Supporting Information

Selective Synthesis of [7]- and [8]Cycloparaphenylenes

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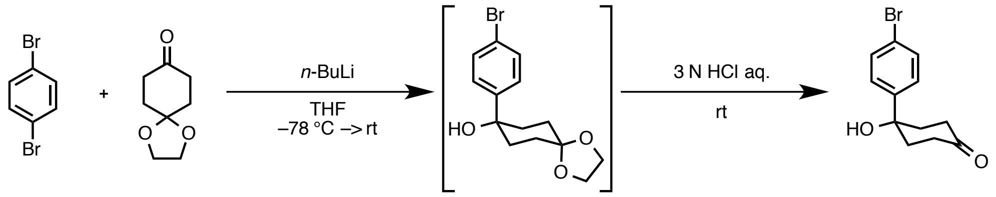
1. Experimental Section

General

Unless otherwise noted, all materials including dry dimethyl sulfoxide (DMSO) were obtained from commercial suppliers and used without further purification. Tetrahydrofuran (THF), dichloromethane, 1,4-dioxane, dimethyl formamide (DMF), and *m*-xylene 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 and dichloromethane was freshly distilled from phosphorous pentoxide (P_2O_5) under air.

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). Flash column chromatography was performed with KANTO silica gel 60N (40–100 μm), Merck, or Fluka silica gel 60 (40–63 μm). Preparative thin-layer chromatography (PTLC) was performed using Wako-gel® B5-F silica coated plates (0.75 mm) prepared in our laboratory. High-resolution mass spectra (HRMS) were obtained from JEOL JMS700 (fast atom bombardment mass spectrometry, FAB-MS) or Bruker Daltonics Ultraflex III TOF/TOF (MALDI-TOF-MS) with tetracyanoquinodimethane as matrix. Melting points were measured on a MPA100 Optimelt automated melting point system. Nuclear magnetic resonance (NMR) spectra were recorded on 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), or $CHDCl_2$ (δ 5.32 ppm). Chemical shifts for ^{13}C NMR are expressed in ppm relative to $CDCl_3$ (δ 77.0 ppm), or CD_2Cl_2 (δ 53.8 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, m = multiplet, br = broad signal, brs = broad singlet), coupling constant (Hz), and integration.

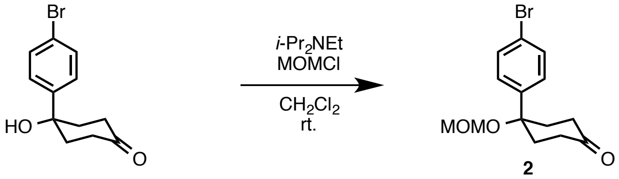
Synthesis of 4-(4-chloropheny)-4-hydroxycyclohexanone



To a 100-mL round-bottom flask containing a magnetic stirring bar were added 1,4-dibromobenzene (3.89 g, 16.5 mmol), and dry THF (30 mL). A solution of *n*-butyllithium in hexane (10 mL, 1.6 M, 16.0 mmol) was added at –78 °C in 15 min. After stirring the mixture at –78 °C for 1 h, 1,4-cyclohexanedione monoethyleneketal (2.34 g, 15.0 mmol) was added as solid, and the resultant mixture was further stirred at –78 °C for 1 h. After warmed up to room temperature, a 3 M solution of hydrochloric acid (10 mL) was added, and stirred for 1 day. The mixture was neutralized with saturated $NaHCO_3$ aqueous solution, extracted with EtOAc, washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by three times recrystallization ($CHCl_3$) to afford 4-(4-bromopheny)-4-hydroxycyclohexanone (3.33 g, 83%) as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 1.74–1.96 (brs, 1H), 2.11–2.18 (m, 2H), 2.26 (td, J = 13.8 Hz, 4.8 Hz, 2H), 2.32–2.40 (m, 2H), 2.90 (td, J = 14.4 Hz, 5.4 Hz, 2H), 7.40 (dd, J = 9.0 Hz, 1.2 Hz, 2H), 7.50 (dd, J = 9.0 Hz, 1.2 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 37.2 (CH_2), 38.5 (CH_2), 71.9 (4°), 121.5 (4°), 126.3 (CH), 131.6 (CH), 146.1 (4°), 211.0 (4°); HRMS (FAB) *m*/*z* calcd for $C_{12}H_{13}BrO_2Na$ $[M+Na]^+$: 290.9997, found ; 291.0002; mp: 154.8–156.2 ºC.

Synthesis of 2

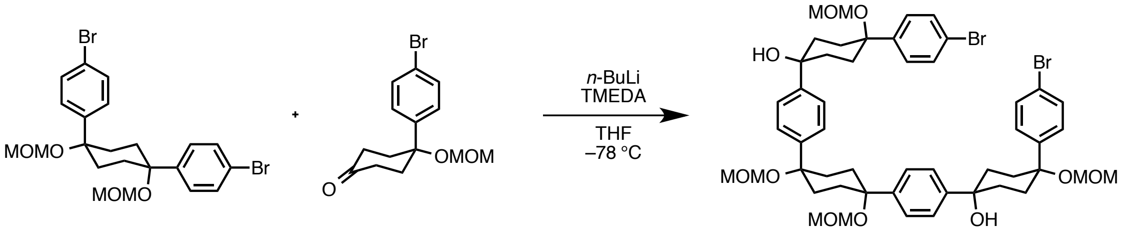


2

To a 50-mL round-bottom flask containing a stirring bar were added 4-(4-bromopheny)-4-hydroxycyclohexanone (5.87 g, 22.7 mmol), dry CH_2Cl_2 (25 mL), diisopropylethylamine (8.40 mL, 45.5 mmol), and chloromethyl methylether (3.50 mL, 45.5 mmol). After stirring at room temperature for 48 h, the mixture was quenched with saturated NH_4Cl aqueous solution, extracted with CH_2Cl_2, dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (pentane/EtOAc = 2:1 – EtOAc) to afford 4-(4-bromophenyl)-4-methoxymethoxycyclohexanone **2** (5.5 g, 80%) as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 2.15 (td, *J* = 13.2 Hz, 4.8 Hz, 2H), 2.32–2.38 (m, 2H), 2.39–2.45 (m, 2H), 2.91 (td, *J* = 14.4 Hz, 6.0 Hz, 2H), 3.43 (s, 2H), 4.52 (s, 3H), 7.33 (d, *J* = 9.0 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 36.1 (CH_2), 37.2 (CH_2), 56.6 (CH_3), 77.3 (4°), 92.9 (CH_2), 121.9 (4°), 127.8 (CH), 131.7 (CH), 142.9 (4°), 211.1 (4°); HRMS (FAB) *m/z* calcd for $C_{14}H_{17}BrO_3Na$ $[M+Na]^+$: 335.0259, found; 335.0261; mp: 74.5–75.8 ºC.

Synthesis of 3

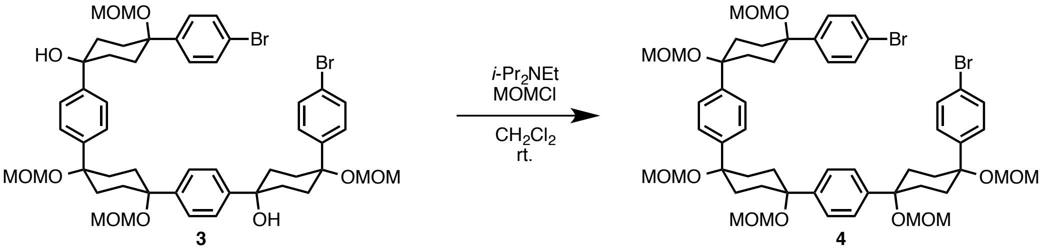


1 **2** **3**

To a 200-mL round-bottom flask containing a magnetic stirring bar were added **1** (2.07 g, 4.03 mmol), *N*,*N*,*N*',*N*'-tetramethylethylenediamine (1.2 mL, 8.05 mmol), and dry THF (80 mL). A solution of *n*-butyllithium in hexane (5.0 mL, 1.6 M, 8.0 mmol) was added at –78 °C. After stirring the mixture at –78 °C for 1 h, **2** (4.43 g, 8.43 mmol) in 20 mL of THF was added, and the resultant mixture was further stirred at –78 °C for 1 h. After warmed up to room temperature, the mixture was quenched with saturated NH_4Cl aqueous solution, extracted with EtOAc, dried over with Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by column chromatography (hexane/EtOAc = 1:1, then EtOAc) to afford **3** (2.13 g, 54%) as a white solid.

^{1}H NMR (600 MHz, CD_2Cl_2) δ 1.60 (brs, 2H), 1.82–2.37 (m, 24H), 3.30 (s, 6H), 3.32 (s, 6H), 4.33 (s, 4H), 4.37 (s, 4H), 7.32 (m, 8H), 7.37 (d, *J* = 9.0 Hz, 4H), 7.48 (d, *J* = 9.0 Hz, 4H); ^{13}C NMR (150 MHz, CD_2Cl_2) δ 32.9 (CH_2), 33.2 (CH_2), 35.7 (CH_2), 55.9 (CH_3), 56.0 (CH_3), 72.2 (4°), 78.16 (4°), 78.20 (4°), 92.2 (CH_2), 92.3 (CH_2), 121.9 (4°), 125.2 (CH), 127.1 (CH), 129.6 (CH), 131.7 (CH), 141.2 (4°), 146.7 (4°); HRMS (FAB) *m*/*z* calcd for $C_{50}H_{62}Br_2O_{10}Na$ $[M+Na]^+$: 1003.2607, found; 1003.2615.

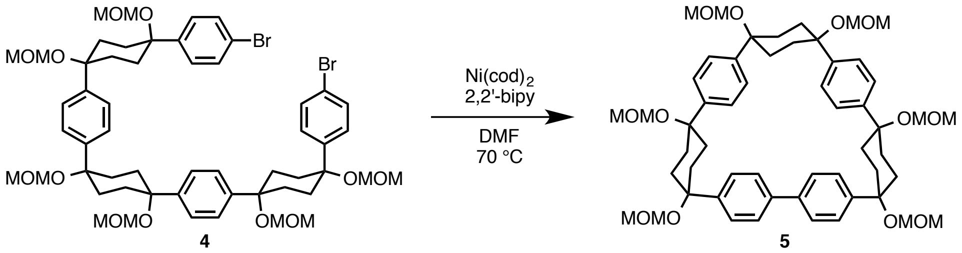
Synthesis of 4



To a 50-mL round-bottom flask containing a stirring bar were added **3** (704 mg, 718 μmol), dry CH_2Cl_2 (20 mL), diisopropylethylamine (1.32 mL, 7.18 μmol) and chloromethyl methylether (540 μL, 7.18 mmol). After stirring at room temperature for 48 h, the mixture was quenched with saturated NH_4Cl aqueous solution, extracted with CH_2Cl_2, dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (pentane/EtOAc = 1:2) to afford **4** (688 mg, 90%) as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 1.73–2.44 (br, 24H), 3.36 (s, 6H), 3.37 (s, 6H), 3.38 (s, 6H), 4.36 (s, 4H), 4.38 (s, 4H), 4.40 (s, 4H), 7.27–7.41 (m, 12H), 7.44 (d, *J* = 9.0 Hz, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 32.7 (CH_2), 32.8 (CH_2), 32.9 (CH_2), 55.9 (CH_3), 56.0 (CH_3), 56.1 (CH_3), 77.8 (4°), 77.9 (4°), 92.0 (CH_2), 92.1 (CH_2), 92.2 (CH_2), 121.7 (4°), 126.6 (CH), 126.8 (CH), 128.8 (CH), 131.5 (CH), 141.9 (4°); HRMS (FAB) *m*/*z* calcd for $C_{54}H_{70}Br_2O_{12}Na$ $[M+Na]^+$: 1091.3132, found; 1091.3146.

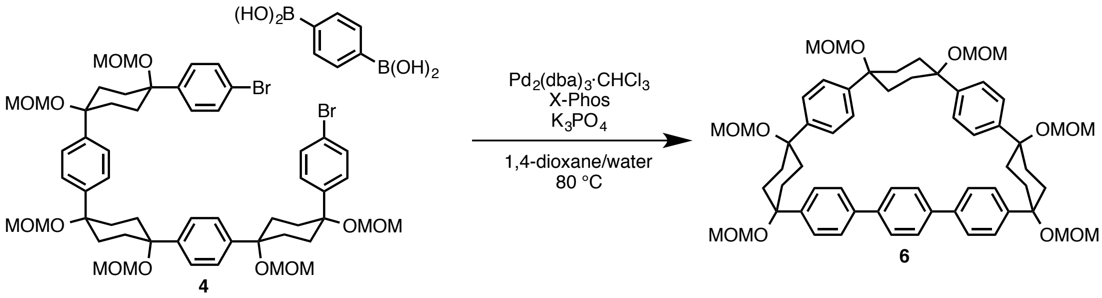
Synthesis of 5



To a 200-mL Schlenk tube containing a magnetic stirring bar were added **4** (269 mg, 251 μmol), Ni(cod)$_2$ (140 mg, 509 μmol), and 2,2'-bipyridyl (79.5 mg, 509 μmol). Then to this flask was added dry DMF (100 mL). The reaction mixture was stirred at 70 °C for 40 h. After cooled down to room temperature, the mixture was extracted with EtOAc, washed with brine, dried over with Na$_2$SO$_4$, and concentrated under reduced pressure. The crude product was purified by column chromatography (hexane/EtOAc = 1:1 – 1:4) to afford **5** (154 mg, 67%) as a white solid

^{1}H NMR (600 MHz, CDCl$_3$) δ 1.41 (t, *J* = 13.2 Hz, 4H), 1.63–2.24 (br, 12H), 2.35 (t, *J* = 13.2 Hz, 4H), 2.56 (d, *J* = 12.6 Hz, 4H), 3.37 (s, 6H), 3.38 (s, 6H), 3.46 (s, 6H), 4.44 (s, 4H), 4.49 (s, 4H), 4.66 (s, 4H), 7.07 (br, 4H), 7.15 (br, 4H), 7.58 (d, *J* = 8.4 Hz, 4H), 7.73 (d, *J* = 8.4 Hz, 4H); ^{13}C NMR (150 MHz, CDCl$_3$) δ 32.6 (CH$_2$), 33.3 (CH$_2$), 34.0 (CH$_2$), 55.4 (CH$_3$), 55.9 (CH$_3$), 56.3 (CH$_3$), 78.3 (4°), 78.5 (4°), 92.1 (CH$_2$), 92.3 (CH$_2$), 9.26 (CH$_2$), 125.7 (CH), 126.1 (CH), 126.5 (CH), 128.8 (CH), 137.3 (4°), 138.0 (4°), 144.1 (4°); HRMS (FAB) *m*/*z* calcd for $C_{54}H_{70}O_{12}Na$ $[M+Na]^+$: 933.4765, found; 933.4772; mp: 209.9–212.6 ºC.

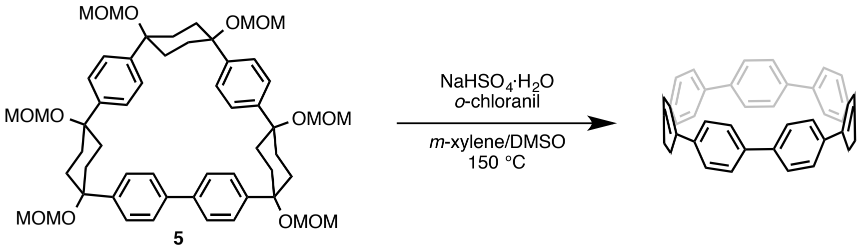
Synthesis of 6



To a 50-mL schlenk tube containing a magnetic stirring bar were added **4** (54.5 mg, 50.9 μmol), 1,4-benzenedibronic acid (10.2 mg, 61.5 μmol), $Pd_2(dba)_3$·$CHCl_3$ (2.1 mg, 2.0 μmol), X-Phos (2-dicyclohexylphosphino-2',4',6'-triisopropylbiphenyl, 4.9 mg, 10 μmol), and K_3PO_4 (44.8 mg, 211 μmol) and the flask was evacuated and backfilled with nitrogen three times. Then to this flask was added dry dioxane (19 mL) and degassed water (1 mL). The reaction mixture was stirred at 80 °C for 36 h. After cooled down to room temperature, the mixture was extracted with EtOAc, washed with brine, dried over with Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by PTLC (hexane/EtOAc = 1:1) to afford **6** (13.1 mg, 27%) as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 1.26 (td, *J* = 14.4 Hz, 2.4 Hz, 4H), 1.90 (br, 4H), 2.10 (d, *J* = 13.2 Hz, 4H), 2.24 (m, 4H), 2.37 (td, *J* = 13.2 Hz, 2.4 Hz, 4H), 2.58 (d, *J* = 12.0 Hz, 4H), 3.32 (s, 6H), 3.396 (s, 6H), 3.403 (s, 6H), 4.21 (s, 4H), 4.32 (s, 4H), 4.69 (s, 4H), 7.07 (d, *J* = 8.4 Hz, 4H), 7.21 (d, *J* = 8.4 Hz, 4H), 7.60 (d, *J* = 8.4 Hz, 4H), 7.65 (d, *J* = 9.0 Hz, 4H), 7.70 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 32.4 (CH_2), 32.8 (CH_2), 33.4 (CH_2), 55.4 (CH_3), 56.1 (CH_3), 56.4 (CH_3), 76.6 (4°), 77.7 (4°), 78.4 (4°), 125.8 (CH), 126.5 (CH), 126.6 (CH), 127.4 (CH), 128.8 (CH), 136.8 (4°), 138.5 (4°), 138.7 (4°), 144.0 (4°); HRMS (FAB) *m/z* calcd for $C_{60}H_{74}O_{12}Na$ $[M+Na]^+$: 1009.5078, found; 1009.5083; mp: over 155 ºC started to melt.

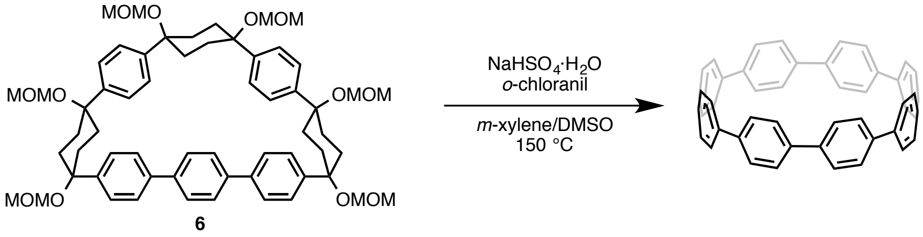
Synthesis of [7]CPP



To a 20-mL Schlenk tube containing a magnetic stirring bar were added **5** (14.0 mg, 15.4 μmol), $NaHSO_4 \cdot H_2O$ (34.2 mg, 248 μmol), dry *m*-xylene (3.0 mL) and dry DMSO (0.5 mL). The reaction mixture was stirred at 150 °C for 96 h under air. After cooled down to room temperature, the mixture was passed through short pad of silica ($CHCl_3$), and concentrated under reduced pressure. The crude product was purified by PTLC (hexane/CH_2Cl_2 = 1:1) to afford [7]CPP (1.4 mg, 17%) as a yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48 (s, 28H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 127.4 (CH), 136.8 (4°); HRMS (MALDI) *m*/*z* calcd for $C_{42}H_{28}$ $[M]^+$: 532.2191, found; 532.2181.

Synthesis of [8]CPP



To a 20-mL Schlenk tube containing a magnetic stirring bar were added **6** (13.6 mg, 13.8 μmol), $NaHSO_4 \cdot H_2O$ (33.3 mg, 241 μmol), dry *m*-xylene (3.0 mL) and dry DMSO (0.5 mL). The reaction mixture was stirred at 150 °C for 72 h under air. After cooled down to room temperature, the mixture was passed through short pad of silica ($CHCl_3$), and concentrated under reduced pressure. The crude product was purified by PTLC (hexane/CH_2Cl_2 = 1:1) to afford [8]CPP (1.0 mg, 12%) as a yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48 (s, 32H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 127.4 (CH), 137.6 (4°); HRMS (MALDI) *m*/*z* calcd for $C_{48}H_{32}$ $[M]^+$: 608.2504, found; 608.2501.

2. X-ray Crystal Structure Analysis of [7]CPP·cyclohexane

Recrystallization of [7]CPP from chloroform/hexane yielded colorless crystals suitable for X-ray crystal structure analysis. Details of the crystal data and a summary of the intensity data collection parameters are listed in Table S1. 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 = 0.71075 Å) was used. The structures were solved by direct methods with (SIR-97)[S1] and refined by full-matrix least-squares techniques against F^2 (SHELXL-97).[S2] The intensities were corrected for Lorentz and polarization effects. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using AFIX instructions. CCDC 963468 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www. ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystallographic data and structure refinement details for [7]CPP·cyclohexane

	[7]CPP·cyclohexane
formula	$C_{48}H_{40}$
fw	616.80
T (K)	113(2)
λ (Å)	0.71075
cryst syst	Orthorhombic
space group	*Pnma*
a, (Å)	18.340(7)
b, (Å)	22.335(8)
c, (Å)	8.218(3)
α, (deg)	90°
β, (deg)	90°
γ, (deg)	90°
V, (Å^3)	3366(2)
Z	4
D_{calc}, (g / cm^3)	1.217
μ (mm^{-1})	0.069
F(000)	1312
cryst size (mm)	0.20 × 0.20 × 0.05
2θ range, (deg)	3.27–25.00
reflns collected	36989
indep reflns/R_{int}	3039/0.0346
params	232
GOF on F^2	1.078
R_1, wR_2 [I>2σ(I)]	0.0648, 0.1742
R_1, wR_2 (all data)	0.0679, 0.1772

[S1] A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, *J. Appl. Crystallogr.*, 1999, **32,** 115–119.

[S2] G. M. Sheldrick, University of Göttingen: Göttingen, Germany, 1997.

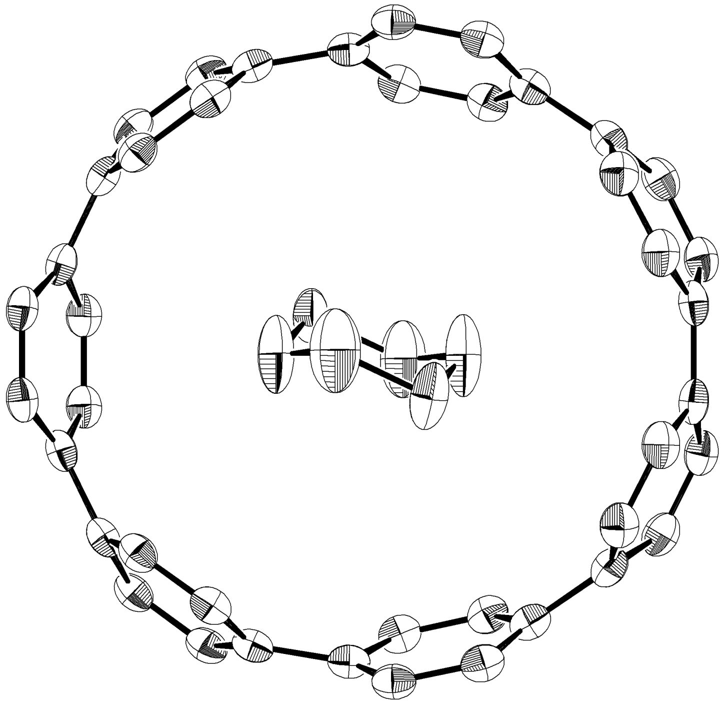


Fig. S1. ORTEP drawing of [7]CPP·cyclohexane with 50% thermal ellipsoids. All hydrogen atoms and the other part of disordered cyclohexane molecule are omitted for clarity. Half of the entire structure constitutes an asymmetric unit.

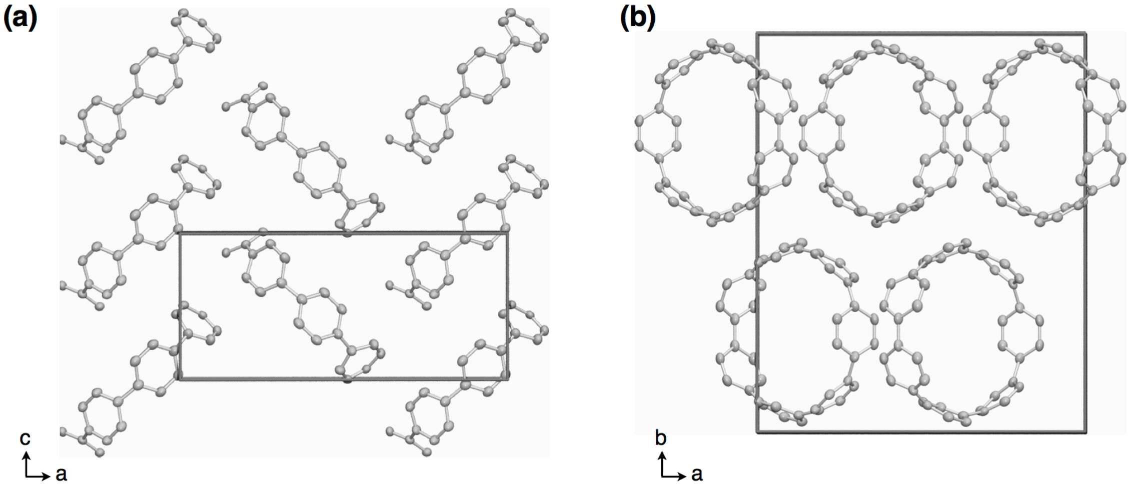


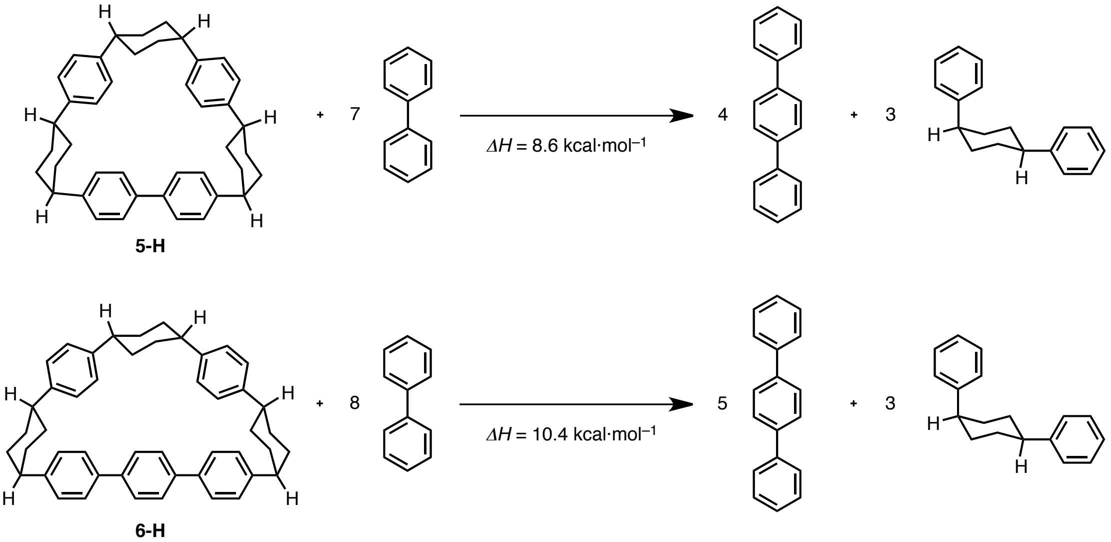
Fig. S2. Packing structure of [7]CPP·cyclohexane on (a) *ac* plane and (b) *ab* plane. All hydrogen atoms and cyclohexane molecule are omitted for clarity.

3. Photophysical Properties

UV/vis absorption spectra were recorded on a Shimadzu UV- 3510 spectrometer with a resolution of 0.5 nm. Emission spectra were measured with an F-4500 Hitachi spectrometer with a resolution of 0.4 nm. Dilute solutions in degassed spectral grade chloroform in a 1 cm square quartz cell were used for measurements.

4. Computational Study

The Gaussian 09 program[S3] running on a SGI Altix4700 system was used for optimization with B3LYP/6-31G(d).[S4] Structures were optimized without any symmetry assumptions. Zero-point energy, enthalpy, and Gibbs free energy at 298.15 K and 1 atm were estimated from the gas-phase studies. Harmonic vibration frequency calculation at the same level was performed to verify all stationary points as local minima (with no imaginary frequency).



Scheme S1. Model structure of **5-H**, **6-H** and homodesmotic reactions for calculation of strain energies for **5-H** and **6-H**.

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

compound	*E*	*E* + *ZPE*	*H*	*G*
5-H	-1628.22073428	-1627.440481	-1627.406471	-1627.502735
6-H	-1859.27515236	-1858.414500	-1858.375559	-1858.483945

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

S3) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09, Revision A.02*, Gaussian, Inc., Wallingford CT, 2009.

S4) (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; (b) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.

Table S4. Cartesian coordinates for **5-H**, and **6-H**.

5-H

C	-5.896881	-1.295028	0.129777
C	-6.027588	-0.283519	1.291209
C	-4.951503	0.816958	1.249955
C	-4.823811	1.544298	-0.116640
C	-4.910454	0.564226	-1.315370
C	-6.031005	-0.475463	-1.179045
H	-5.155429	1.563408	2.028452
H	-7.024408	0.172348	1.217090
H	-6.003433	-0.787323	2.265505
H	-6.753605	-1.983881	0.184521
H	-5.669013	2.242898	-0.202321
H	-5.043936	1.144761	-2.237061
H	-3.956579	0.036608	-1.423945
H	-7.009604	0.024826	-1.164468
H	-6.038996	-1.126457	-2.060462
H	-3.982087	0.378060	1.502568
C	-3.530126	2.348670	-0.164777
C	-3.508497	3.742894	-0.266715
C	-2.292193	1.688534	-0.088810
C	-2.300682	4.451704	-0.280822
H	-4.447547	4.289633	-0.330339
C	-1.094543	2.391628	-0.102118
H	-2.260898	0.604676	-0.009953
H	-2.321624	5.537481	-0.354421
H	-0.161600	1.837763	-0.032554
C	-4.608830	-2.131132	0.161043
C	-3.796309	-2.229449	1.300174
C	-4.155987	-2.802583	-0.987664
C	-2.541171	-2.835405	1.256205
H	-4.111472	-1.777881	2.234786
C	-2.907848	-3.417359	-1.035394
H	-4.771879	-2.818376	-1.882371
C	-2.040812	-3.393185	0.070263
H	-1.912069	-2.802517	2.141323
H	-2.591553	-3.900980	-1.955662
C	-0.615936	-3.793273	-0.037714
C	0.119885	-4.281355	1.054748
C	0.091032	-3.565101	-1.227871
C	1.502232	-4.441164	0.981507
H	-0.391816	-4.525723	1.981984
C	1.471655	-3.733303	-1.297014
H	-0.433853	-3.182044	-2.098297
H	2.025045	-4.801361	1.863152
H	1.964180	-3.504900	-2.235900
C	3.759612	-4.197491	-0.213328
C	4.420676	-3.677314	1.087419
C	4.401981	-3.413873	-1.379939
H	4.039188	-5.256291	-0.325882
C	4.218893	-2.166555	1.278077
H	5.494672	-3.904325	1.032400
H	4.045500	-4.212133	1.966768
C	4.220872	-1.892635	-1.243156
H	5.475277	-3.650338	-1.385981
H	4.018739	-3.753424	-2.349355
C	4.761961	-1.334478	0.099345
H	4.697658	-1.845718	2.212135
H	3.144747	-1.974678	1.393099
H	4.720224	-1.391277	-2.080624
H	3.158347	-1.633788	-1.319684
H	5.857412	-1.458228	0.084861
C	2.225702	-4.124531	-0.181023
C	4.456055	0.160096	0.209914
C	3.679033	0.706793	1.235347
C	4.920732	1.053684	-0.770756
C	3.327367	2.060286	1.248538
H	3.319953	0.079061	2.043896
C	4.558012	2.397434	-0.764373
H	5.567683	0.689484	-1.566136
H	2.726782	2.419910	2.076406
H	4.934811	3.043267	-1.554544
C	3.291616	4.403584	0.151058
C	2.376093	4.897537	1.293312
C	2.592294	4.736771	-1.192489
H	4.213990	5.002323	0.191512
C	0.934767	4.358470	1.224557
H	2.813534	4.661425	2.271721
H	2.347056	5.994543	1.233881
C	1.201575	4.097433	-1.299346
H	3.210904	4.418780	-2.039545
H	2.501335	5.830148	-1.269043
C	0.256734	4.538611	-0.156823
H	0.923678	3.292771	1.472724
H	0.322567	4.851927	1.990492
H	1.311727	3.006175	-1.286819
H	0.743595	4.350190	-2.263985
H	0.052178	5.610968	-0.294960
C	3.717344	2.933148	0.227936
C	-1.070176	3.792805	-0.193286

6-H

C	-6.990737	-1.283957	0.078898
C	-7.056272	-0.302566	1.272587
C	-5.903751	0.718695	1.273034
C	-5.765346	1.499052	-0.058728
C	-5.846373	0.553407	-1.282348
C	-7.031654	-0.420520	-1.207662
H	-6.043155	1.434825	2.093066
H	-8.014386	0.231204	1.205939
H	-7.081913	-0.837999	2.229500
H	-7.903159	-1.899410	0.098885
H	-6.618232	2.191134	-0.125602
H	-5.911342	1.157219	-2.196366
H	-4.917148	-0.023195	-1.360532
H	-7.975496	0.143002	-1.205518
H	-7.056700	-1.044455	-2.107864
H	-4.960437	0.202302	1.478051
C	-4.488372	2.329418	-0.078947
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C	-3.226099	1.716180	-0.014251
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C	-2.052922	2.465999	-0.026123
H	-3.154265	0.632918	0.048063
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H	-1.645042	-3.295715	-2.069968
C	0.197889	-4.753921	0.991458
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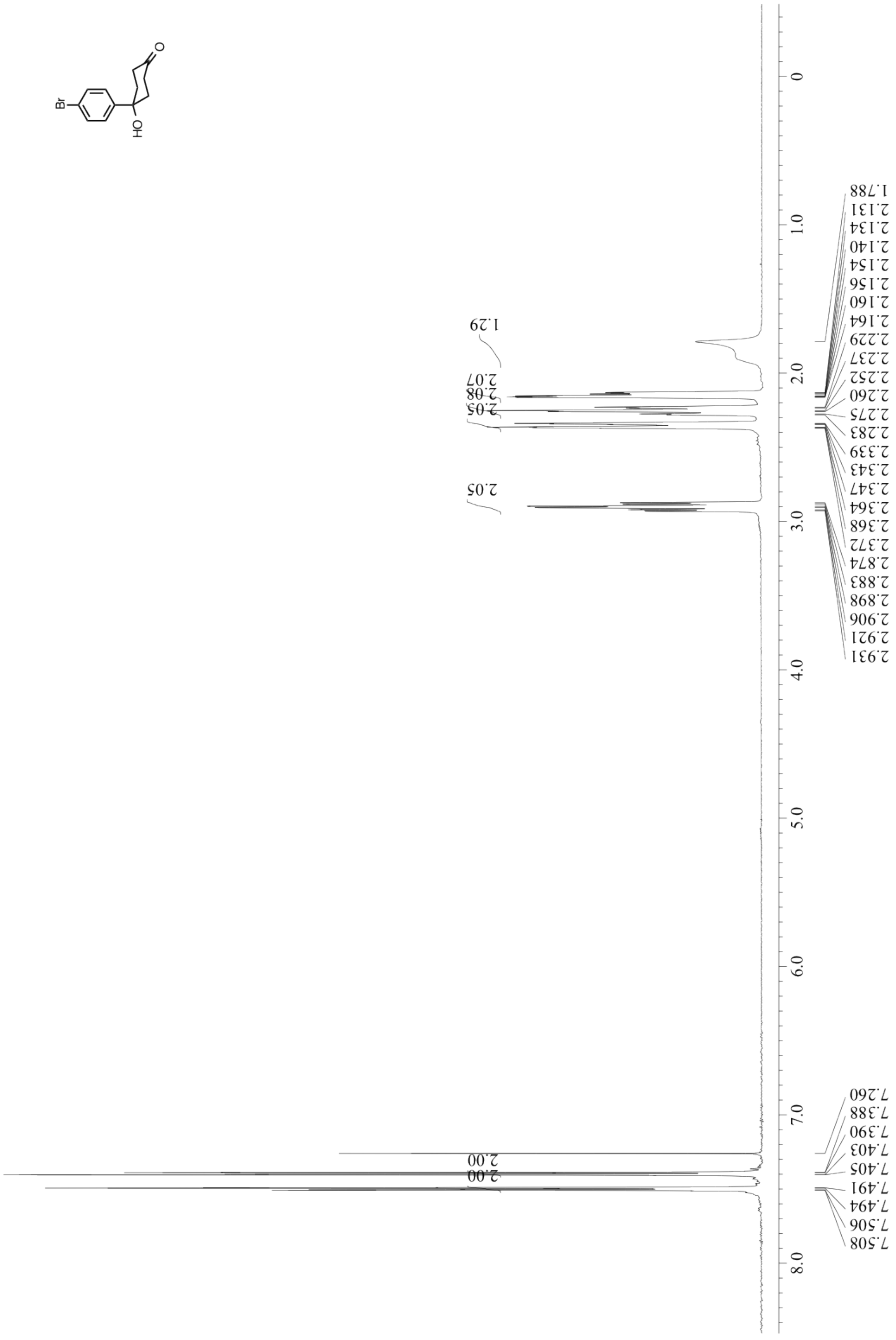
C	0.950972	-4.298309	-0.105002
H	0.789135	-3.479862	-2.094798
H	0.707774	-5.167711	1.857483
C	2.418416	-4.095466	-0.038707
C	3.018449	-3.661474	1.152427
C	3.232910	-4.142660	-1.182748
C	4.325699	-3.177896	1.170563
H	2.429557	-3.616856	2.064226
C	4.535355	-3.653188	-1.159080
H	2.831347	-4.537266	-2.112432
H	4.720262	-2.810732	2.111962
H	5.112930	-3.680742	-2.078886
C	6.453790	-2.380579	-0.052943
C	6.784085	-1.524116	1.191254
H	4.856910	-0.613383	1.518625
H	5.738671	0.386011	-2.086199
H	4.587208	-0.582990	-1.179205
H	6.913148	1.024171	-0.027659
C	5.094210	-3.090060	0.001337
C	4.931436	1.795079	0.138552
C	3.876248	1.887300	1.051022
C	5.066929	2.849674	-0.780418
C	2.988487	2.969192	1.039870
H	3.727806	1.113928	1.797635
C	4.178521	3.919615	-0.797050
H	5.889710	2.833116	-1.492987
H	2.202505	2.991486	1.787179
H	4.330180	4.719166	-1.520029
C	2.187616	5.228030	0.049386
C	1.241078	5.427757	1.256720
C	1.365399	5.292768	-1.266874
H	2.861801	6.096766	0.034493
C	-0.037192	4.568977	1.236345
H	1.786841	5.268105	2.195143
H	0.936900	6.483995	1.259793
C	0.141250	4.366693	-1.268123
H	2.010841	5.063474	-2.122877

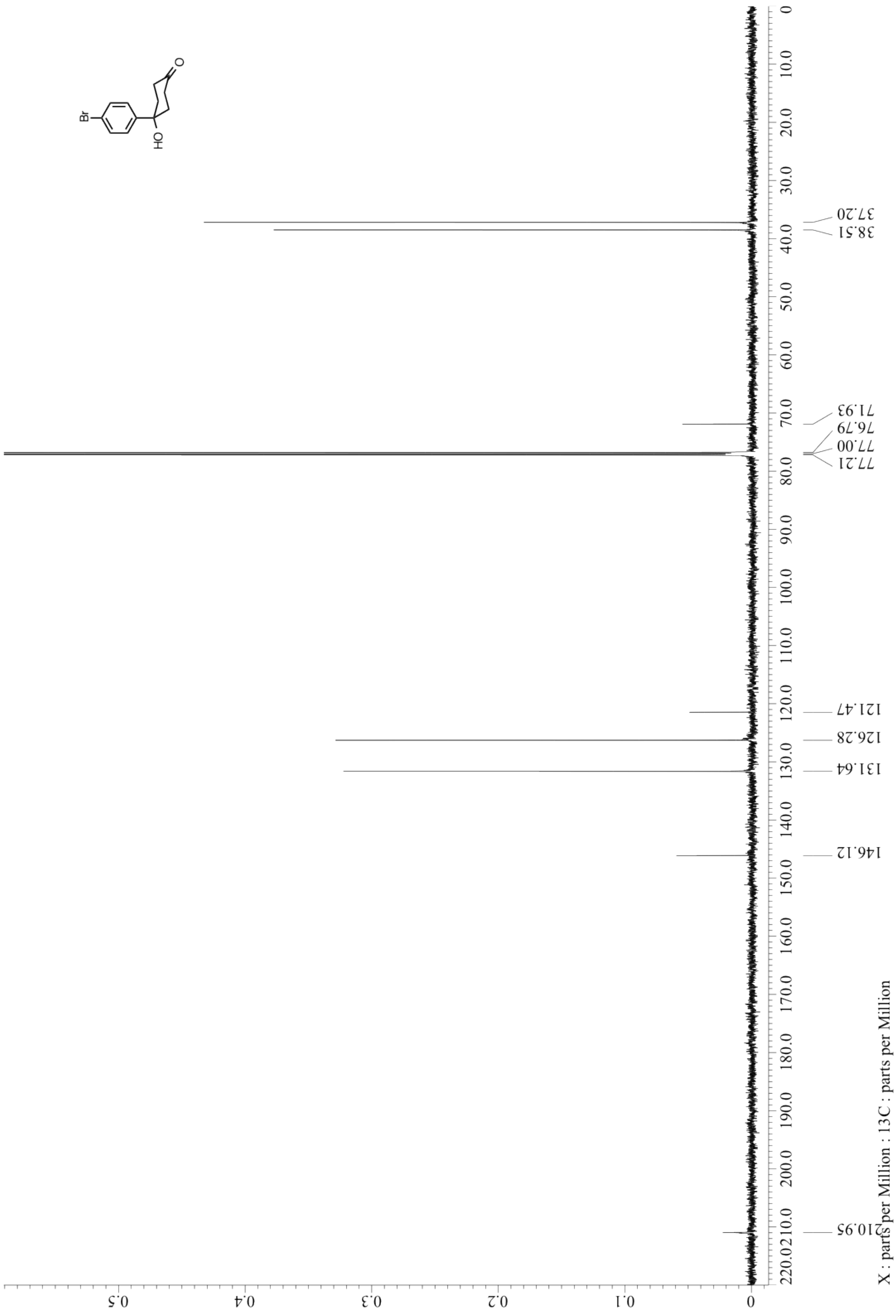
H	-3.404270	5.562979	-0.230509
H	-1.098109	1.947929	0.025202
C	-5.778272	-2.225410	0.106108
C	-5.007650	-2.429280	1.259792
C	-5.348794	-2.886648	-1.057522
C	-3.798306	-3.120762	1.219646
H	-5.312207	-1.989461	2.203432
C	-4.144126	-3.583100	-1.103503
H	-5.941825	-2.824201	-1.965426
C	-3.304620	-3.656161	0.020575
C	6.570981	-1.450349	-1.287481
H	7.233076	-3.152661	-0.143533
C	5.882874	-0.281895	1.328128
H	7.831012	-1.202873	1.101534
H	6.735413	-2.123771	2.108274
C	5.629965	-0.240383	-1.192375
H	7.611101	-1.099487	-1.350276
H	6.379738	-1.997864	-2.216594
C	5.895834	0.612351	0.073970
H	6.190804	0.302716	2.204770
H	1.021732	6.328550	-1.404233
C	-0.809565	4.695665	-0.095995
H	0.203539	3.511545	1.398793
H	-0.687058	4.866178	2.069314
H	0.467890	3.320409	-1.196105
H	-0.395657	4.462027	-2.220128
H	-1.105825	5.750424	-0.206066
C	3.105622	4.004969	0.108751
C	-2.084286	3.867129	-0.102389

4. Spectra of Products

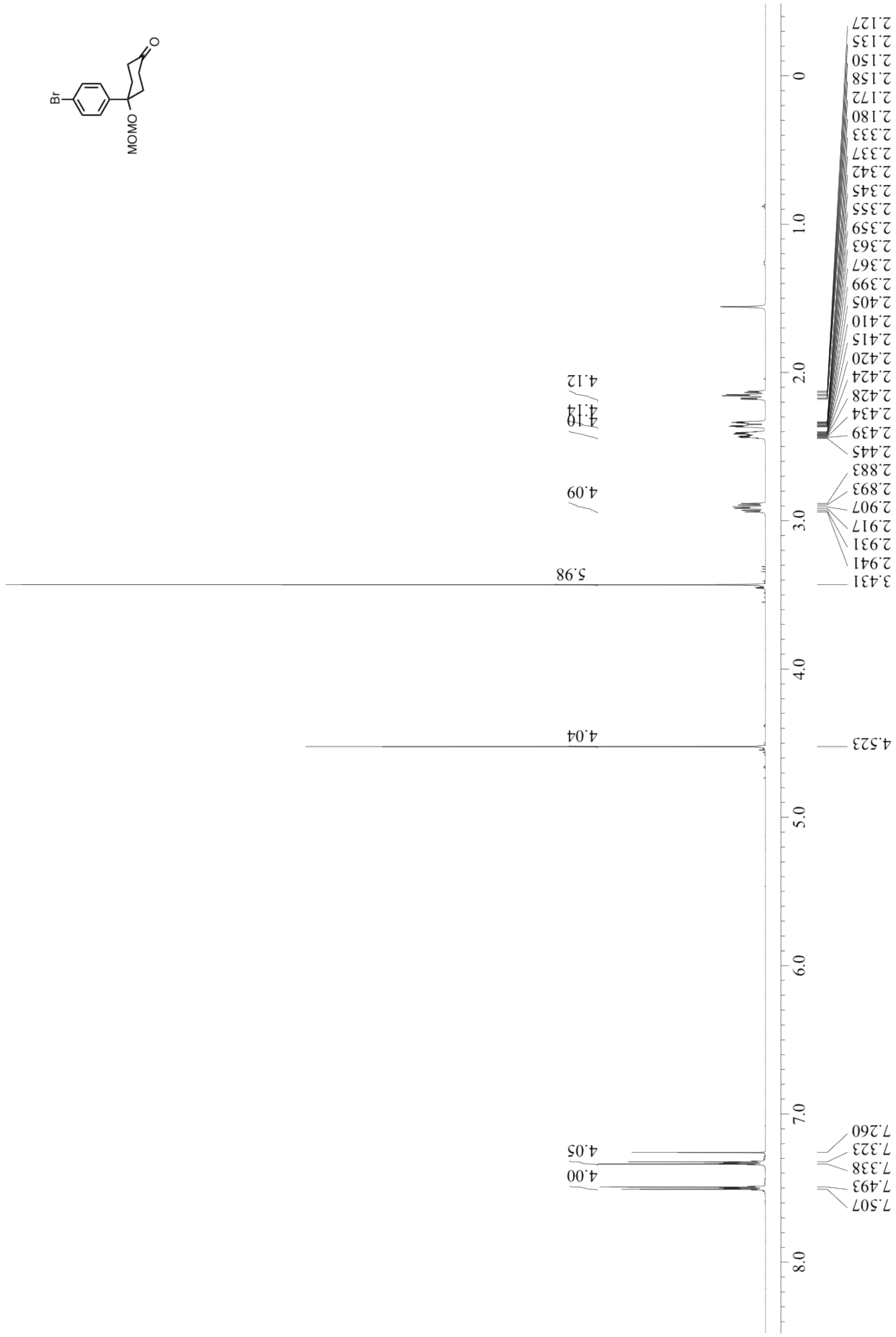
^{1}H NMR spectrum of 4-(4-bromopheny)-4-hydroxycyclohexanone ($CDCl_3$)



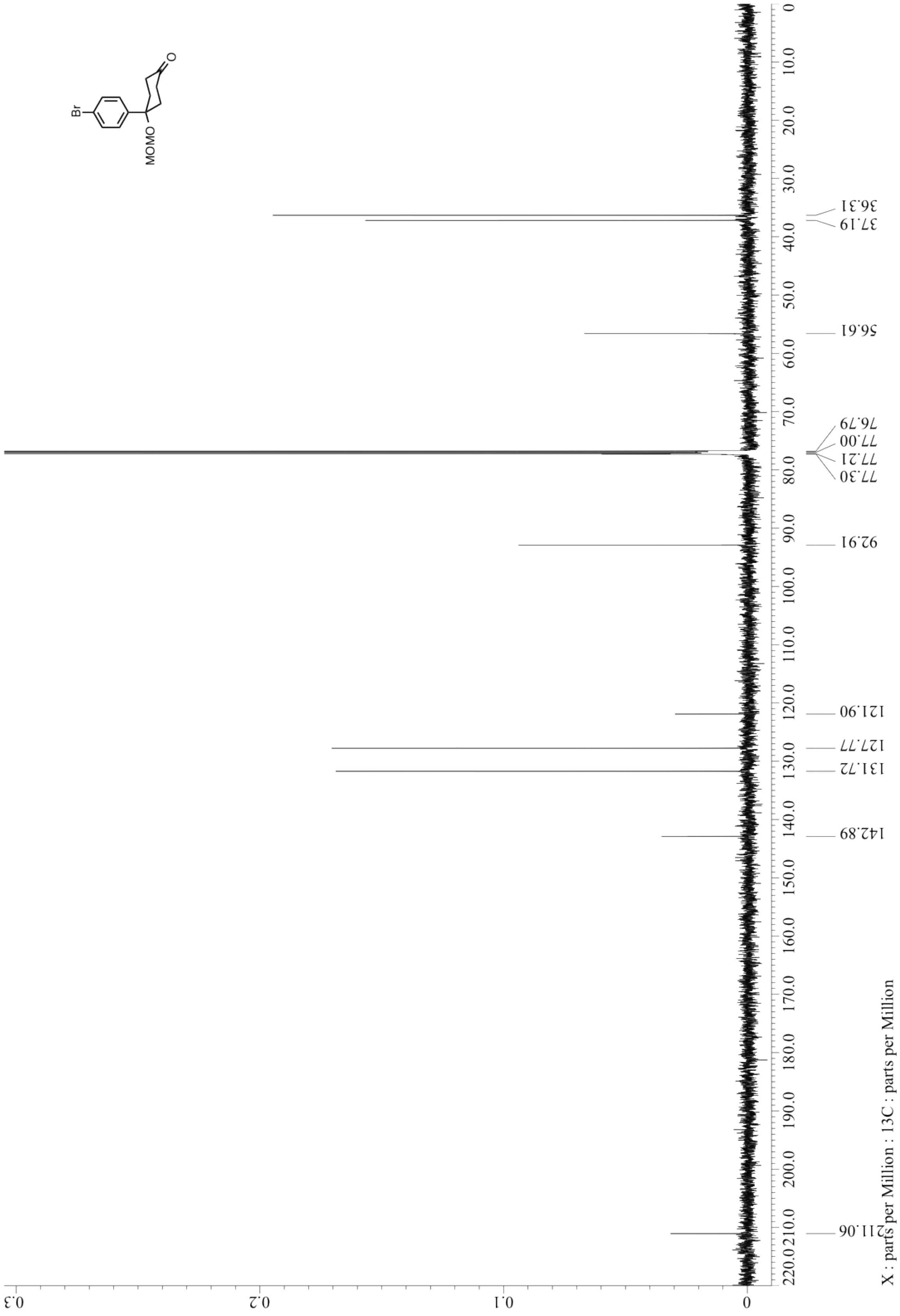
^{13}C NMR spectrum of 4-(4-bromopheny)-4-hydroxycyclohexanone (CDCl$_3$)



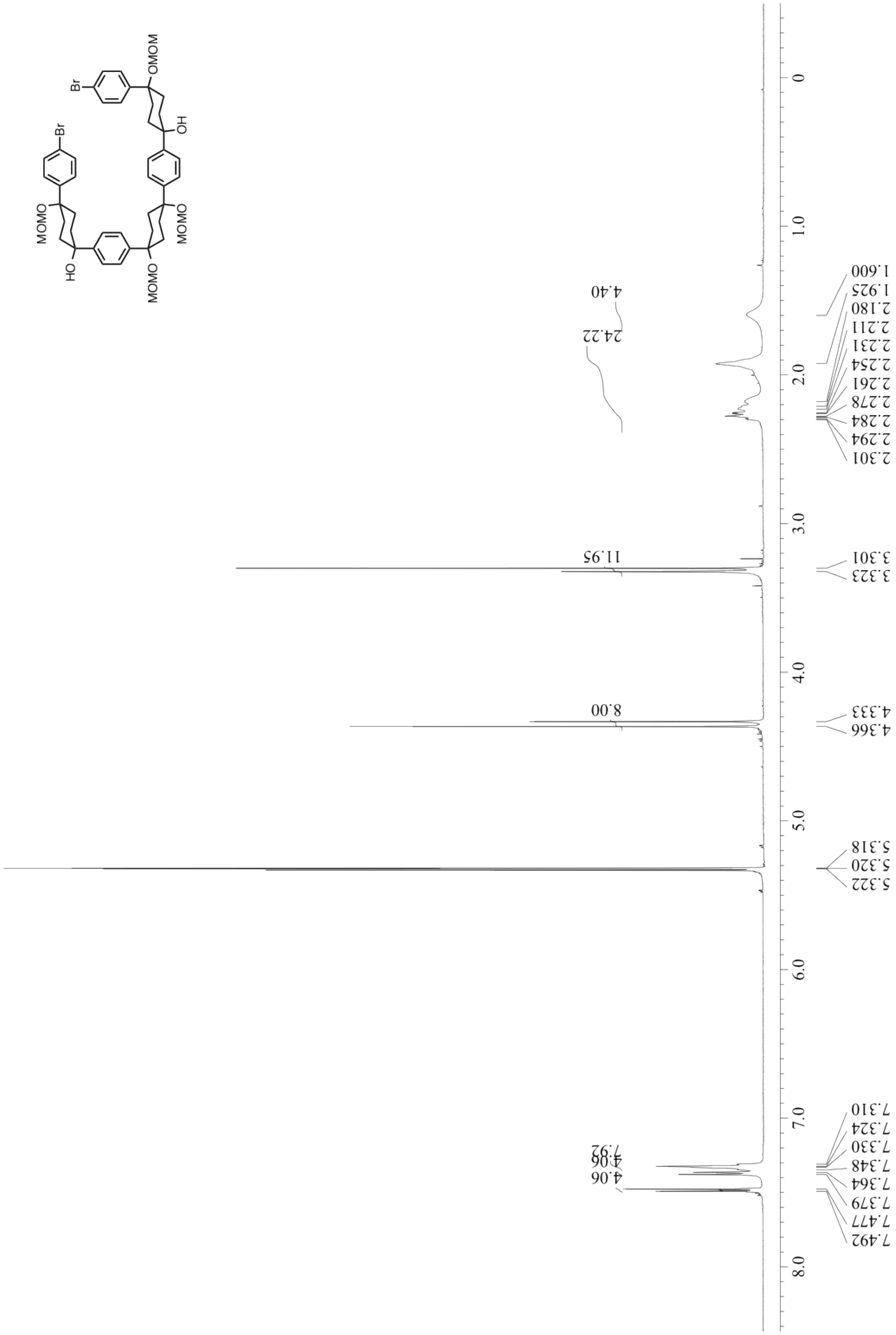
^{1}H NMR spectrum of **2** ($CDCl_3$)



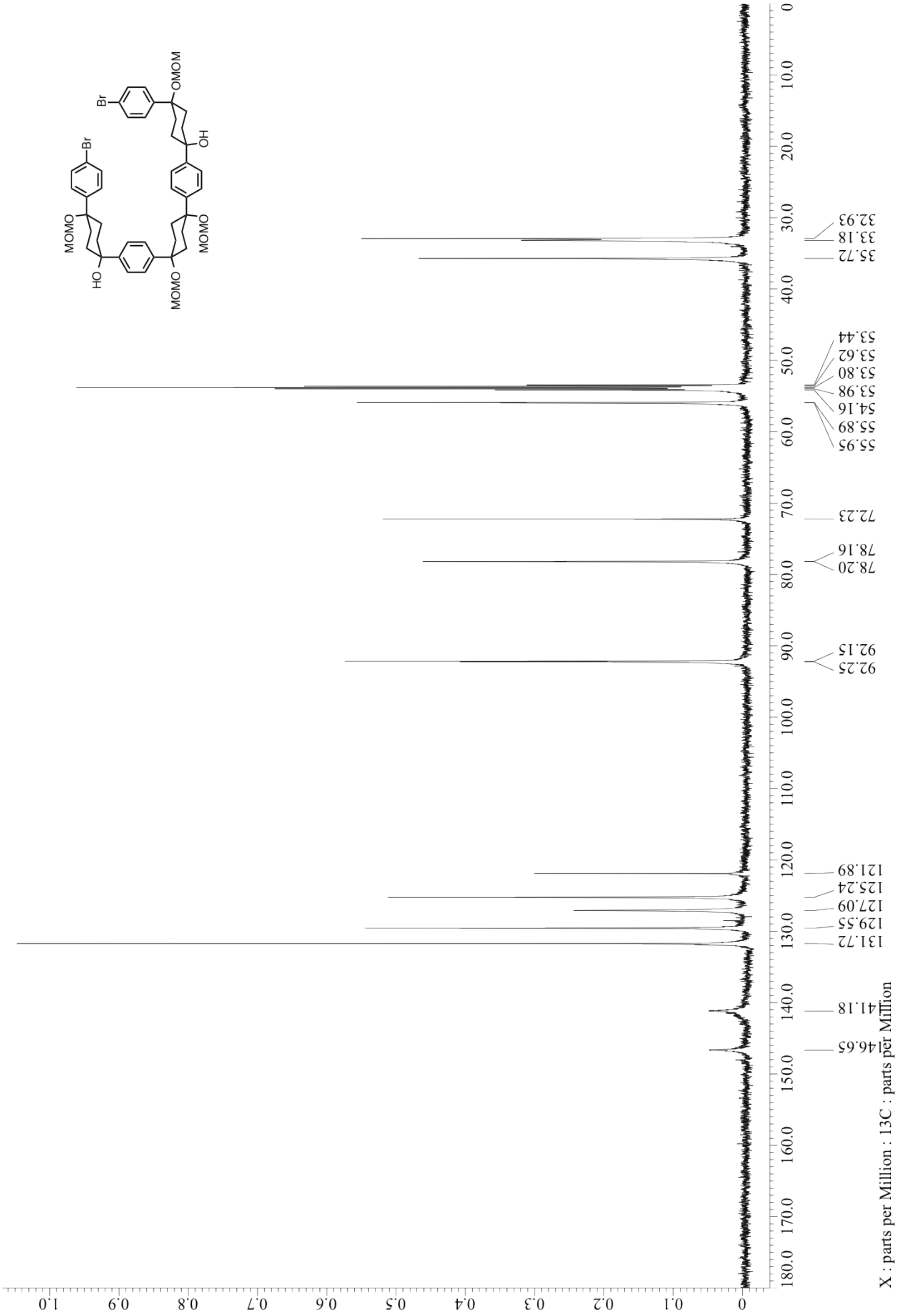
^{13}C NMR spectrum of **2** (CDCl$_3$)



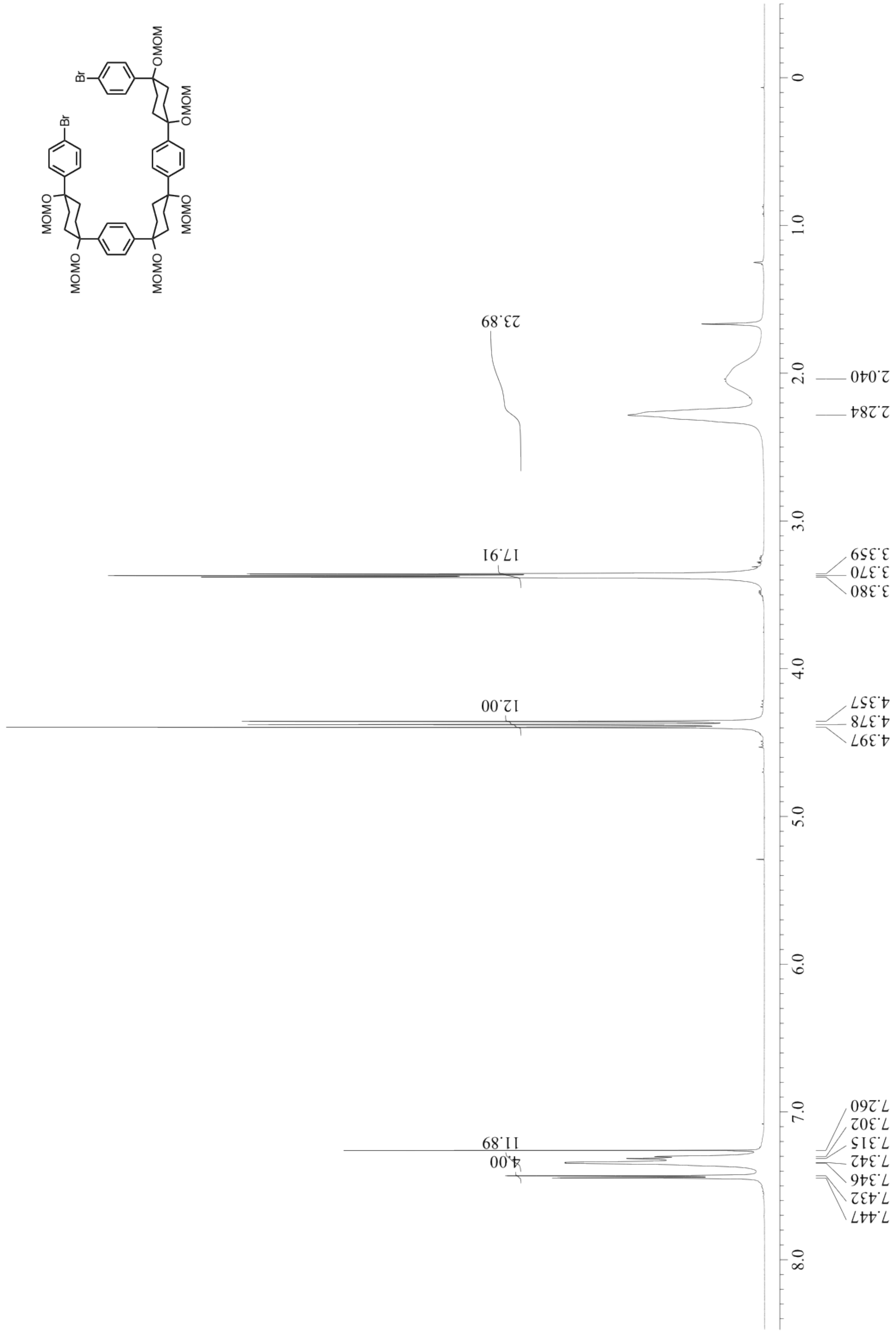
^{1}H NMR spectrum of **3** (CD_2Cl_2)



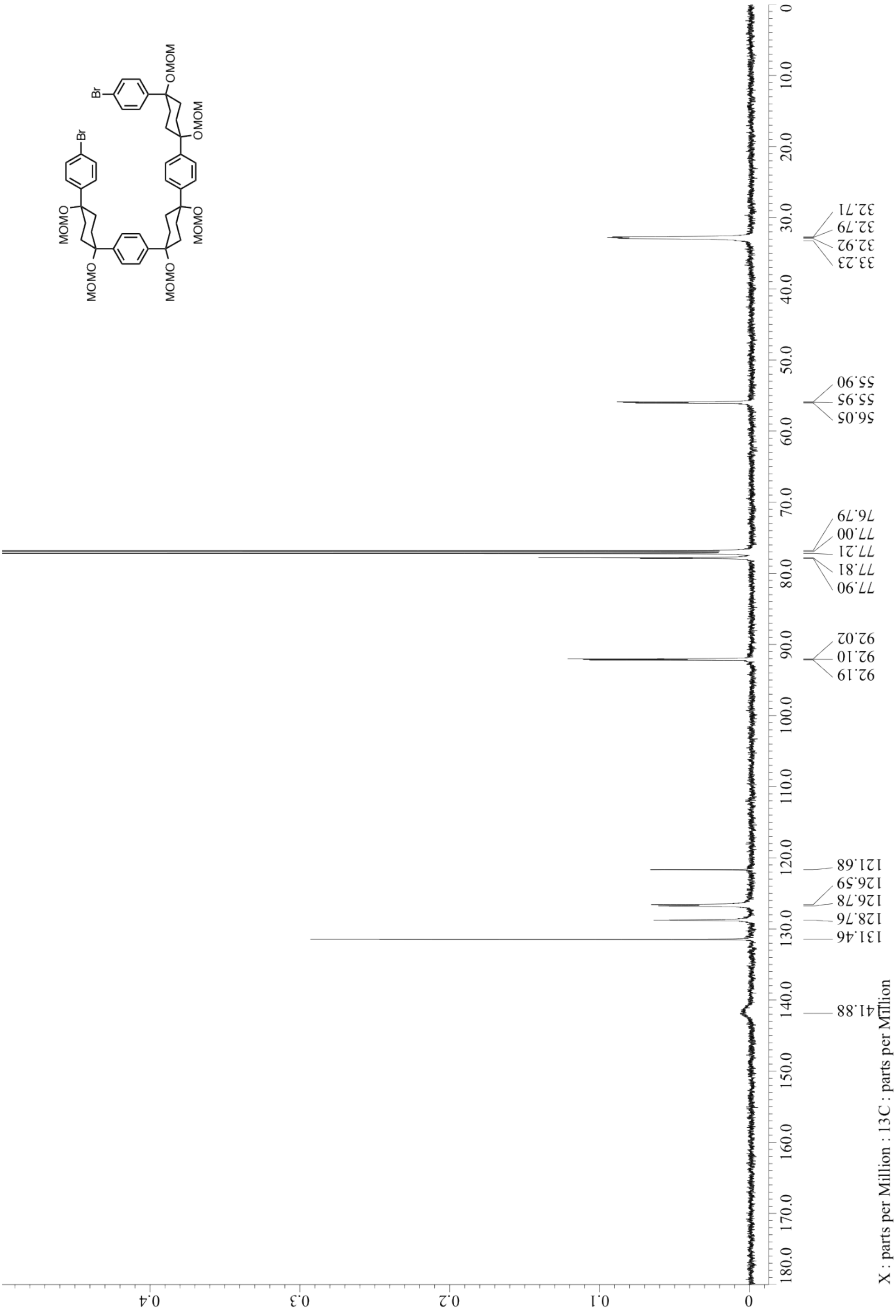
^{13}C NMR spectrum of **3** (CD_2Cl_2)



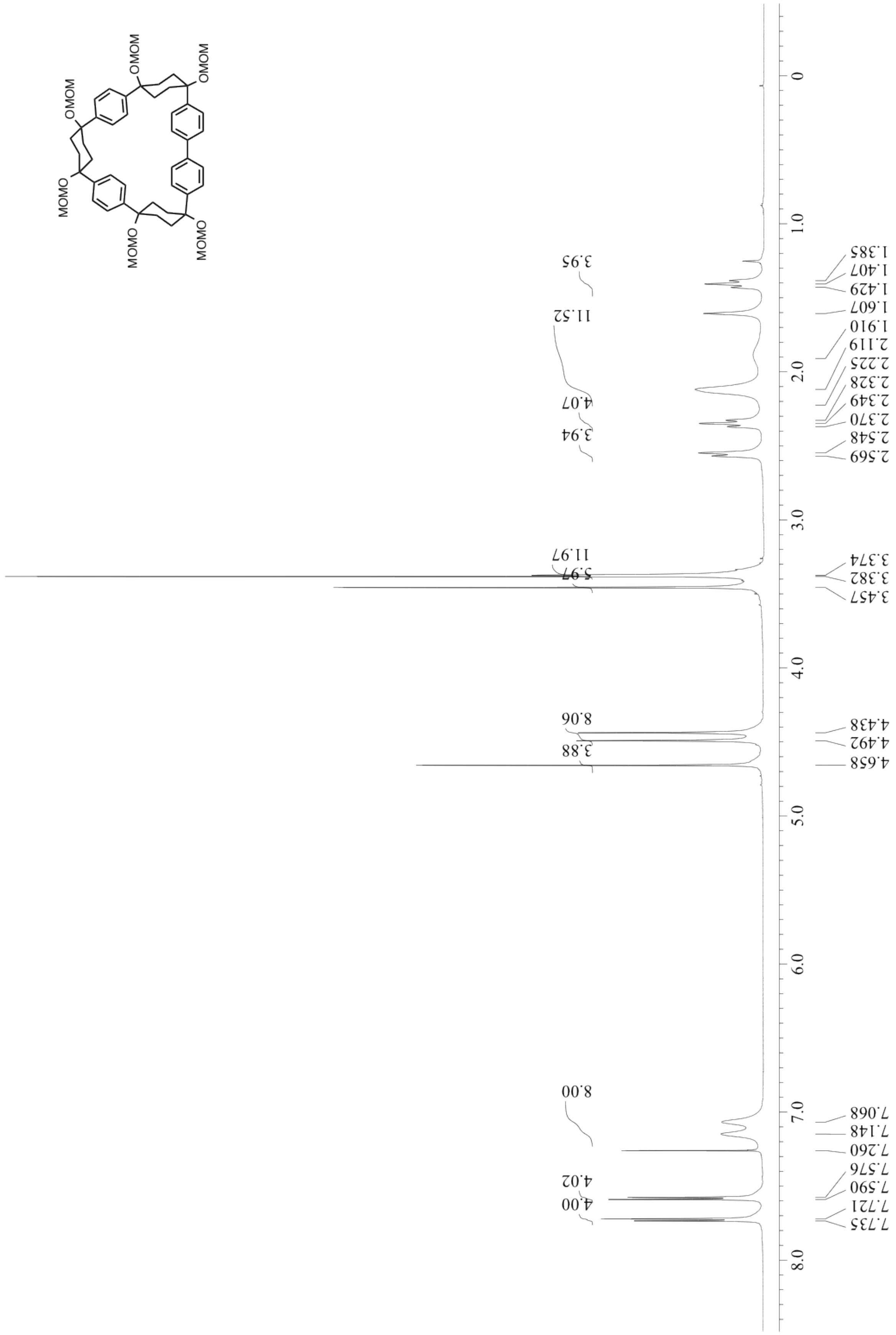
^{1}H NMR spectrum of **4** ($CDCl_3$)



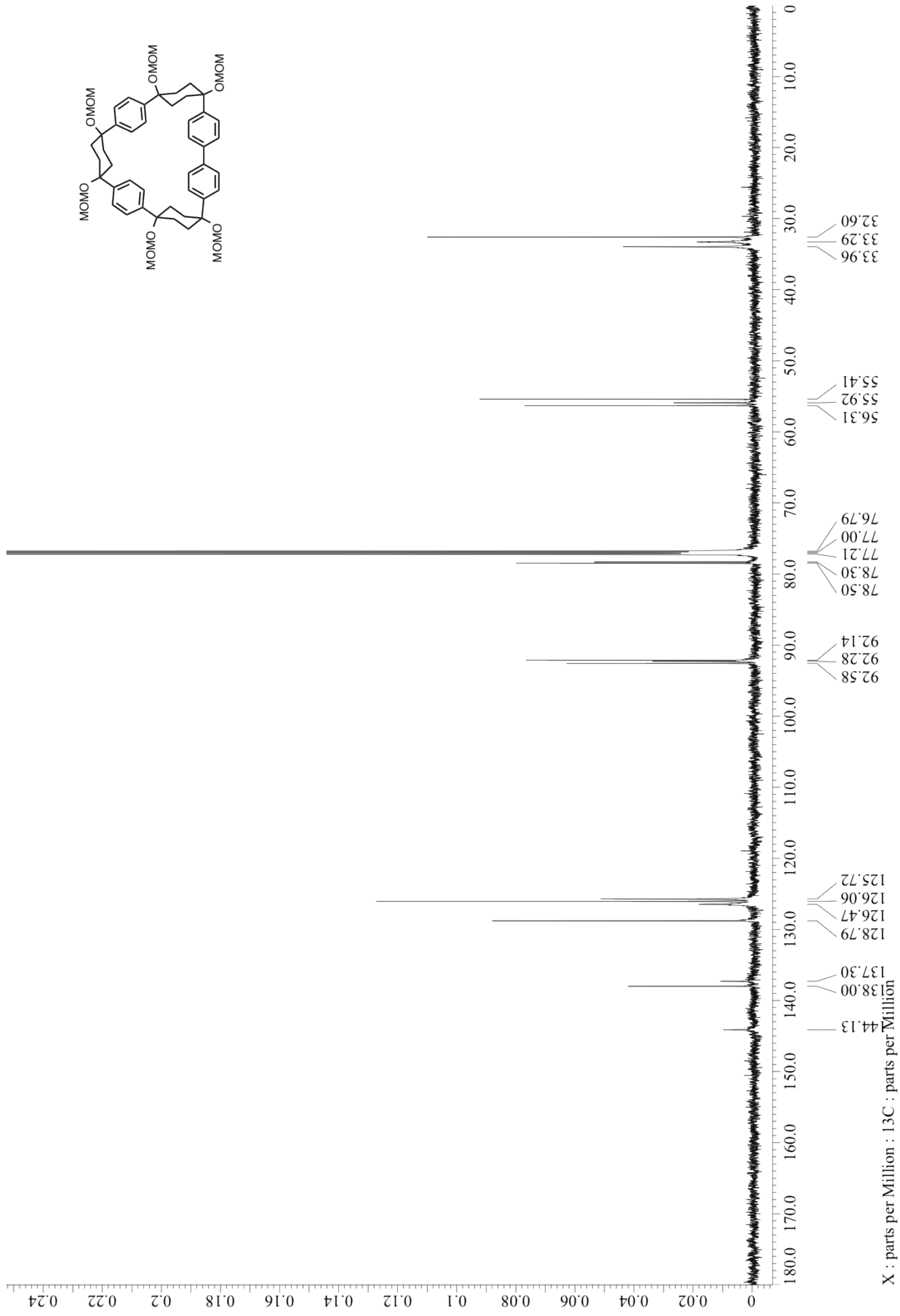
^{13}C NMR spectrum of **4** (CDCl$_3$)



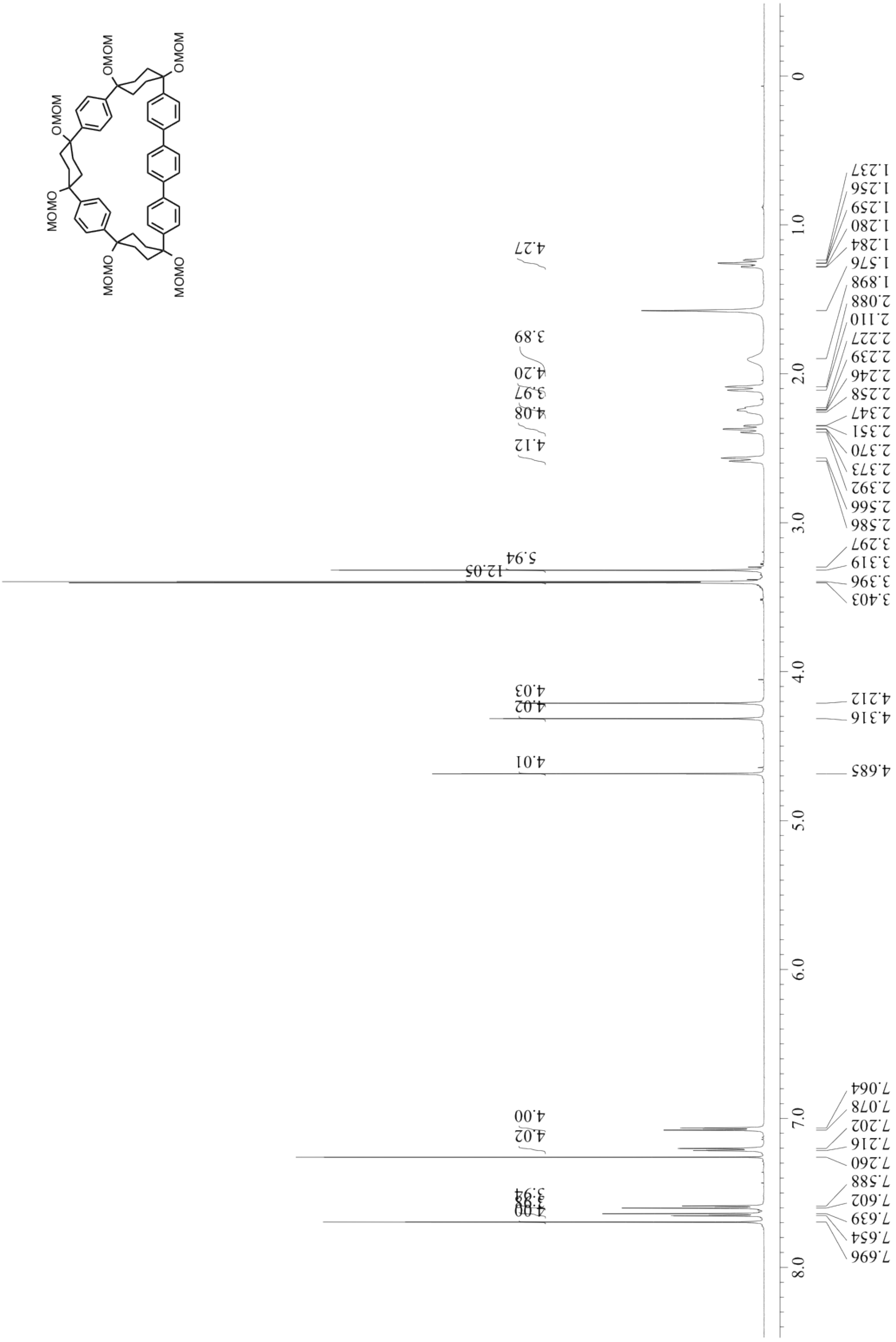
^{1}H NMR spectrum of **5** (CDCl$_3$)



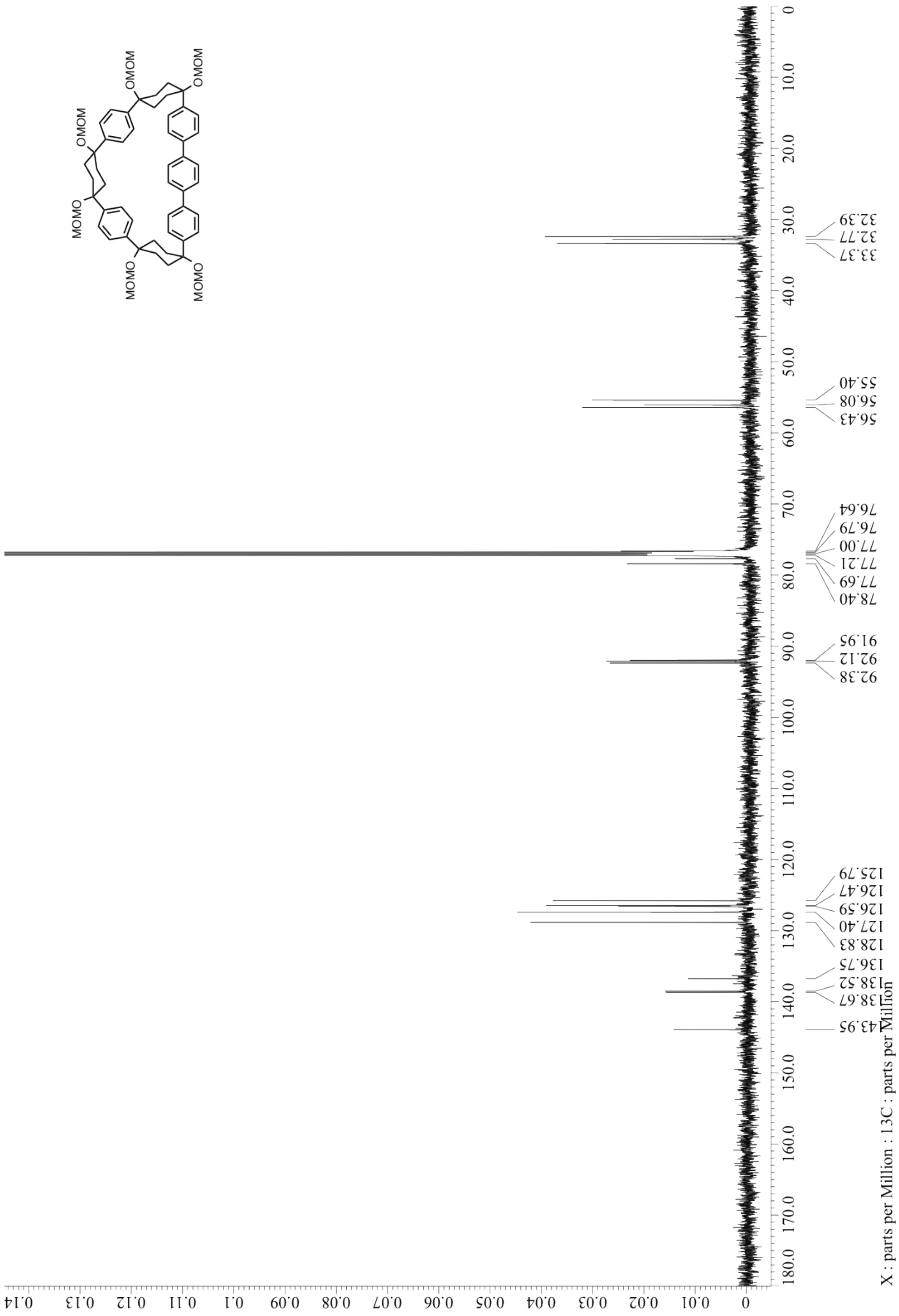
^{13}C NMR spectrum of **5** ($CDCl_3$)



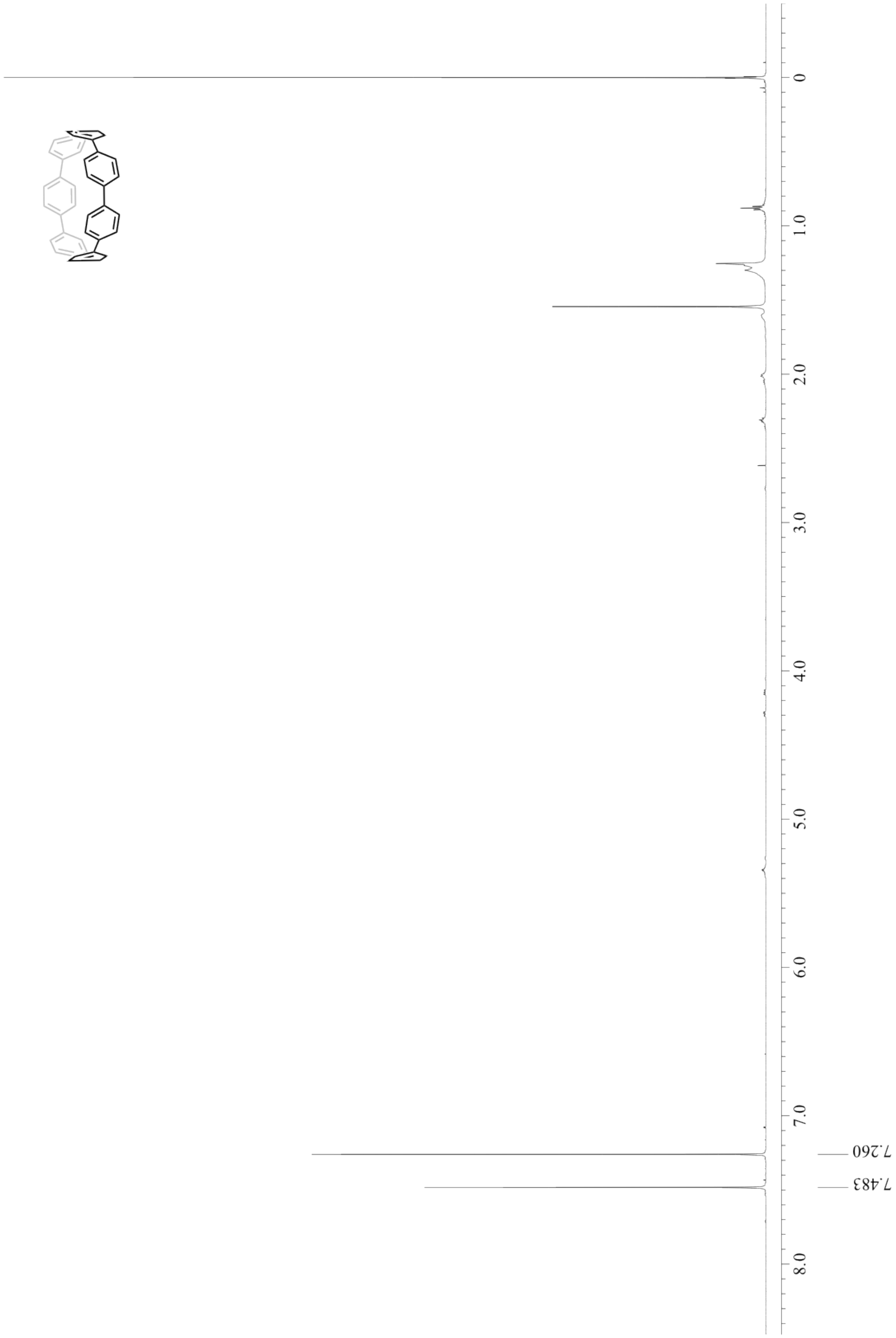
^{1}H NMR spectrum of **6** (CDCl$_3$)



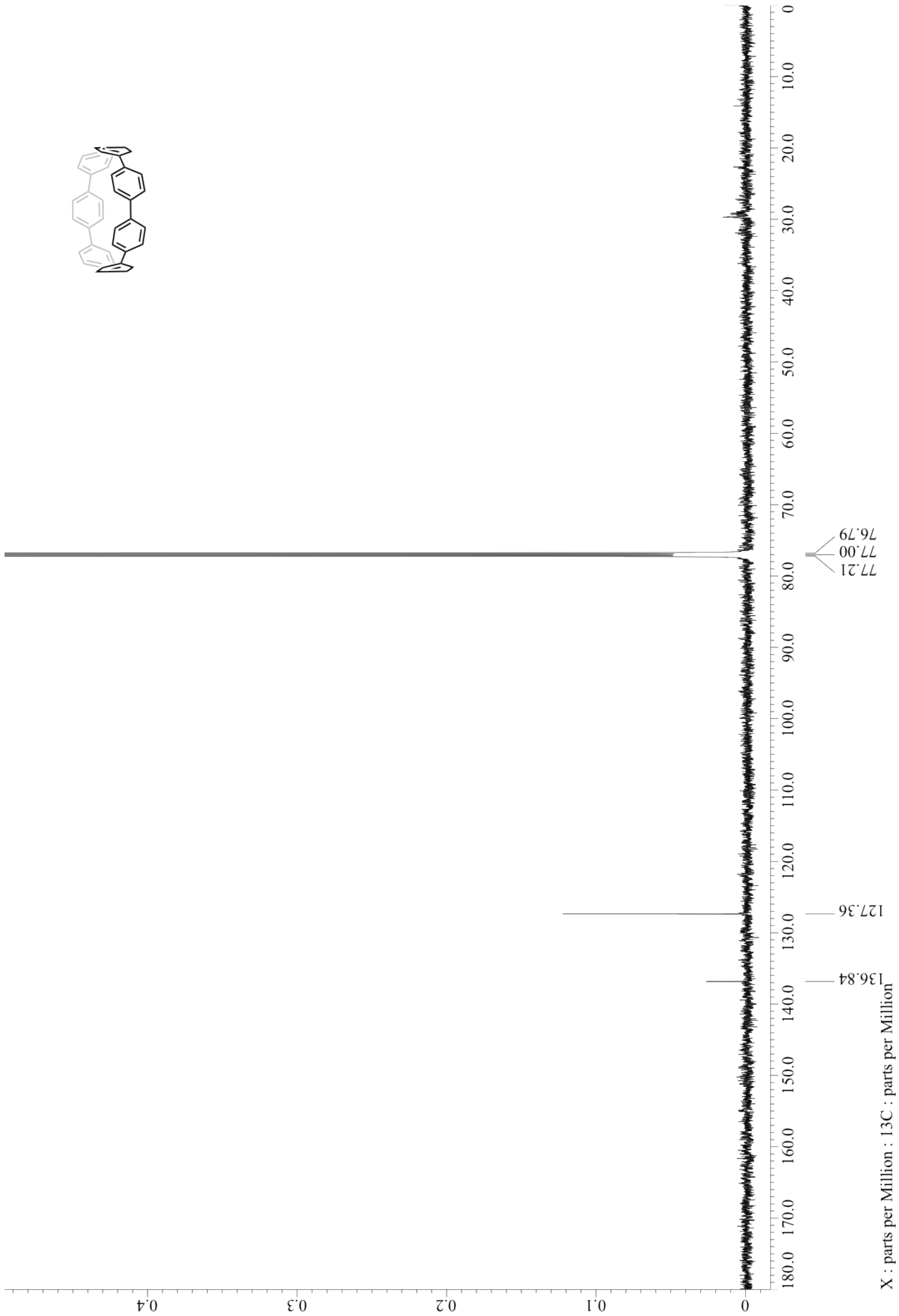
^{13}C NMR spectrum of **6** (CDCl$_3$)



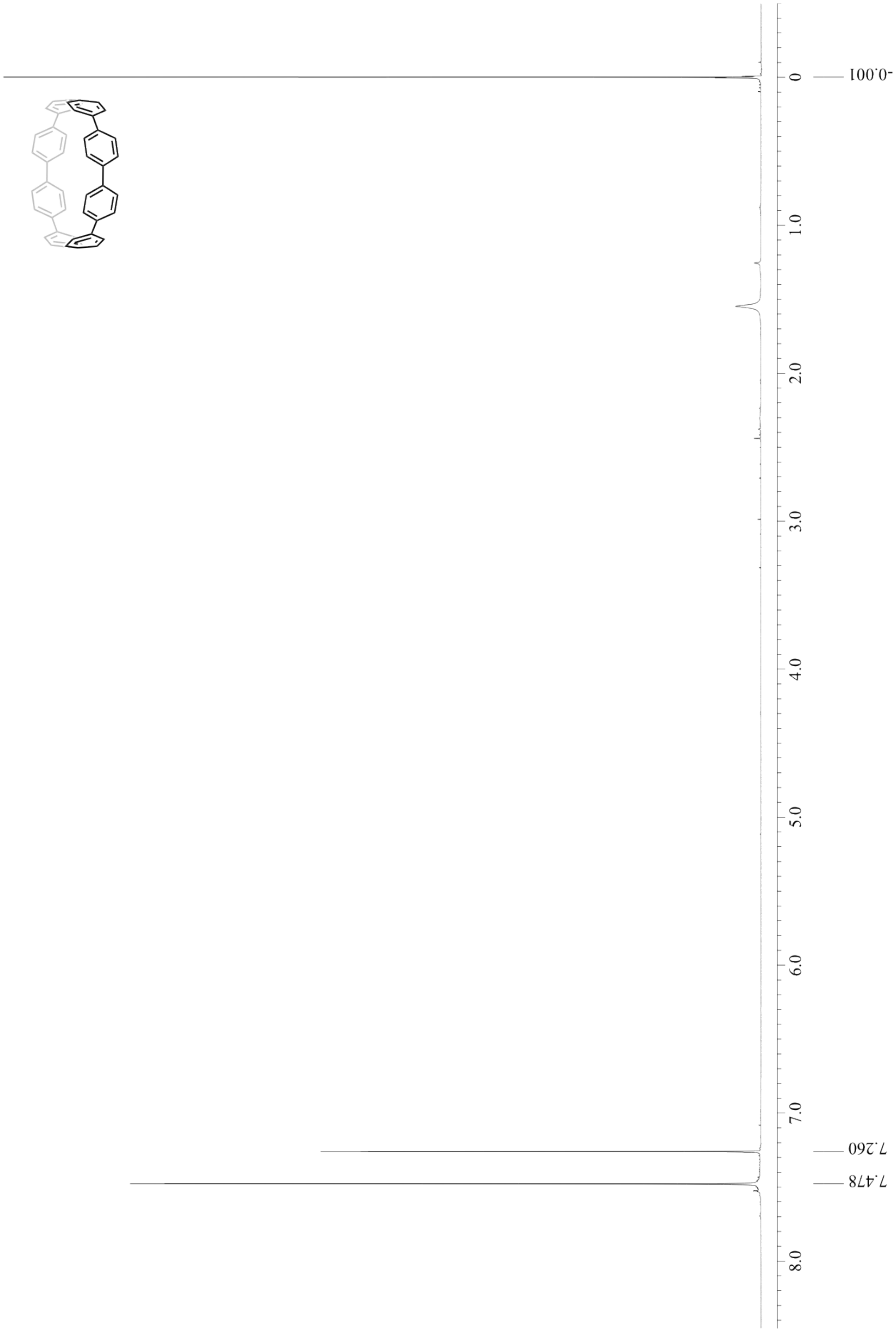
^{1}H NMR spectrum of **[7]CPP** ($CDCl_3$)



^{13}C NMR spectrum of **[7]CPP** ($CDCl_3$)



^{1}H NMR spectrum of **[8]CPP** (CDCl$_3$)



^{13}C NMR spectrum of **[8]CPP** (CDCl$_3$)