007	5.440048	0.909279	C	1.310370	7.455136	-3.506371
C	-1.454253	-5.861724	-0.196977	C	-2.277240	5.508856	-0.200571	C	4.303747	6.259003	1.697699
C	-2.408777	-6.266274	0.708389	C	-2.714698	4.722664	-1.257466	C	6.320213	4.331395	1.877735
C	-3.747981	-5.845191	0.604161	C	-3.860423	3.910605	-1.150398	C	5.231629	6.321664	2.714275
C	0.002482	-5.940407	0.134349	C	-4.591603	3.846147	0.024083	C	6.249993	5.347024	2.806064
C	0.979375	-6.664045	-0.626781	C	-4.300898	4.798578	1.056794	C	7.456836	1.738419	-1.969465
C	2.377033	-6.363699	-0.457385	C	-3.148793	5.651377	0.935658	C	7.706652	-1.030301	-1.679319
C	2.776898	-5.360717	0.488754	C	-5.434419	2.636968	0.264279	C	8.189425	1.011523	-2.882225
C	1.815500	-4.852456	1.348185	C	-6.547125	2.245905	-0.550227	C	8.319024	-0.386905	-2.732989
C	0.447611	-5.133622	1.167504	C	-7.070414	0.905888	-0.454129	C	6.595029	-2.972428	2.679800
C	4.075831	-4.629968	0.417013	C	-5.450143	0.423792	1.278752	C	4.787552	-5.103507	2.760346
C	4.372900	-3.973296	-0.766991	C	-4.978142	1.744526	1.220198	C	6.497501	-3.755275	3.809721
C	5.249488	-2.873522	-0.797579	C	-6.424240	-0.050770	0.408099	C	5.579371	-4.827914	3.853314
C	5.872824	-2.405396	0.351288	C	-6.545115	-1.523094	0.264837	C	3.324402	-7.077768	-1.240351
C	5.795086	-3.224336	1.532797	C	-6.037125	-4.657062	2.281704	C	0.606624	-7.663518	-1.566200
C	4.875231	-4.330738	1.571081	C	-6.821840	-2.026508	2.676947	C	2.926888	-8.047869	-2.133846
C	6.294306	-0.976787	0.384390	C	-6.845984	-2.904561	3.738994	C	1.554041	-8.343370	-2.298516
C	6.943050	-0.315871	-0.717411	C	-6.479086	-4.243161	3.523743	H	-6.798261	-1.537327	-1.867693
C	6.822211	1.112038	-0.863189	C	-3.640128	-4.194509	-2.768369	H	-6.057560	-3.779630	-2.191271
C	6.078264	1.866088	0.107320	C	-0.973347	-4.789284	-2.373634	H	-2.112602	-6.843195	1.580432
C	5.683228	1.215291	1.266867	C	-1.353563	-4.178088	-3.543467	H	-4.380282	-6.124122	1.427489
C	5.782476	-0.179974	1.399608	C	-2.715496	-3.907950	-3.749926	H	2.102037	-4.109164	2.086179
C	5.457767	3.191987	-0.171076	C	-8.226605	0.582672	-1.214369	H	-0.280051	-4.601551	1.773680
C	4.664533	3.309598	-1.303300	C	-7.172566	3.161800	-1.439105	H	3.797534	-4.201465	-1.659450
C	3.644615	4.275466	-1.390733	C	-8.819008	1.503325	-2.051697	H	5.304651	-2.287852	-1.709536
C	3.388129	5.156969	-0.350515	C	-8.278837	2.802454	-2.176285	H	5.139037	1.767894	2.026403

H	5.301322	-0.647541	2.252334	H	-0.614129	-3.922677	-4.297333	H	7.111569	3.590668	1.938627
H	4.714749	2.541599	-2.069272	H	-3.052916	-3.464630	-4.683156	H	5.186772	7.128453	3.440891
H	2.947034	4.214928	-2.220616	H	-8.661966	-0.405262	-1.104749	H	6.985917	5.405423	3.603497
H	-0.615671	5.136456	1.820196	H	-6.772102	4.168667	-1.508464	H	7.374771	2.816310	-2.070678
H	1.812637	4.997627	1.757599	H	-9.711619	1.232250	-2.609150	H	7.821370	-2.102908	-1.557315
H	-2.083458	4.609943	-2.133402	H	-8.749435	3.524277	-2.838373	H	8.680646	1.516333	-3.709713
H	-4.081073	3.211623	-1.952395	H	-5.996984	4.283484	2.293832	H	8.912385	-0.955140	-3.444274
H	-4.948411	-0.270513	1.943947	H	-2.053299	7.271169	1.857964	H	7.309671	-2.156022	2.645093
H	-4.148102	2.030586	1.859602	H	-5.517347	5.960298	4.037995	H	4.094383	-5.938776	2.784177
H	-5.877435	-5.716461	2.143129	H	-3.544400	7.472289	3.807823	H	7.134594	-3.552409	4.666369
H	-7.179281	-1.010298	2.807907	H	-1.874868	7.142247	-2.346564	H	5.508118	-5.444598	4.745208
H	-7.196394	-2.577726	4.714015	H	3.077450	6.806144	-2.490012	H	4.379083	-6.857644	-1.105717
H	-6.572643	-4.970597	4.325766	H	-0.632812	8.035119	-4.277335	H	-0.448270	-7.890956	-1.688358
H	-4.660615	-3.966269	-3.006630	H	1.856523	7.862832	-4.352765	H	3.670147	-8.593371	-2.709060
H	0.071731	-5.017047	-2.214129	H	3.529839	7.016301	1.620265	H	1.247334	-9.113108	-3.001599

[9]CN (TS_{rac})

C	-5.473779	2.671275	-1.652415	C	4.810170	-4.866616	-0.906949	C	-2.567023	5.920103	-1.130297
C	-6.176619	1.461863	-1.738214	C	5.826464	-3.846468	-0.894251	C	-3.868451	5.307700	-1.206320
C	-6.834691	0.852317	-0.664537	C	5.841306	-2.870302	0.160860	C	-3.387825	4.078944	0.825641
C	-7.098321	1.776910	0.439976	C	5.011600	-3.085645	1.252213	C	-2.123787	4.688215	0.906652
C	-6.281856	2.967529	0.580526	C	4.017526	-4.078691	1.238060	C	-4.237994	4.300389	-0.248318
C	-6.868767	-0.672946	-0.667488	C	6.441451	-1.514842	0.019201	C	-5.364886	3.353510	-0.453506
C	-6.246029	-1.310668	-1.745856	C	6.118378	-0.782809	-1.114686	C	-8.174031	1.663787	1.357531
C	-5.580207	-2.541208	-1.657920	C	6.141644	0.623292	-1.114305	C	-6.473233	3.819804	1.701940
C	-5.480036	-3.217302	-0.454465	C	6.488681	1.343648	0.020039	C	-7.475518	3.602951	2.619152
C	-6.382348	-2.800917	0.581281	C	7.085347	0.623333	1.112443	C	-8.363615	2.532769	2.412412
C	-7.164219	-1.588262	0.436830	C	7.061419	-0.815273	1.112091	C	-4.759622	5.740997	-2.225952
C	-4.377153	-4.191158	-0.247500	C	5.931991	2.717431	0.162739	C	-2.226225	6.913892	-2.088309
C	-4.032846	-5.210596	-1.202315	C	5.945871	3.693114	-0.892828	C	-4.396537	6.712296	-3.132666
C	-2.745866	-5.852875	-1.125996	C	4.959511	4.742151	-0.906810	C	-3.114630	7.302080	-3.066214
C	-1.827363	-5.486037	-0.085561	C	3.969765	4.801324	0.134925	C	-0.100369	6.975888	2.073324
C	-2.271681	-4.625884	0.906914	C	4.145338	3.980259	1.239503	C	2.677062	6.670529	2.159160
C	-3.520914	-3.986984	0.825162	C	5.110072	2.958652	1.254573	C	0.616890	7.472320	3.139126
C	-0.369346	-5.796808	-0.130086	C	2.645269	5.463111	-0.029706	C	2.020911	7.321109	3.180817
C	0.357263	-5.358658	-1.225957	C	1.917008	5.177754	-1.176071	C	5.000763	5.695702	-1.959624
C	1.756032	-5.219525	-1.174575	C	0.522255	5.352363	-1.227977	C	6.913184	3.656980	-1.932835
C	2.477202	-5.522451	-0.028244	C	-0.193285	5.809795	-0.132685	C	5.959624	5.633561	-2.947253
C	1.787113	-6.185730	1.044782	C	0.542720	6.308983	0.994977	C	6.925690	4.603240	-2.934249
C	0.354020	-6.312924	0.998137	C	1.972091	6.145268	1.042226	C	7.699531	1.291145	2.205657
C	3.819145	-4.896274	0.134810	C	-1.658418	5.534809	-0.087845	C	7.652861	-1.503661	2.205070

C	8.272401	0.589832	3.244384	H	3.424210	4.017885	2.049826	H	8.753333	1.123695	4.059594
C	8.248750	-0.822313	3.244117	H	5.094411	2.248339	2.075064	H	8.711537	-1.372285	4.059122
C	6.794036	-3.839262	-1.934689	H	2.405746	4.674451	-2.004475	H	7.569620	-3.079838	-1.914653
C	4.823826	-5.822258	-1.958604	H	-0.015203	4.988167	-2.098670	H	4.070005	-6.603332	-1.958226
C	6.778806	-4.786456	-2.935178	H	-3.653947	3.330687	1.565977	H	7.541050	-4.770614	-3.709513
C	5.783650	-5.788738	-2.946632	H	-1.454207	4.395388	1.709861	H	5.782670	-6.542317	-3.729582
C	2.478706	-6.727647	2.162132	H	-8.936947	0.929327	1.176203	H	3.561281	-6.653563	2.187481
C	-0.305643	-6.961591	2.077604	H	-5.839850	4.696024	1.790285	H	-1.385204	-7.066525	2.037111
C	1.806400	-7.359702	3.184894	H	-7.615386	4.285023	3.453185	H	2.360434	-7.780347	4.019766
C	0.398940	-7.474747	3.143916	H	-9.223315	2.401496	3.064100	H	-0.127052	-7.980891	3.948939
C	-2.429625	-6.857472	-2.081132	H	-5.753367	5.307025	-2.266447	H	-1.464691	-7.349814	-2.014268
C	-4.935627	-5.627286	-2.218594	H	-1.250235	7.383992	-2.021778	H	-5.919375	-5.171076	-2.258687
C	-3.328339	-7.228518	-3.056267	H	-5.102866	7.035117	-3.892819	H	-3.068369	-8.009712	-3.765521
C	-4.596611	-6.609974	-3.122396	H	-2.835645	8.074612	-3.777730	H	-5.311692	-6.919430	-3.879915
H	-4.873194	2.974018	-2.504468	H	-1.176827	7.108723	2.032300	H	-6.107920	-0.793161	-2.684359
H	-6.041111	0.932848	-2.670364	H	3.757348	6.568395	2.185010	H	-4.997101	-2.867665	-2.513314
H	-1.594751	-4.346953	1.708887	H	0.103849	7.993022	3.943223	C	-8.245857	-1.448019	1.343628
H	-3.768238	-3.230082	1.563213	H	2.585284	7.728465	4.015356	C	-6.599796	-3.643957	1.704748
H	-0.171080	-4.982190	-2.097012	H	4.269546	6.497992	-1.960491	C	-8.464147	-2.310102	2.398791
H	2.257335	-4.730143	-2.003821	H	7.666676	2.875632	-1.911818	H	-9.327201	-2.159344	3.041754
H	5.016573	-2.374297	2.071948	H	5.980454	6.385960	-3.731064	C	-7.601467	-3.398931	2.615865
H	3.295373	-4.094627	2.048188	H	7.687530	4.564799	-3.708187	H	-7.762748	-4.074614	3.451220
H	5.671925	-1.288800	-1.965074	H	7.730940	2.376376	2.198264	H	-8.994263	-0.701134	1.148219
H	5.712083	1.144147	-1.964398	H	7.647968	-2.589301	2.197151	H	-5.989886	-4.536192	1.798072

1,1'-binaphtyl (C)

C	-0.826504	1.508873	1.424336	C	-4.042065	-1.197330	-1.406505	C	4.163638	0.055520	-0.649005
C	-0.664492	0.344611	0.693680	C	-2.792524	-1.856132	-1.495876	C	3.163866	-1.665019	0.827289
C	-1.785175	-0.195376	-0.022042	H	-5.118327	0.460913	-0.579264	C	2.792528	1.856128	-1.495879
C	-3.050701	0.478926	0.055275	H	-4.901498	-1.593698	-1.940568	H	0.740302	1.877983	-0.898719
C	-3.163869	1.665020	0.827284	H	-2.699441	-2.752559	-2.103184	H	2.163172	-3.080232	2.083580
C	-2.073274	2.172017	1.493736	C	0.664492	-0.344605	0.693681	C	4.042068	1.197324	-1.406505
H	-0.740298	-1.877982	-0.898715	C	1.785176	0.195378	-0.022041	H	5.118327	-0.460919	-0.579260
H	0.023593	1.913690	1.966834	C	0.826501	-1.508868	1.424339	H	4.127771	-2.165862	0.879526
C	-1.694947	-1.368465	-0.822254	C	3.050701	-0.478927	0.055278	H	2.699448	2.752554	-2.103189
C	-4.163637	-0.055524	-0.649007	C	1.694951	1.368465	-0.822257	H	4.901502	1.593690	-1.940569
H	-4.127776	2.165860	0.879520	C	2.073269	-2.172014	1.493741				
H	-2.163178	3.080235	2.083574	H	-0.023599	-1.913683	1.966836				

1,1'-binaphtyl (TS1)

C	-0.129958	1.594684	1.598327	C	-0.144256	0.748832	-0.833088	C	0.010609	-1.780705	0.193544
C	-0.010609	1.780705	0.193544	C	0.144256	-0.748832	-0.833088	C	0.129958	-1.594684	1.598327

C	-0.076384	-2.609391	2.510143	C	0.144256	3.155160	-0.226986	H	-0.864679	0.520362	-2.839885
C	-0.412236	-3.908637	2.079507	C	0.412566	4.171129	0.730943	H	0.497298	-0.656300	1.972525
C	-0.412566	-4.171129	0.730943	C	0.412236	3.908637	2.079507	H	0.052273	-2.404952	3.569850
C	-0.144256	-3.155160	-0.226986	C	0.076384	2.609391	2.510143	H	-0.603902	-4.698418	2.800413
C	0.065290	-3.528060	-1.578526	H	-0.497298	0.656300	1.972525	H	-0.573662	-5.182902	0.366008
C	0.500759	-2.584550	-2.471008	H	-0.052273	2.404952	3.569850	H	-0.046242	-4.571375	-1.862668
C	0.538036	-1.229081	-2.089921	H	0.603902	4.698418	2.800413	H	0.783205	-2.858286	-3.483852
C	-0.538036	1.229081	-2.089921	H	0.573662	5.182902	0.366008	H	0.864679	-0.520362	-2.839885
C	-0.500759	2.584550	-2.471008	H	0.046242	4.571375	-1.862668				
C	-0.065290	3.528060	-1.578526	H	-0.783205	2.858286	-3.483852				

1,1'-binaphtyl (TS2)

C	1.553106	-2.425353	-0.329419	C	1.771701	0.639740	-0.457874	H	-3.054961	3.926500	-0.187897
C	0.195884	-2.006774	-0.164871	C	2.006694	-3.692496	-0.021470	H	-1.503896	5.666708	0.738134
C	-0.381815	-0.661617	-0.388663	C	1.137001	-4.678243	0.476967	H	0.916047	5.117148	0.889774
C	0.381815	0.661617	-0.388663	C	-0.195884	-4.367502	0.570556	H	2.733707	3.747458	0.519819
C	-0.195884	2.006774	-0.164871	C	-0.695032	-3.081754	0.225975	H	3.702721	1.572608	-0.245793
C	-1.553106	2.425353	-0.329419	C	-2.101865	-2.912248	0.229122	H	3.054961	-3.926500	-0.187897
C	-2.006694	3.692496	-0.021470	C	-2.628596	-1.721258	-0.178143	H	1.503896	-5.666708	0.738134
C	-1.137001	4.678243	0.476967	C	-1.771701	-0.639740	-0.457874	H	-0.916047	-5.117148	0.889774
C	0.195884	4.367502	0.570556	H	-2.274677	0.269527	-0.703920	H	-2.733707	-3.747458	0.519819
C	0.695032	3.081754	0.225975	H	2.274677	-0.269527	-0.703920	H	-3.702721	-1.572608	-0.245793
C	2.101865	2.912248	0.229122	H	2.289306	-1.788058	-0.783199				
C	2.628596	1.721258	-0.178143	H	-2.289306	1.788058	-0.783199				

3'

C	-4.496994	1.979504	0.484664	C	3.965636	2.905230	0.486802	C	-0.235236	-6.450718	-1.198372
C	-3.325586	2.765497	0.493363	C	4.062337	1.497899	0.498857	C	-1.518330	-5.795788	-1.207794
C	-3.188530	3.877907	-0.313854	C	4.960672	0.822446	-0.303985	C	-1.766515	-4.700074	-0.311935
C	-4.264104	4.209214	-1.207053	C	5.787784	1.587477	-1.195745	C	-0.731678	-4.262347	0.491299
C	-5.473878	3.427347	-1.190407	C	5.713124	3.026069	-1.183026	C	0.535124	-4.882713	0.476429
C	-1.912944	4.655270	-0.256530	C	4.994662	-0.671050	-0.246665	C	-3.077496	-3.984275	-0.249463
C	-1.852162	6.018137	0.191189	C	6.141555	-1.407206	0.205372	C	-3.121945	-2.647653	-0.597974
C	-0.590003	6.716502	0.200298	C	6.112930	-2.849463	0.213106	C	-4.322470	-1.911819	-0.556527
C	0.604509	6.021670	-0.190984	C	4.914953	-3.534492	-0.184897	C	-5.519212	-2.487027	-0.178072
C	0.503991	4.696699	-0.566186	C	3.820634	-2.782964	-0.564403	C	-5.522565	-3.868467	0.214548
C	-0.733548	4.024771	-0.605142	C	3.859639	-1.375281	-0.601247	C	-4.287049	-4.612892	0.201665
C	2.818303	6.419564	1.042580	C	4.126493	-5.520169	-1.483299	C	-6.970592	-0.764959	1.051945
C	4.060418	5.767219	0.988412	C	2.982997	-6.202109	-1.534752	C	-7.025530	0.636776	0.992496
C	3.887312	5.684102	-1.525612	C	2.960716	-6.403200	0.978265	C	-6.869706	0.519245	-1.520948
C	2.724086	6.332280	-1.480419	C	4.147335	-5.655116	1.039252	C	-6.850666	-0.812012	-1.470790
C	4.777363	3.682833	-0.313171	C	0.801698	-5.972404	-0.326884	C	-5.576312	2.292208	-0.315957

C	-4.159352	5.284636	-2.132312	C	4.338641	6.086956	3.390326	H	-7.592437	-6.351041	1.364494
C	-6.528712	3.813535	-2.066458	C	3.092575	6.716710	3.448742	H	-5.429559	-7.602779	1.424870
C	-6.399502	4.876027	-2.932649	H	-4.552492	1.123800	1.149337	H	-3.459792	-5.728679	-2.158333
C	-5.195652	5.612008	-2.976462	H	-2.517785	2.499655	1.169642	H	0.904304	-8.080321	-2.077943
C	-3.013887	6.698530	0.651972	H	1.399878	4.161109	-0.865918	H	-3.044924	-7.621606	-3.671530
C	-0.592731	8.080616	0.614700	H	-0.764288	2.991615	-0.940052	H	-0.853107	-8.819109	-3.599839
C	-1.742443	8.712975	1.031035	H	4.328181	5.443977	-2.490375	H	1.537090	-7.562028	2.097731
C	-2.966304	8.010060	1.063814	H	2.229470	6.614906	-2.408068	H	5.685794	-4.894286	2.342494
C	-7.270559	1.362346	2.169996	H	3.249647	3.382204	1.147749	H	2.679281	-7.272746	4.274284
C	-7.135160	-1.396275	2.296792	H	3.426204	0.931794	1.173700	H	4.768520	-5.904240	4.393017
C	-7.441529	0.727302	3.394031	H	2.909617	-3.289168	-0.869485	H	7.313439	-4.615281	0.632687
C	-7.365434	-0.666603	3.457674	H	2.982598	-0.830523	-0.939763	H	7.315894	0.340449	0.698228
C	-6.701283	-4.552157	0.633589	H	4.621742	-5.230219	-2.408342	H	9.293640	-3.408311	1.371169
C	-4.294722	-5.959641	0.661135	H	2.557205	-6.459653	-2.501802	H	9.298157	-0.909676	1.441833
C	-6.673387	-5.864145	1.049393	H	-0.903330	-3.430848	1.169328	H	6.702211	-0.125141	-2.149073
C	-5.453243	-6.573760	1.076708	H	1.306519	-4.503951	1.138654	H	6.556577	4.829768	-2.056712
C	-2.505785	-6.243098	-2.128785	H	-2.212642	-2.158084	-0.935626	H	8.138267	1.184417	-3.654879
C	-0.044353	-7.554976	-2.077931	H	-4.307388	-0.868481	-0.857175	H	8.079491	3.681163	-3.576622
C	-2.273544	-7.302324	-2.976003	H	-6.882425	1.017472	-2.487524	H	5.770844	5.116631	2.117232
C	-1.032548	-7.974294	-2.940197	H	-6.849922	-1.384992	-2.396394	H	1.382202	7.370630	2.337573
C	2.455058	-6.981102	2.154428	H	-3.235749	5.851527	-2.168032	H	4.936573	5.961312	4.289037
C	4.776304	-5.484820	2.284546	H	-7.459022	3.256500	-2.060540	H	2.704987	7.083812	4.395398
C	3.090462	-6.814434	3.378815	H	-7.223297	5.142662	-3.589398	C	-6.795686	-1.625632	-0.202777
C	4.259598	-6.051801	3.444138	H	-5.087739	6.436752	-3.675662	H	-7.653085	-2.309210	-0.240311
C	7.292459	-3.531256	0.633146	H	-3.954305	6.159566	0.678871	C	-6.844398	1.415953	-0.303572
C	7.310743	-0.743454	0.671458	H	0.334643	8.642419	0.614294	H	-7.702228	2.101087	-0.374847
C	8.413966	-2.853810	1.055399	H	-1.704720	9.753437	1.342522	C	1.989092	6.695433	-0.215207
C	8.419603	-1.442470	1.088367	H	-3.868731	8.504180	1.413295	H	1.826598	7.779709	-0.255981
C	6.671120	0.958199	-2.116221	H	-7.315058	2.447834	2.114434	C	4.649185	5.218820	-0.304928
C	6.576176	3.745577	-2.058739	H	-7.078587	-2.479297	2.353334	H	5.670723	5.621071	-0.375057
C	7.474473	1.691018	-2.959569	H	-7.631163	1.311531	4.290531	C	4.804962	-5.070368	-0.214283
C	7.435874	3.101613	-2.920172	H	-7.490300	-1.182141	4.406240	H	5.825053	-5.472469	-0.253511
C	4.807738	5.619800	2.168632	H	-7.650959	-4.029006	0.637499	C	2.194650	-6.632202	-0.318119
C	2.349210	6.879301	2.285125	H	-3.357968	-6.505069	0.683768	H	2.030275	-7.717391	-0.392615

4

C	1.573006	0.924597	-0.714631	H	1.651993	-0.524140	-2.389617	C	0.983952	2.722690	0.939365
C	-1.421100	0.498120	-1.073379	C	-0.847670	1.526798	-0.096966	H	2.055154	2.870167	1.057485
C	-0.355716	-0.177368	-1.898816	C	0.532911	1.722282	0.061783	C	-1.278971	3.312202	1.507245
H	-0.716704	-0.870174	-2.656939	C	-1.737001	2.329239	0.637832	H	-1.988678	3.920133	2.062149
C	0.954663	0.015325	-1.752000	H	-2.806358	2.172497	0.523768	C	0.096081	3.513674	1.658241

H	0.470536	4.282080	2.329358	H	3.783661	0.851006	-2.176028	H	-0.612313	-1.592087	0.383419
H	2.190031	1.665432	-1.243271	H	2.547483	-1.558184	3.156102	C	-5.916136	-1.484371	0.215496
H	-2.052398	1.049630	-1.780685	C	6.494665	-0.881130	-1.079053	C	-3.813984	-2.519668	0.993213
C	2.524554	0.103768	0.173531	H	6.635976	-1.951185	0.771633	C	-5.857420	0.489752	-1.166872
C	3.852774	-0.210393	-0.275517	H	4.850830	-2.115200	2.421481	H	-3.954708	1.278396	-1.672147
C	2.094289	-0.392753	1.389131	H	6.051120	0.276337	-2.858619	H	-1.917341	-3.313762	1.589188
C	4.696157	-1.023072	0.558640	H	7.503278	-1.130653	-1.397065	C	-6.588065	-0.509414	-0.483347
C	4.390113	0.240729	-1.515398	C	-2.308812	-0.542454	-0.369134	H	-6.465153	-2.258515	0.746833
C	2.926458	-1.193288	2.205165	C	-3.743093	-0.498184	-0.428179	H	-4.397969	-3.275578	1.512890
H	1.093979	-0.152917	1.735928	C	-1.697471	-1.552623	0.350661	H	-6.386724	1.261484	-1.719410
C	6.012648	-1.336721	0.125958	C	-4.495964	-1.509999	0.266429	H	-7.674237	-0.503142	-0.512269
C	4.202097	-1.502189	1.800314	C	-4.480285	0.493571	-1.139138				
C	5.670886	-0.083729	-1.906331	C	-2.440475	-2.538995	1.035059				

ternaphtyl (5)

C	0.705167	0.343651	-1.377840	C	3.702947	0.648814	-0.159662	C	-3.703007	0.648792	-0.159654
C	1.428163	-0.461237	-0.517053	C	3.564899	-1.570502	-1.145299	C	-3.564897	-1.570773	-1.144726
C	0.719543	-1.290427	0.414273	C	5.130009	0.607079	-0.314817	C	-5.130068	0.606970	-0.314808
C	-0.719425	-1.290440	0.414373	C	3.125104	1.801504	0.442204	C	-3.125225	1.801636	0.441984
C	-1.428182	-0.461267	-0.516878	C	4.970517	-1.609261	-1.291112	C	-4.970509	-1.609616	-1.290525
C	-0.705295	0.343633	-1.377754	H	2.970978	-2.416756	-1.479877	H	-2.970949	-2.417084	-1.479110
H	2.483307	-2.099348	1.372711	C	5.905891	1.717400	0.115934	C	-5.905997	1.717369	0.115661
H	1.235020	0.974650	-2.086266	C	5.736855	-0.540806	-0.888932	C	-5.736879	-0.541077	-0.888631
C	1.398760	-2.105091	1.363312	C	3.907262	2.857793	0.852924	C	-3.907428	2.857993	0.852440
C	-1.398475	-2.105082	1.363554	H	2.049537	1.837814	0.578436	H	-2.049668	1.838006	0.578266
H	-1.235244	0.974601	-2.086136	H	5.437995	-2.486454	-1.730213	H	-5.437960	-2.486936	-1.729402
C	-0.706545	-2.883019	2.263353	C	5.312075	2.820077	0.684871	C	-5.312234	2.820202	0.684349
C	0.706985	-2.883034	2.263225	H	6.985308	1.676424	-0.011237	H	-6.985410	1.676322	-0.011521
H	-2.483018	-2.099328	1.373163	H	6.818258	-0.560158	-1.002323	H	-6.818281	-0.560488	-1.002024
H	-1.247934	-3.493331	2.981333	H	3.443789	3.726842	1.312266	H	-3.443995	3.727154	1.311612
H	1.248496	-3.493367	2.981095	H	5.918258	3.661272	1.010221	H	-5.918452	3.661453	1.009486
C	2.922261	-0.472362	-0.600064	C	-2.922279	-0.472467	-0.599783				

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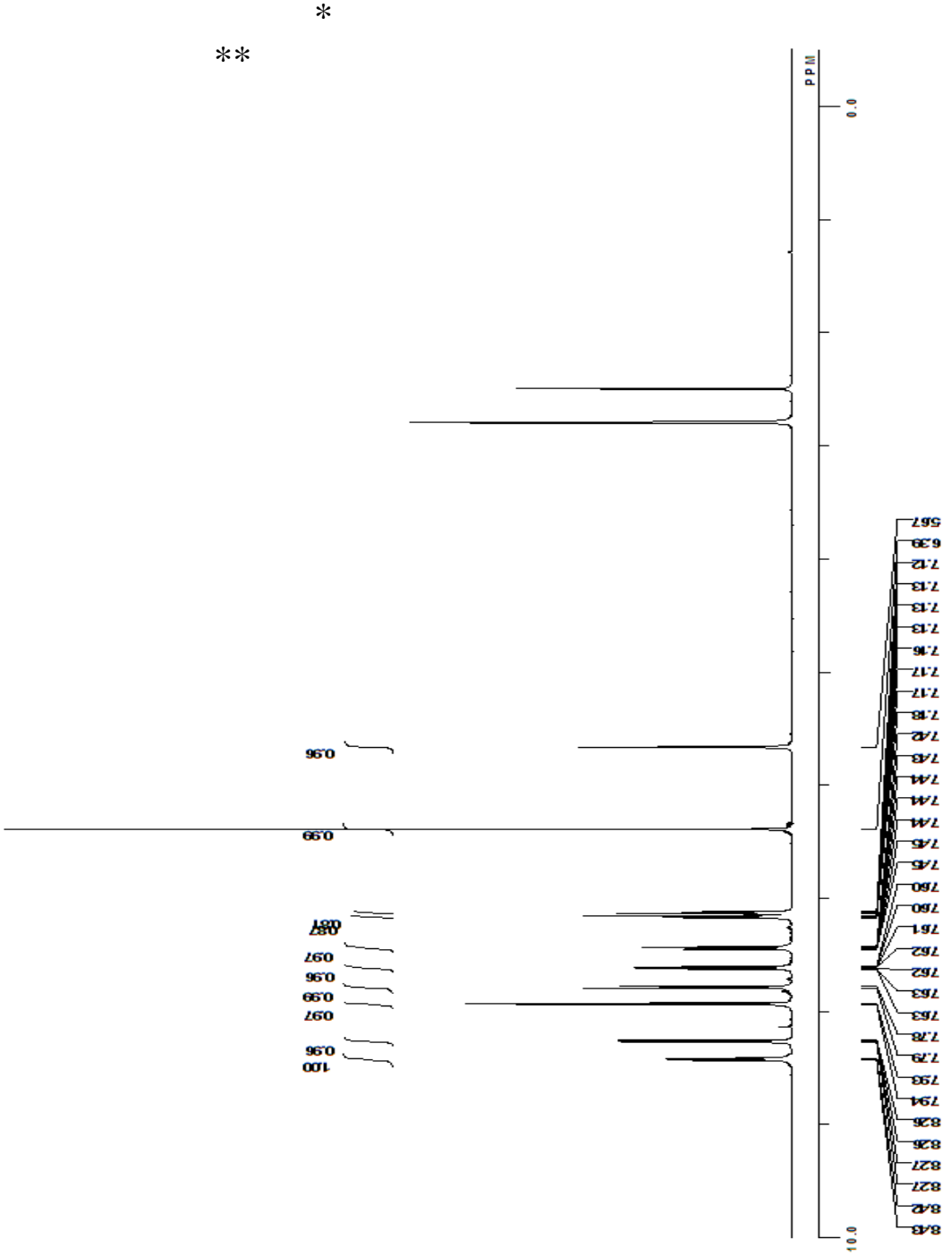
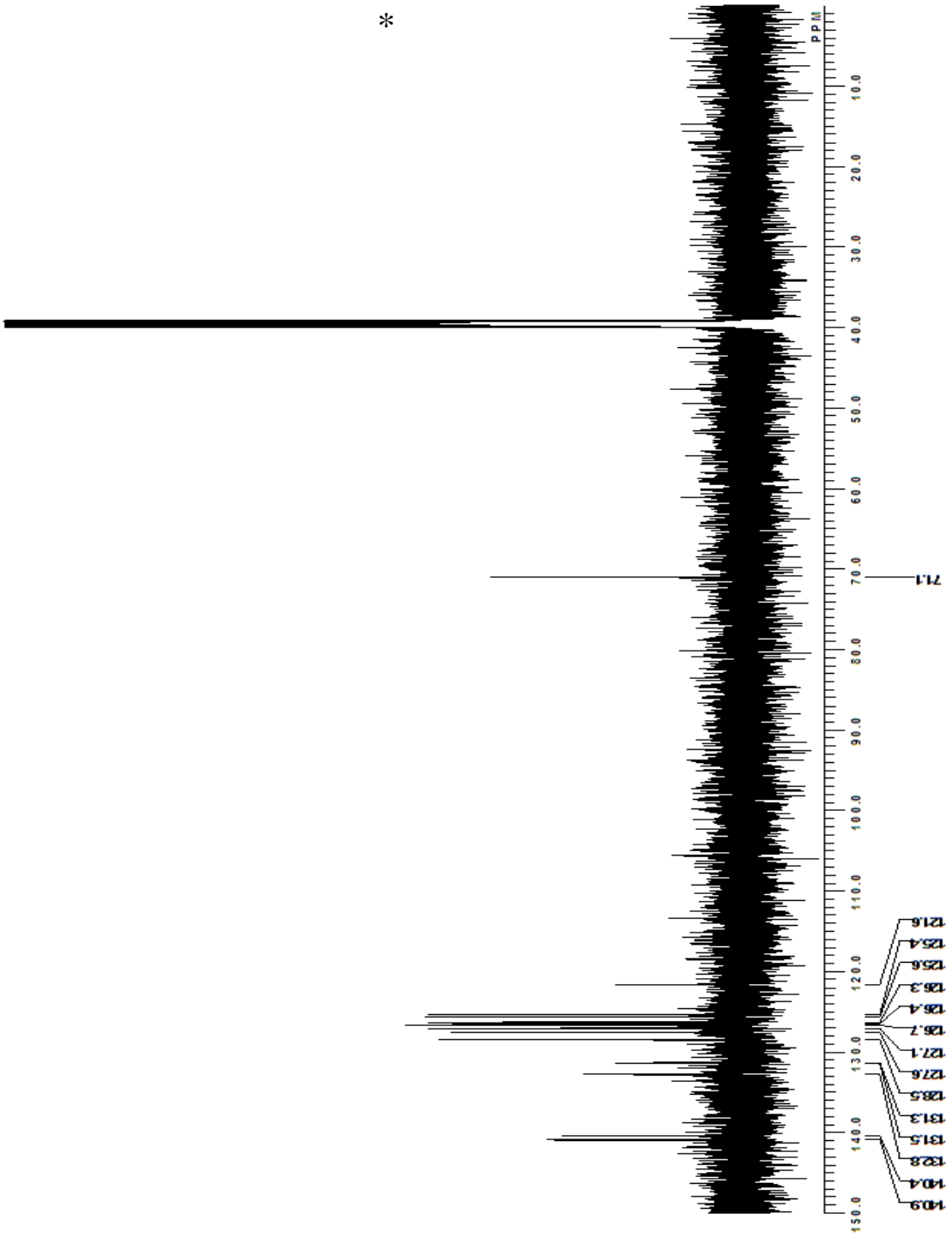
7. ^{1}H and ^{13}C NMR Spectra, and Mass Spectra of Products

^{1}H NMR spectrum of *cis*-**1** (600 MHz, DMSO-d_6, 150 °C)



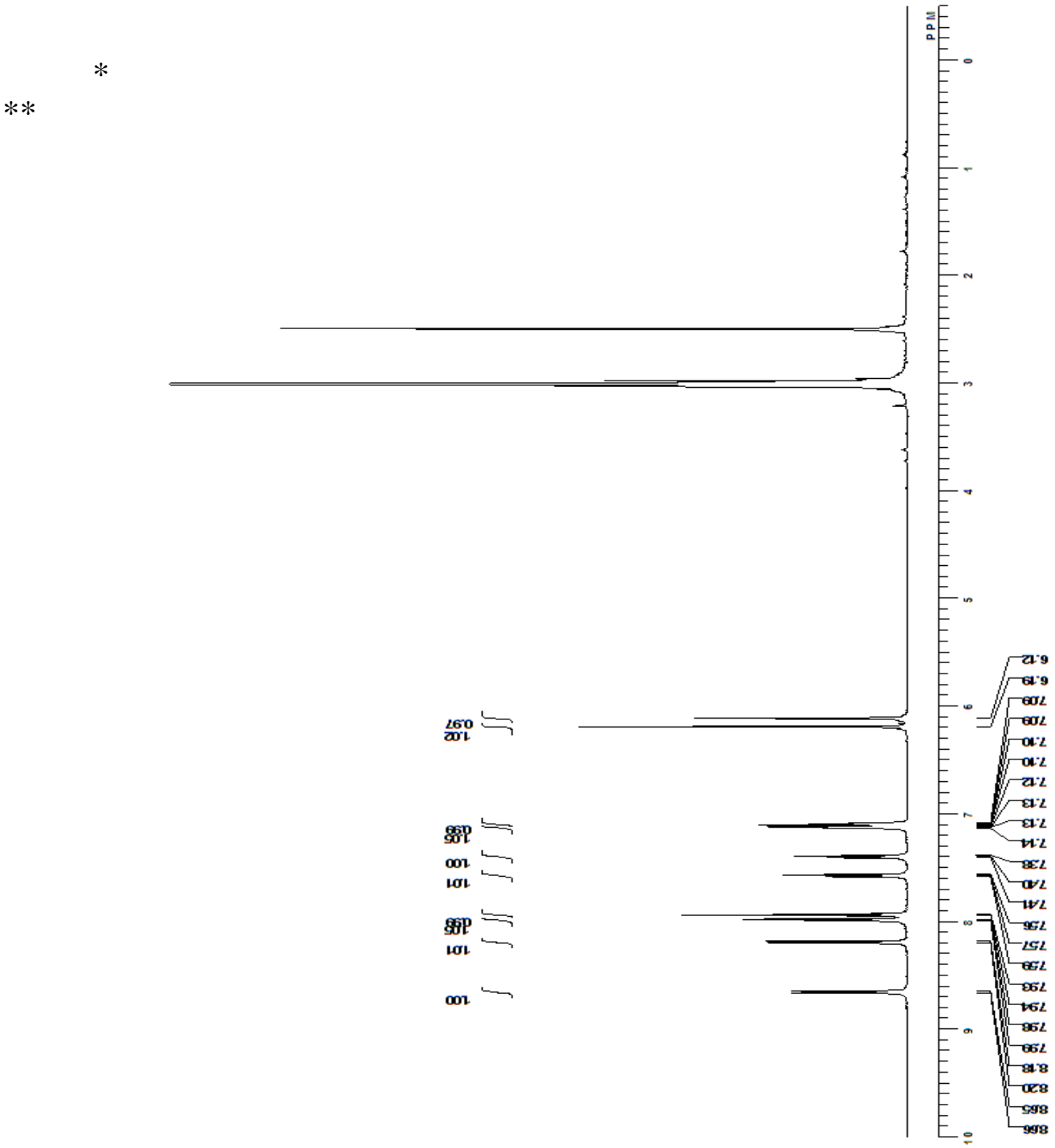
*: DMSO-d_5, **: H_2O

^{13}C NMR spectrum of *cis*-**1** (150 MHz, DMSO-d_6, 120 °C)



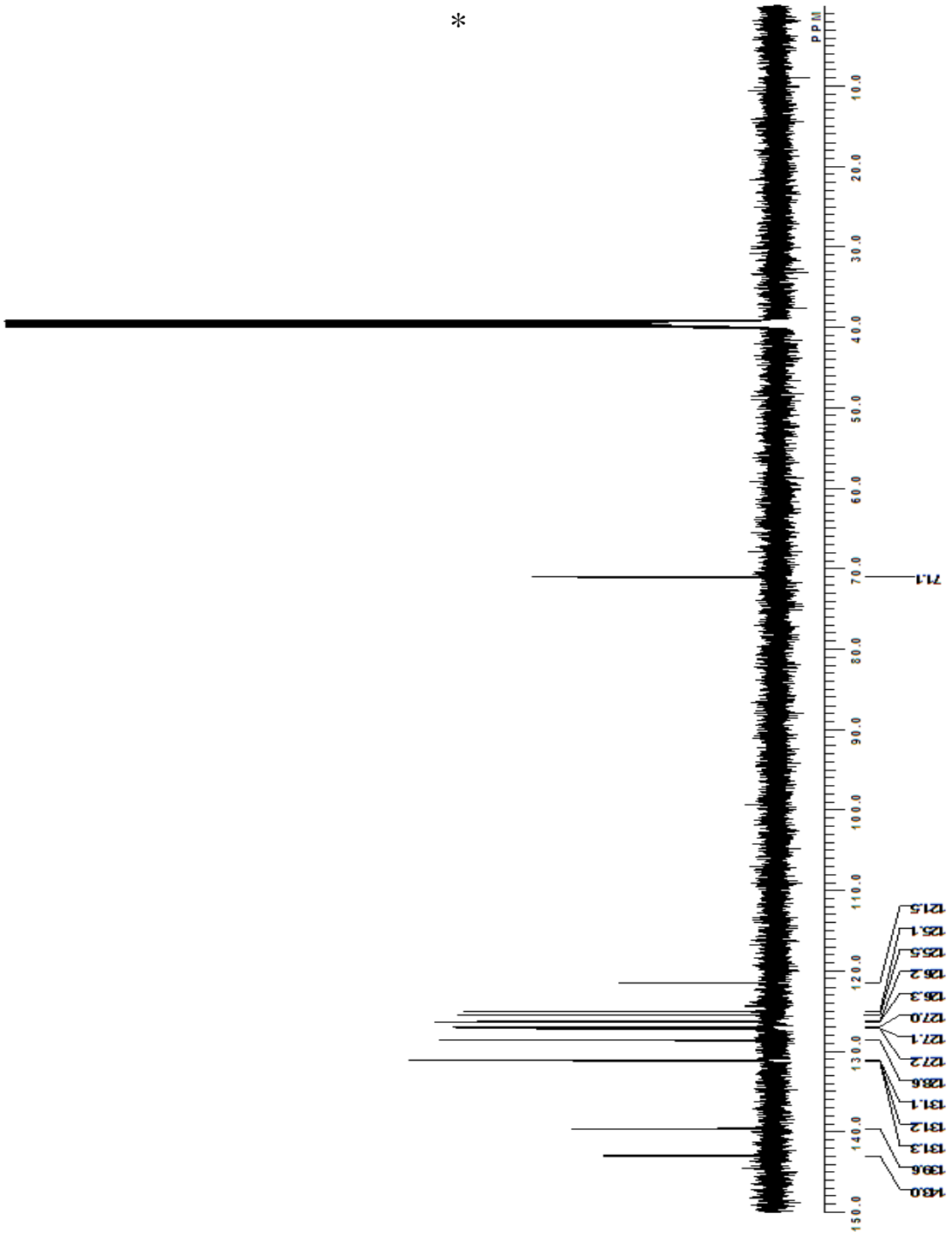
*: DMSO-d_6,

^{1}H NMR spectrum of *trans*-**1** (600 MHz, DMSO-d_6, 100 °C)



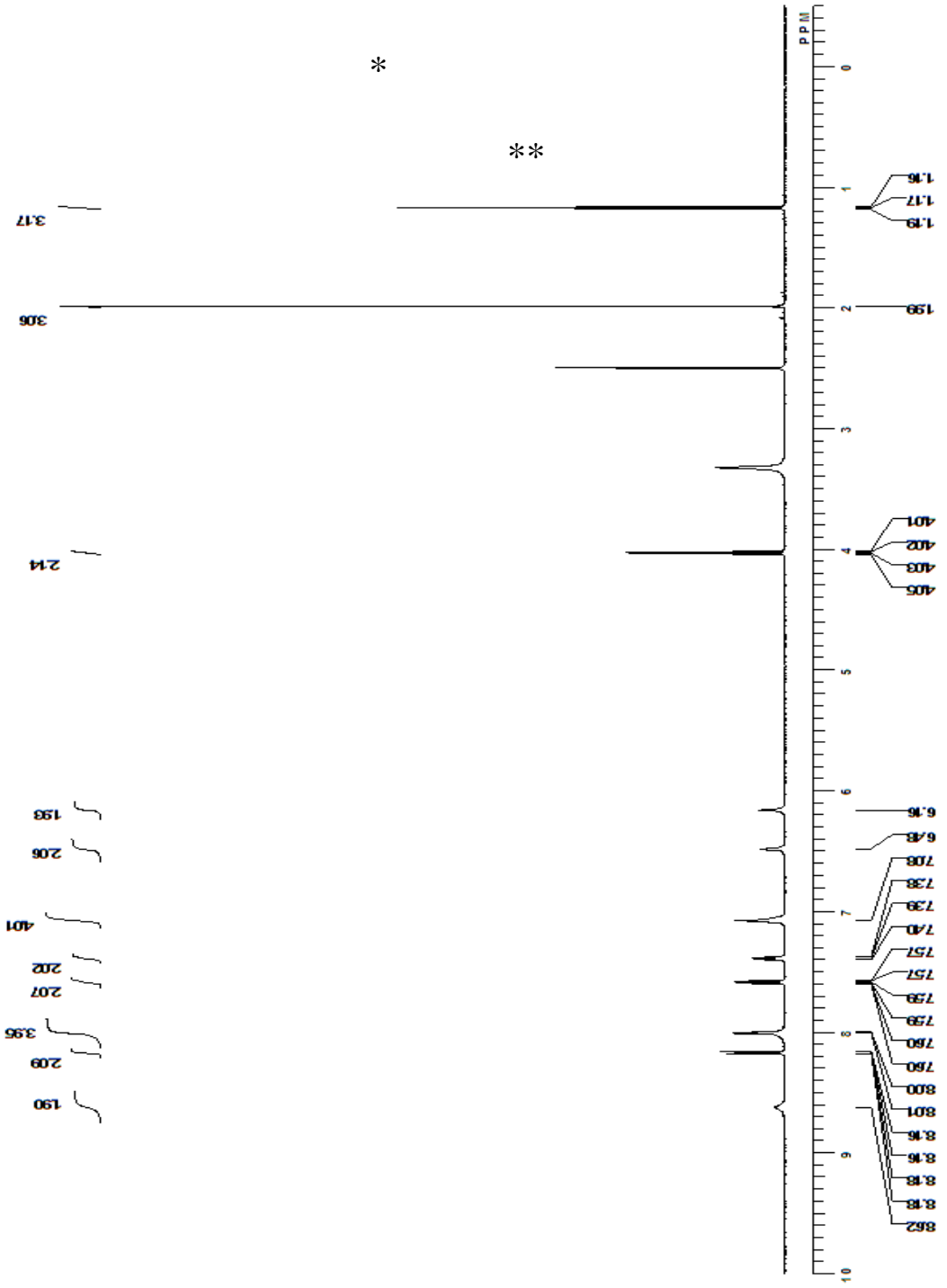
*: DMSO-d_5, **: H_2O

^{13}C NMR spectrum of *trans*-**1** (150 MHz, DMSO-d_6, 100 °C)



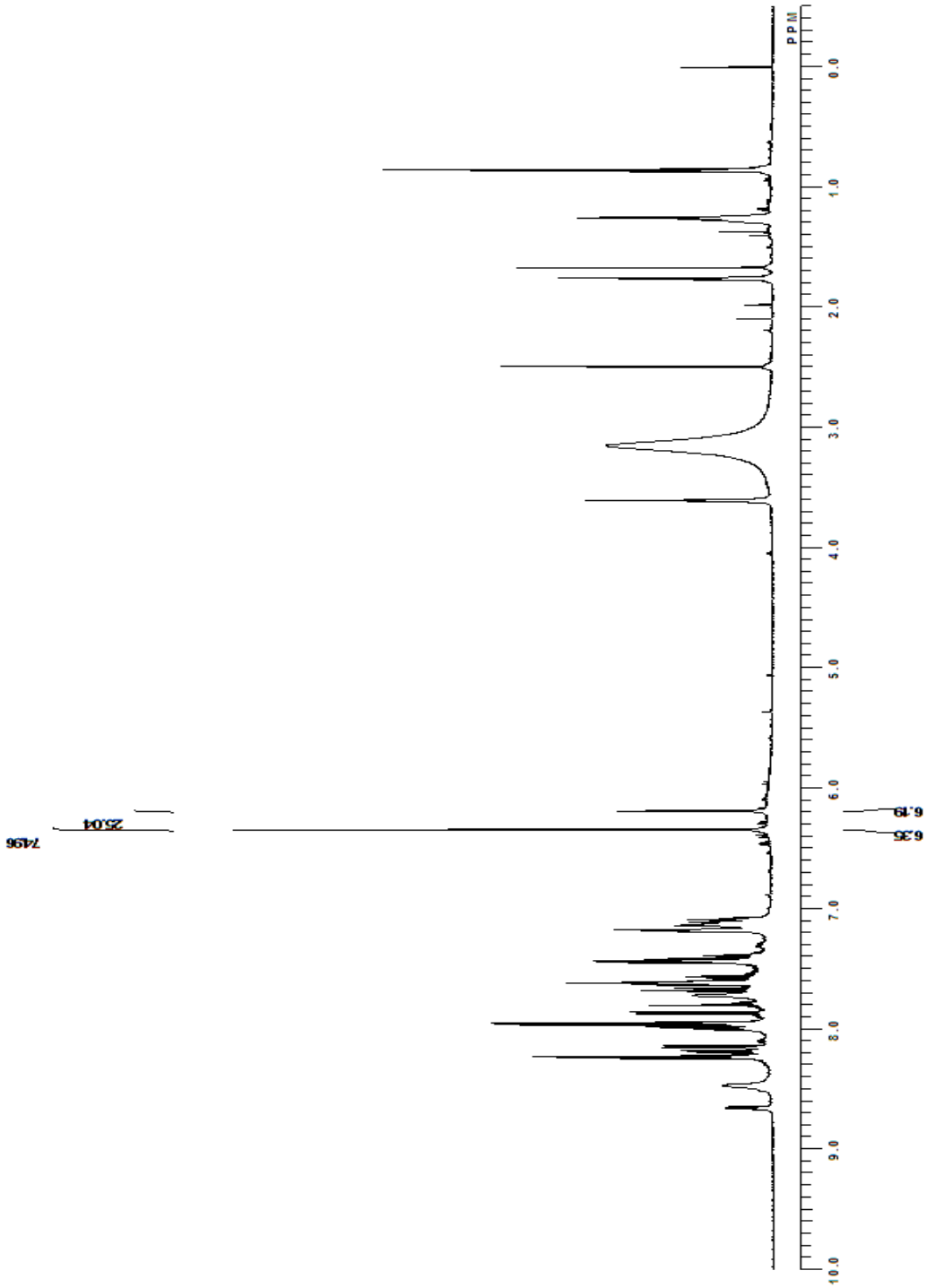
*: DMSO-d_6,

^{1}H NMR spectrum of single crystal of *trans*-**1**·EtOAc (600 MHz, DMSO-d_6)

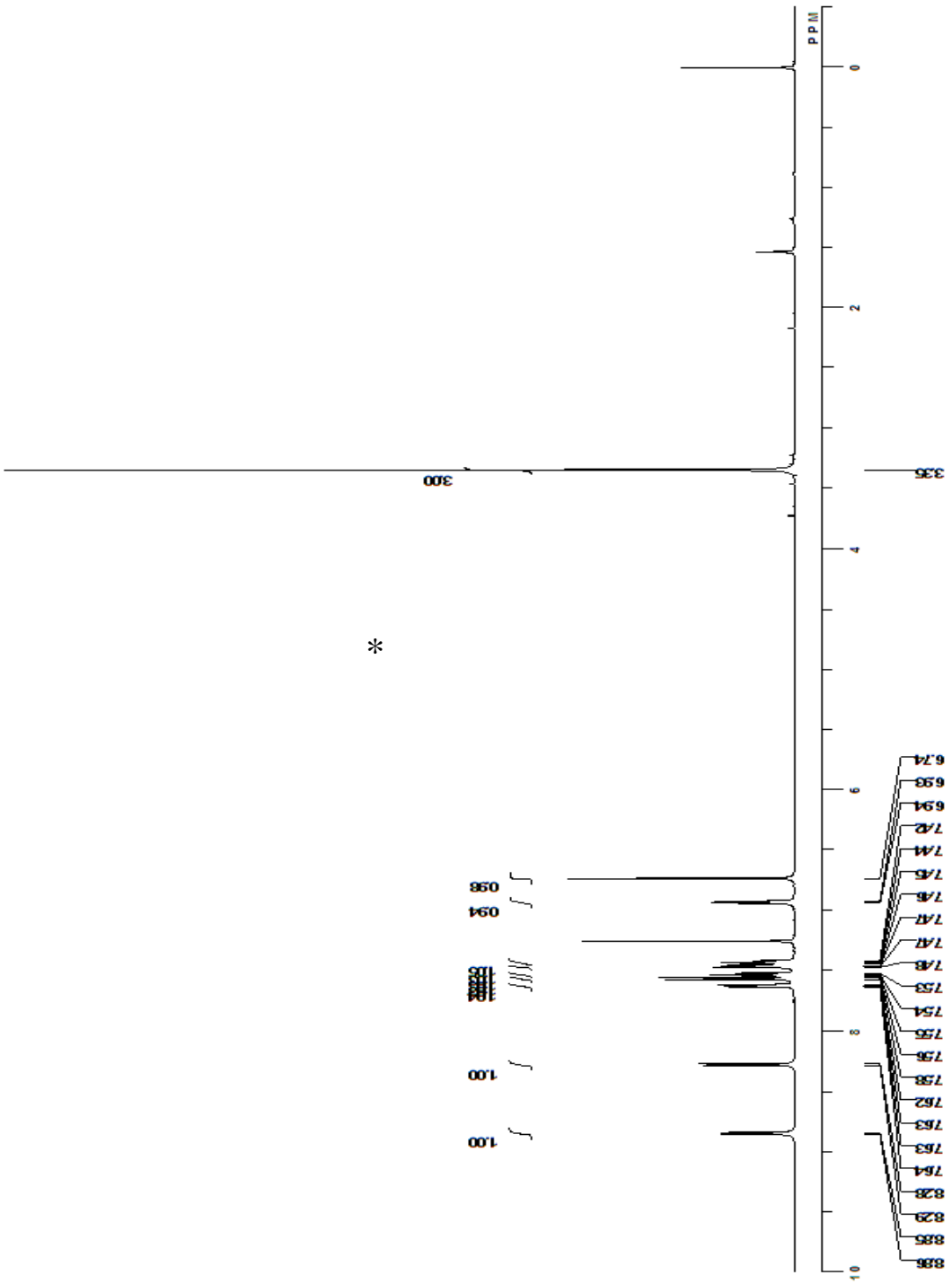


*: DMSO-d_5, **: H_2O

^{1}H NMR spectrum of crude product containing *cis*-**1** and *trans*-**1** (600 MHz, DMSO-d_6, 80 °C)



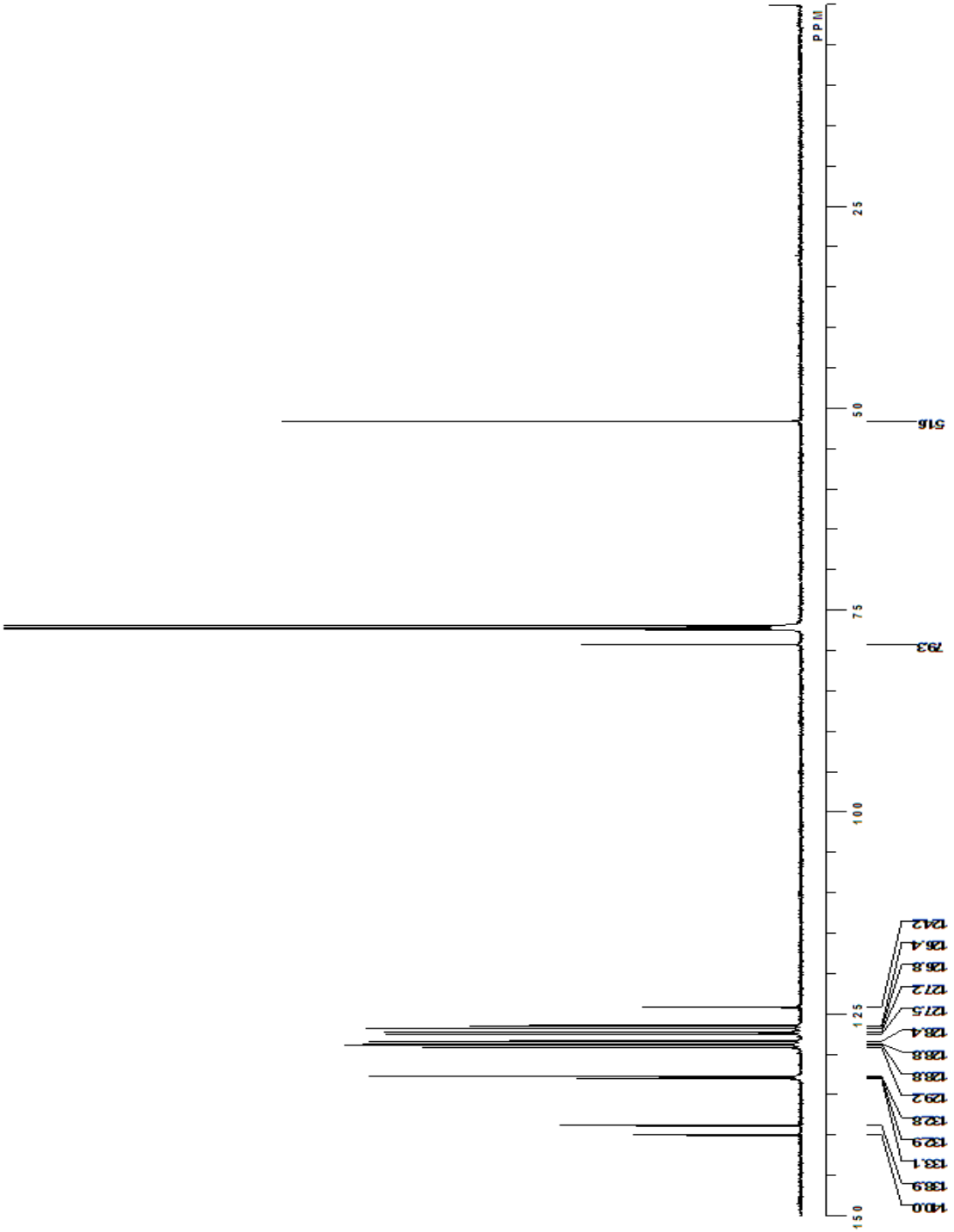
^{1}H NMR spectrum of **2** (600 MHz, $CDCl_3$)



*: $CHCl_3$

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

:



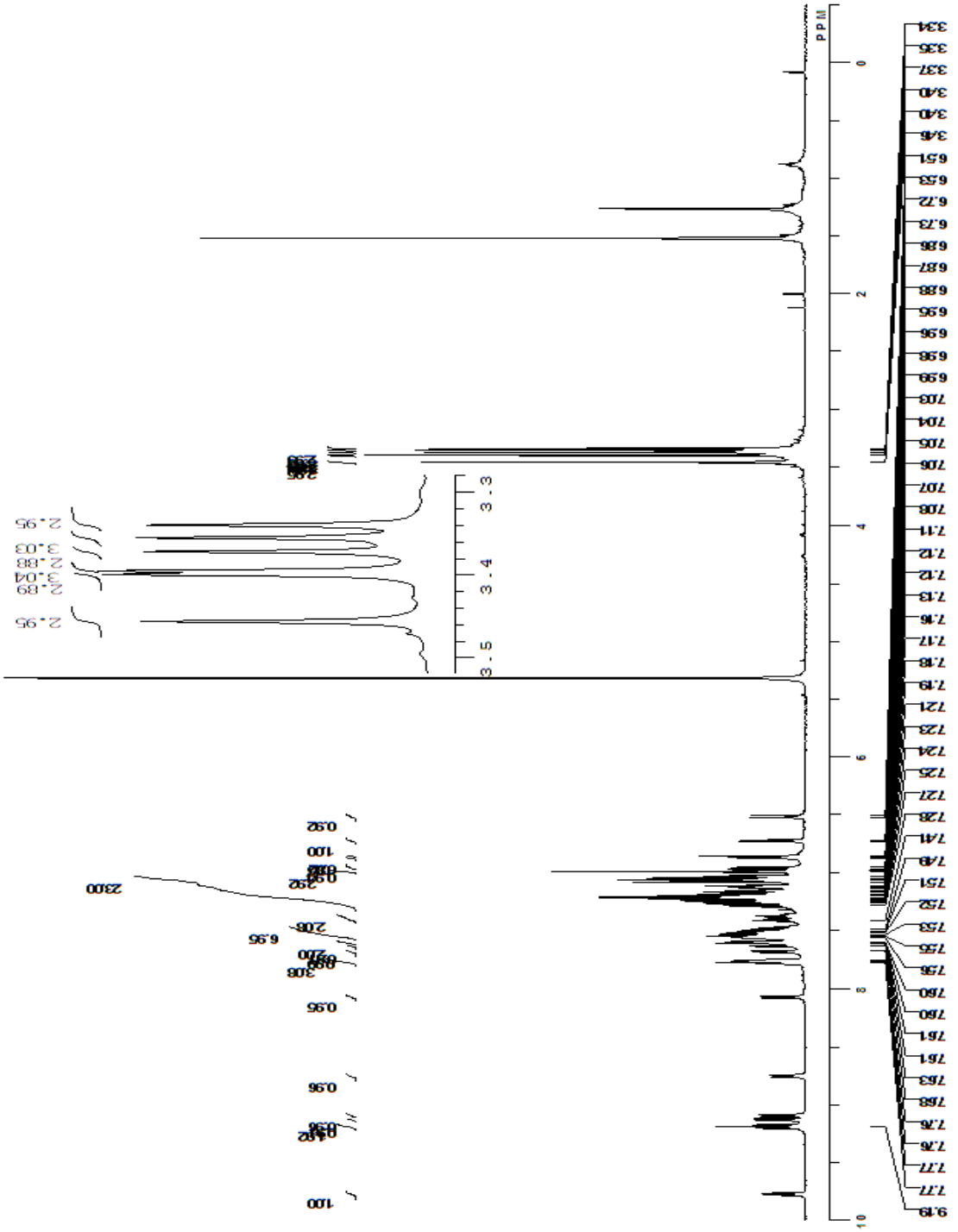
*: $CDCl_3$

***

^{1}H NMR spectrum of **3** (600 MHz, CD_2Cl_2)***

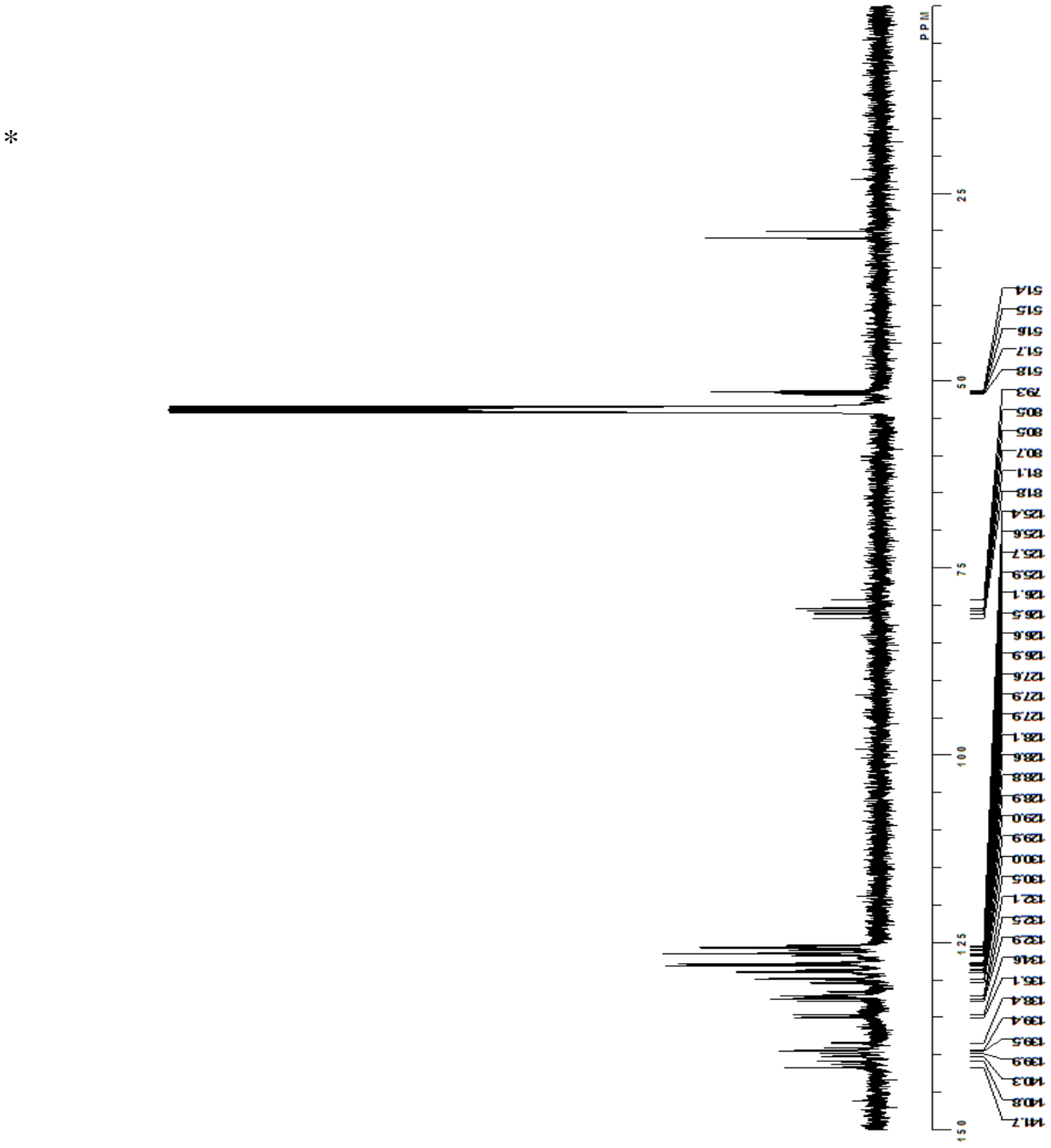
**

*



*: $CHDCl_2$, **: H_2O, ***: hexane

^{13}C NMR spectrum of **3** (600 MHz, CD_2Cl_2)



*: CD_2Cl_2, **: hexane

***

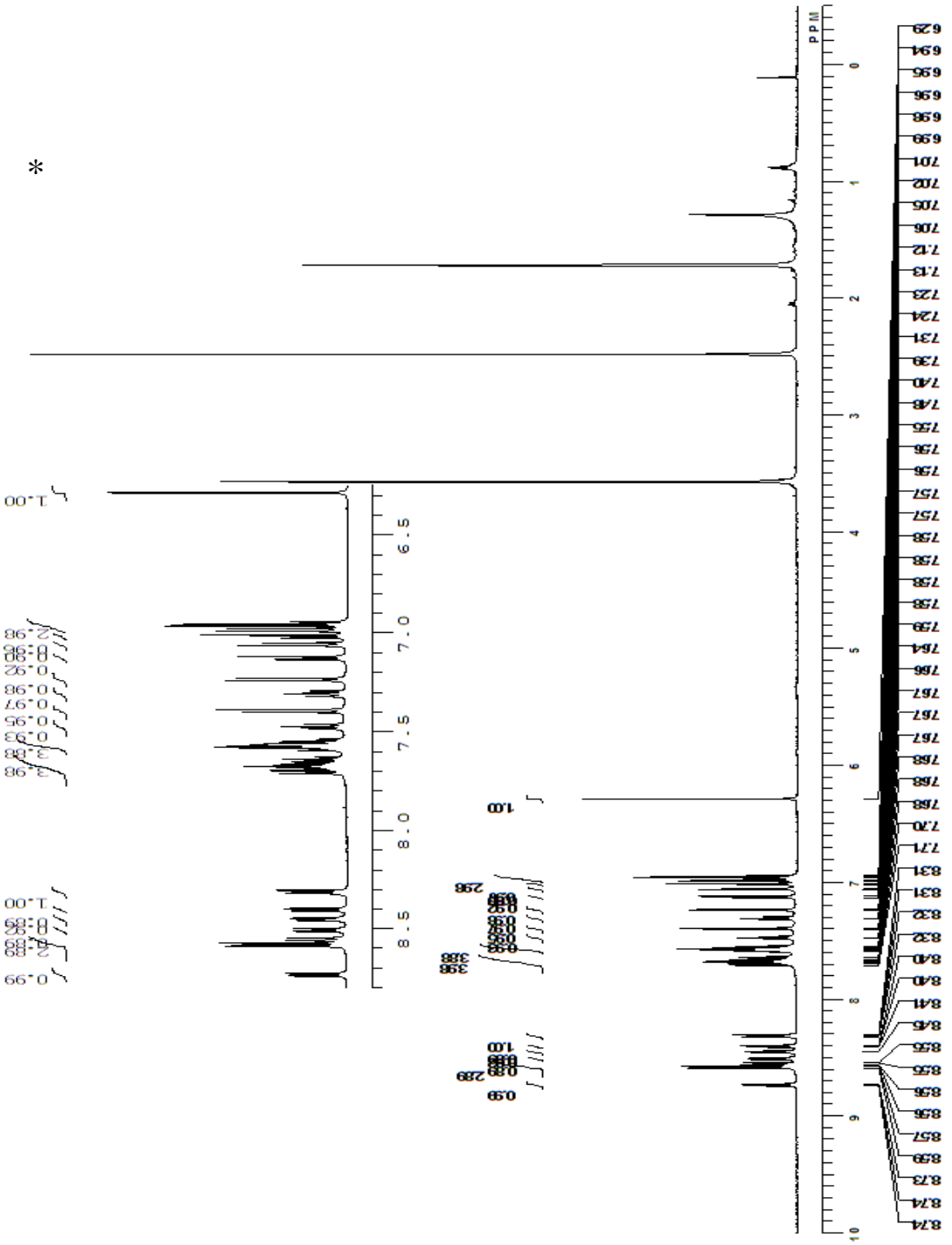
***

^{1}H NMR spectrum of **[9]CN** (600 MHz, THF-d_8)

**

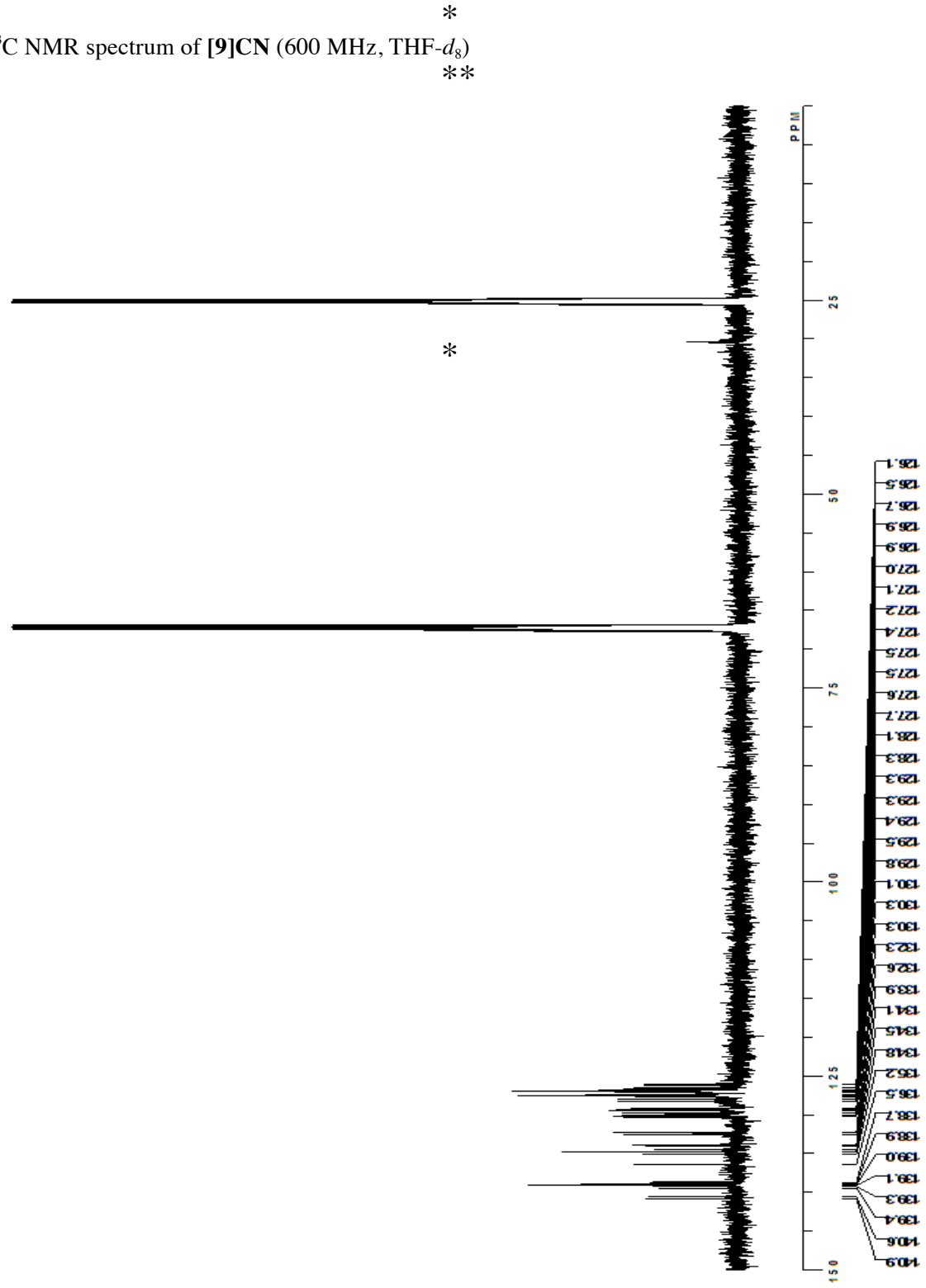
*

*



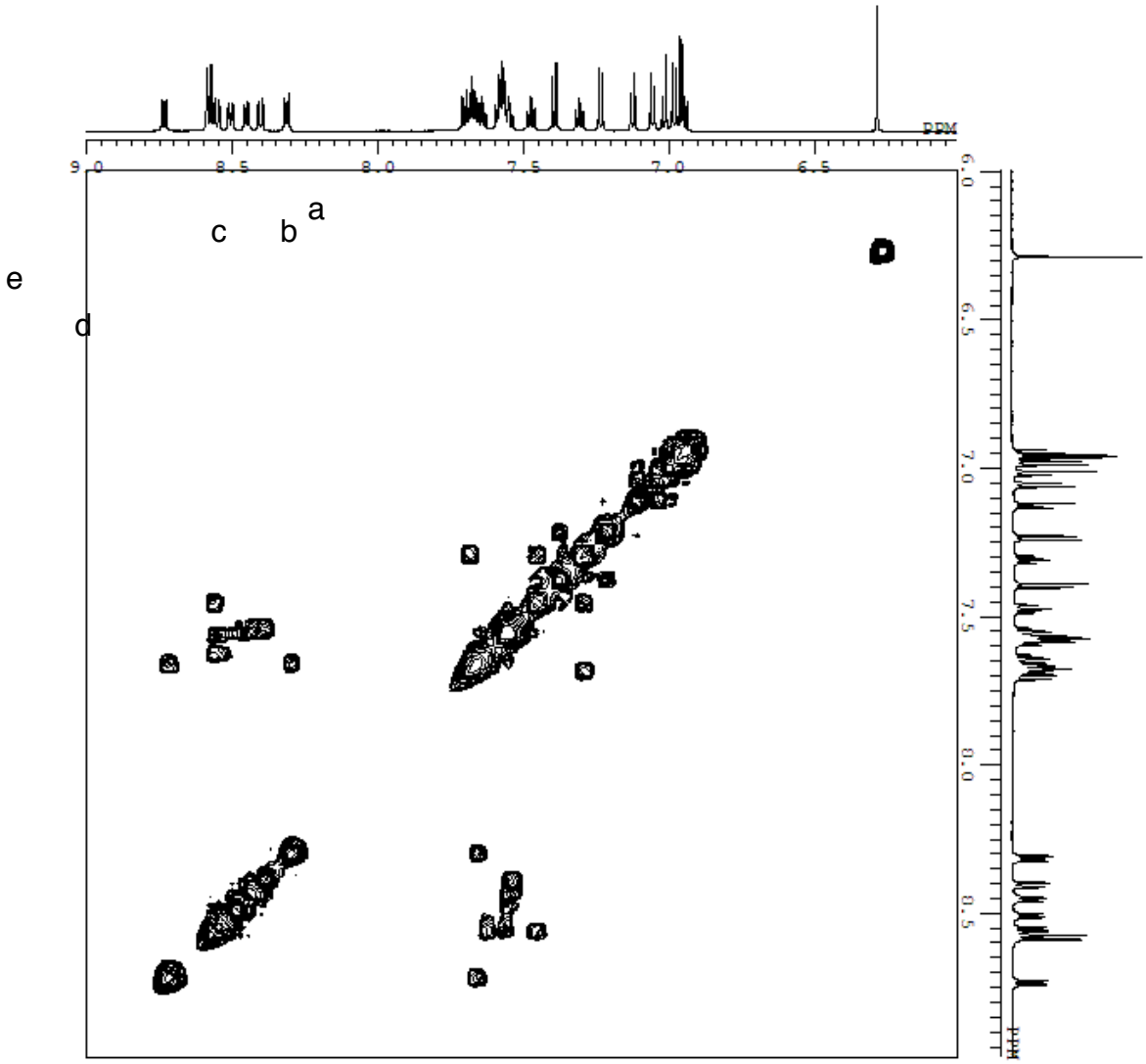
*: THF-d_7 **: H_2O, ***: hexane

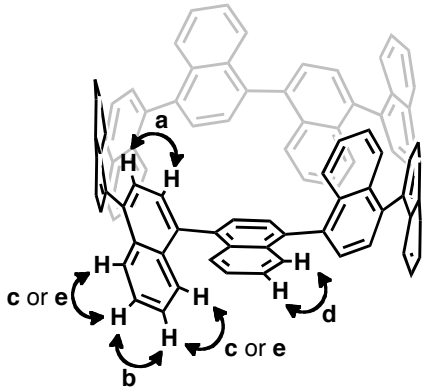
^{13}C NMR spectrum of **[9]CN** (600 MHz, THF-d_8)



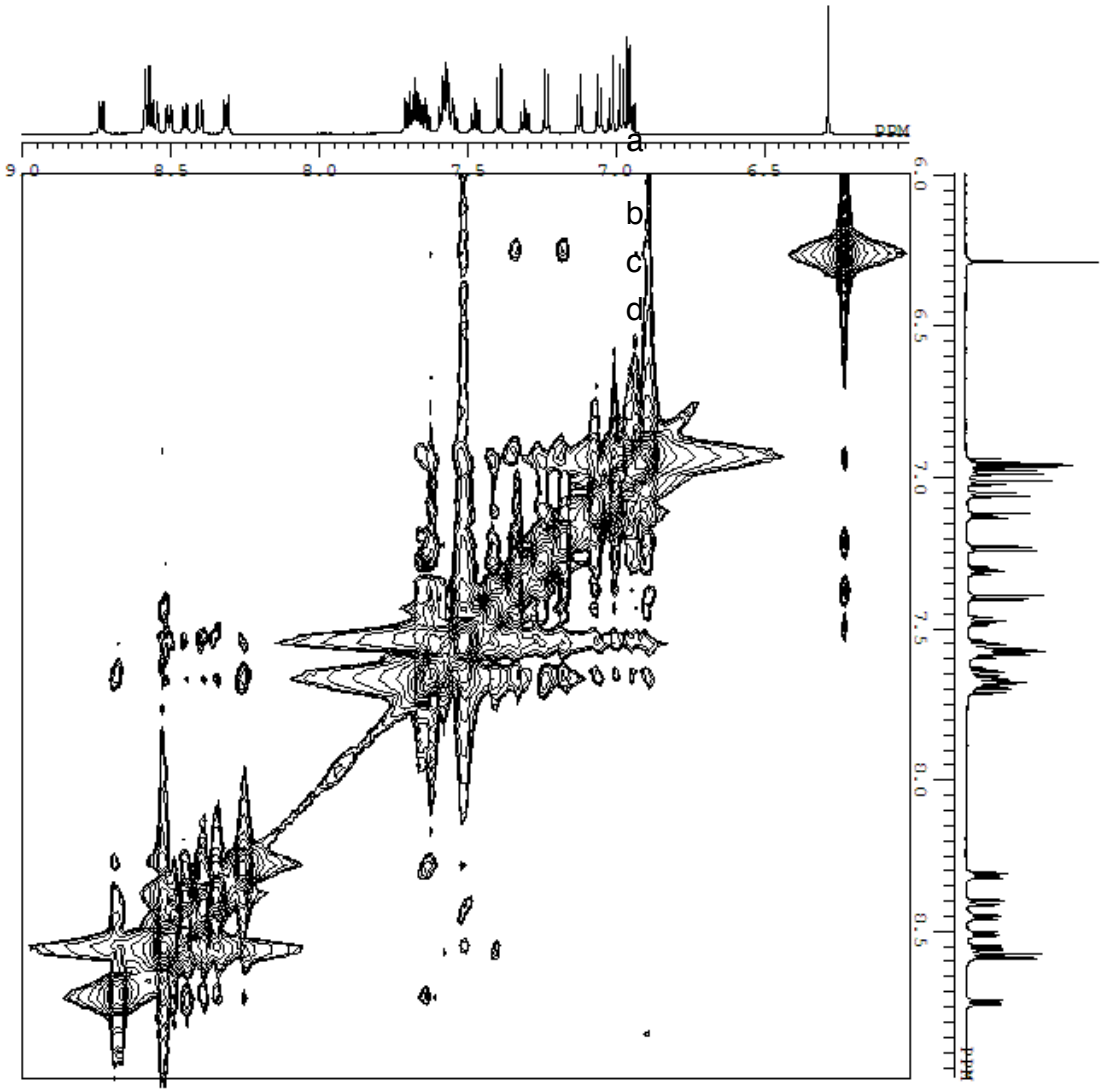
*: THF-d_6, **: hexane

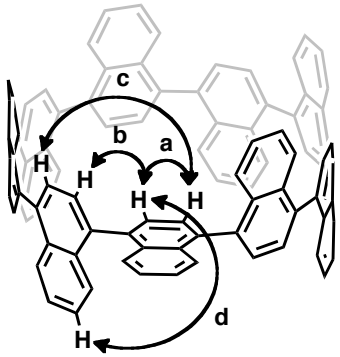
HH COSY spectrum of **[9]CN** (600 MHz, THF-d_8)



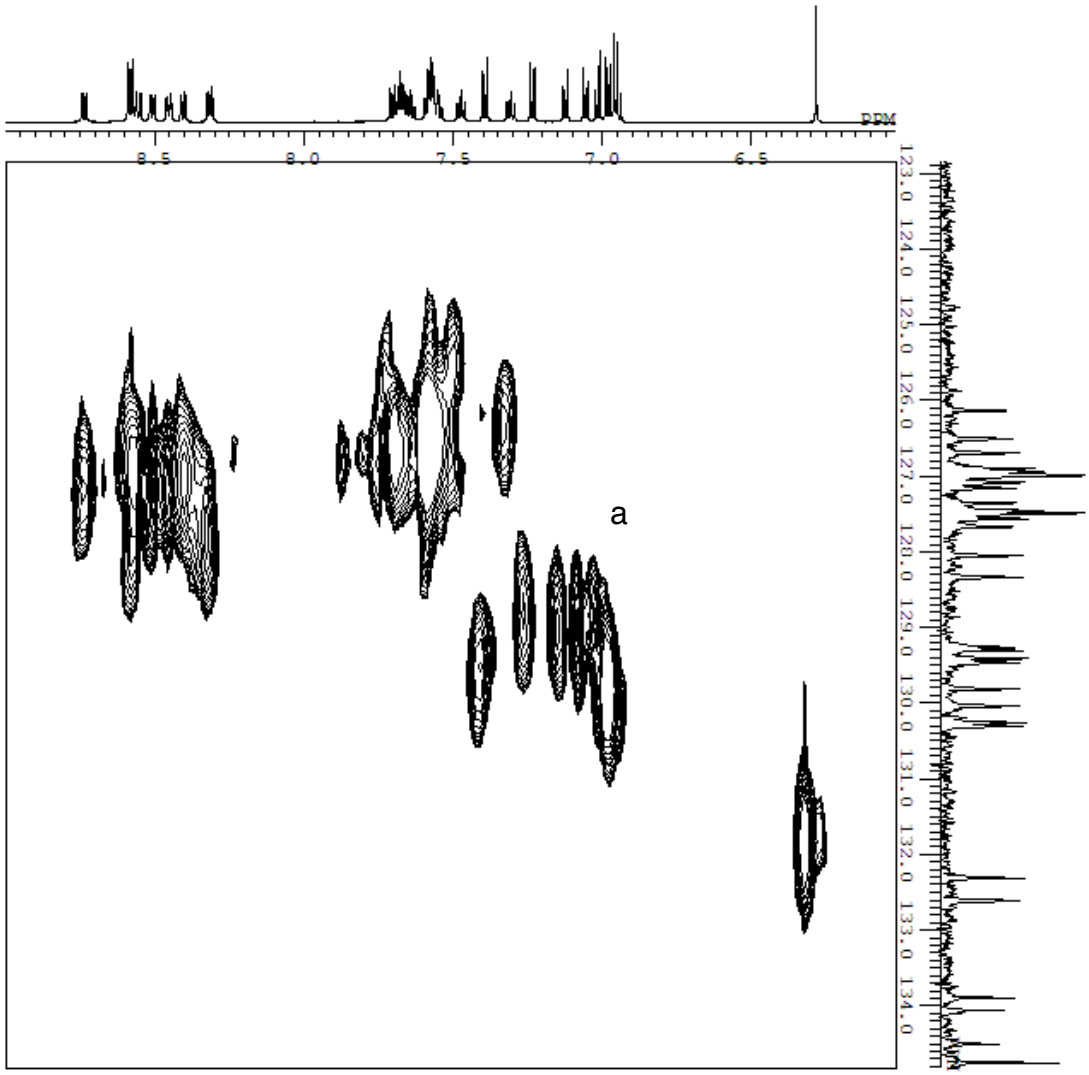


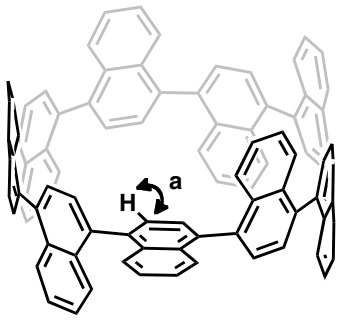
NOESY spectrum of **[9]CN** (600 MHz, THF-d_8)





HMQC spectrum of **[9]CN** (600 MHz, THF-d_8)





Mass spectrum of **[9]CN** (MALDI-TOF MS)