

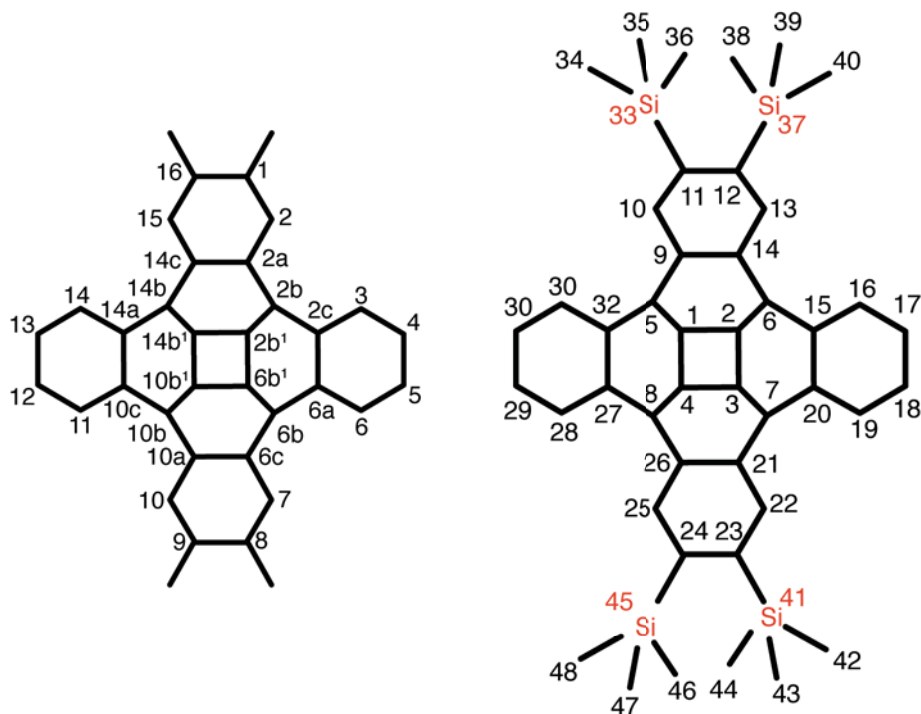
## **Quadrannulene: A Nonclassical Fullerene Fragment\*\***

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## IUPAC nomenclature, IUPAC numbering, and crystallographic numbering

IUPAC recommends the name 1,8,9,16-tetrakis(trimethylsilyl)-5,6:11,12-di[2,3,]naphthalenodibenzo[*b,h*]biphenylene and the numbering below left.



The IUPAC numbering is poorly suited for crystallography. The use of the letters a, b, c, and d conflicts with their to indicate symmetry related atoms, superscripts are not valid for deposition, and the long labels do not work with the most popular crystallographic programs. For this reason, we used an alternative numbering scheme for crystallography (left), arranged to have contiguous numbers in flat rings and TMS groups.

## Synthetic Procedures

All reactions were run under N<sub>2</sub>. Anhydrous ClCl<sub>3</sub> was prepared by drying ClCl<sub>3</sub>•(H<sub>2</sub>O)<sub>7</sub> under vacuum at 140 °C. (1) THF, DME and Et<sub>2</sub>O were distilled from Na and benzophenone.

**Synthesis of 5,5a,5b,6,11,11a,11b,12-octahydro-5,6,11,12-tetrahydroxy-5,6,11,12-tetrakis[(trimethylsilyl)ethynyl]dibenzo[*b,h*]biphenylene (2):** Trimethylsilylacetylene (14.0 mL, 99.1 mmol) was added to a Schlenk flask and THF (20 mL) was added. To this, 1.6 M *n*-BuLi (55.0 mL, 88.0 mmol) was added dropwise at –78 °C. This mixture was stirred for 1 h. Dry CeCl<sub>3</sub> (4.02 g, 16.3 mmol) was added and stirred this again for 30 min. The naphthaquinone dimer **1** (2) (1.00 g, 3.16 mmol) was added in a single dose. The reaction mixture was warmed to room temperature over 12 h and then quenched with a saturated ammonium chloride solution (10 mL) at 0 °C. The mixture was extracted with Et<sub>2</sub>O (30 mL) followed by CHCl<sub>3</sub> (30 mL). The organic extracts were combined and evaporated to dryness. The solid residue was dissolved in chloroform and filtered. The CHCl<sub>3</sub> was evaporated and the resulting residue was washed with acetone to give clean tetraol **1** (1.10 g, 50%) as a single but unidentified diastereomer. mp 225–227 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 0.20 (s, 36H), 3.14 (s, 4H), 3.45 (s, 4H) 7.36 (m, 4H), 7.87 (m, 4H). <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>) δ 0.22, 41.9, 67.7, 91.5, 107.1, 126.9, 128.9, 137.4. Anal. Calcd for C<sub>40</sub>H<sub>52</sub>O<sub>4</sub>Si<sub>4</sub>•H<sub>2</sub>O: C, 66.07, H, 7.48. Found: C, 66.25, H, 7.44.

**Synthesis of 5,6,11,12-tetrakis[(trimethylsilyl)ethynyl]dibenzo[*b,h*]biphenylene:** In a round bottomed flask (250 mL) equipped with a Dean-Stark trap, *p*-TsOH (0.300 g, 1.58 mmol) was added to a solution of **1** (0.500 g, 0.705 mmol) dissolved in toluene (100 mL). Molecular sieves (4 Å, 8–10 beads) were added and solution was refluxed for 8 h with continuous removal of water. The crude reaction became orange-red. This reaction mixture was passed through a silica plug (~10 g SiO<sub>2</sub>). The organic solvents were evaporated and tetraalkyne was purified by column chromatography using hexane: chloroform (8:2). Alternatively, the crude reaction mixture can be washed with hexane to give clean product. (0.150 g, 40%): mp > 295 °C (dec. 280 °C). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 0.38 (s, 36H), 7.45 (m, 4H), 8.20 (m, 4H). <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>) δ 0.4, 100.7, 107.0, 112.2, 127.3, 127.8, 135.4, 145.7. Anal. Calcd for C<sub>40</sub>H<sub>44</sub>Si<sub>4</sub>: C, 75.41, H, 6.96. Found: C, 75.33, H, 7.01. λ<sub>max</sub> (log ε) 462 nm (4.6), 430 nm (4.4) 392 nm (4.4) 363 nm (4.7) 336 nm (5.2) 284 nm (4.9).

**Synthesis of 5,6,11,12-Tetraethynyldibenzo[*b,h*]biphenylene (3):** A methanolic solution of KOH (1.70 g, 30.3 mmol) was added to a solution of **2** (0.200 g, 0.314 mmol) in Et<sub>2</sub>O (200 mL) and methanol (10.0 mL). The mixture was stirred for 1 h, becoming turbid. Water (50 mL) quench, extraction with Et<sub>2</sub>O (2 × 50 mL), and evaporation of the solvent gave **3** (0.110 g, 96.3%) mp 130 °C dec. <sup>1</sup>H NMR δ [400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO] δ 4.90 (s, 4H), 7.63 (m, 4H), 8.12 (m, 4H). <sup>13</sup>C NMR δ [400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO] δ 77.4, 92.3, 111.2, 126.8, 128.8, 134.0, 146.5. HRMS calcd for C<sub>28</sub>H<sub>12</sub> 348.0939, found 348.0878.

**Synthesis of TMS<sub>4</sub>-TBQ:** To a solution of **3** (40.0 mg, 0.115 mmol) in dry DME (50.0 mL), bis(trimethylsilyl)acetylene (5.00 mL) was added. To this solution, Jonas catalyst (40.0 mg, 0.222 mmol) was added. The reaction mixture was stirred at room temperature for 24 h. The reaction was quenched with ferrocenium hexafluorophosphate (72.0 mg, 0.218 mmol). The solvents were evaporated under vacuum. The product was purified by column chromatography with hexane to give TMS<sub>4</sub>-TBQ (2.2 mg, 3%). mp 142 °C dec. <sup>1</sup>H NMR (500 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 0.50 (s, 36H), 7.57 (m, 4H), 8.63 (m, 4H), 8.93 (s, 4H). <sup>13</sup>C NMR δ (500 MHz, CD<sub>2</sub>Cl<sub>2</sub>) 2.2, 127.6 (C<sub>3</sub>, C<sub>6</sub>, C<sub>11</sub>, C<sub>14</sub>), 127.7 (C<sub>4</sub>, C<sub>5</sub>, C<sub>12</sub>, C<sub>13</sub>), 128.8 (C<sub>2b</sub>, C<sub>6b</sub>, C<sub>10b</sub>, C<sub>14b</sub>), 133.9 (C<sub>2</sub>, C<sub>7</sub>, C<sub>10</sub>, C<sub>15</sub>), 140.6 (C<sub>2a</sub>, C<sub>6c</sub>, C<sub>10a</sub>, C<sub>14c</sub>), 141.9

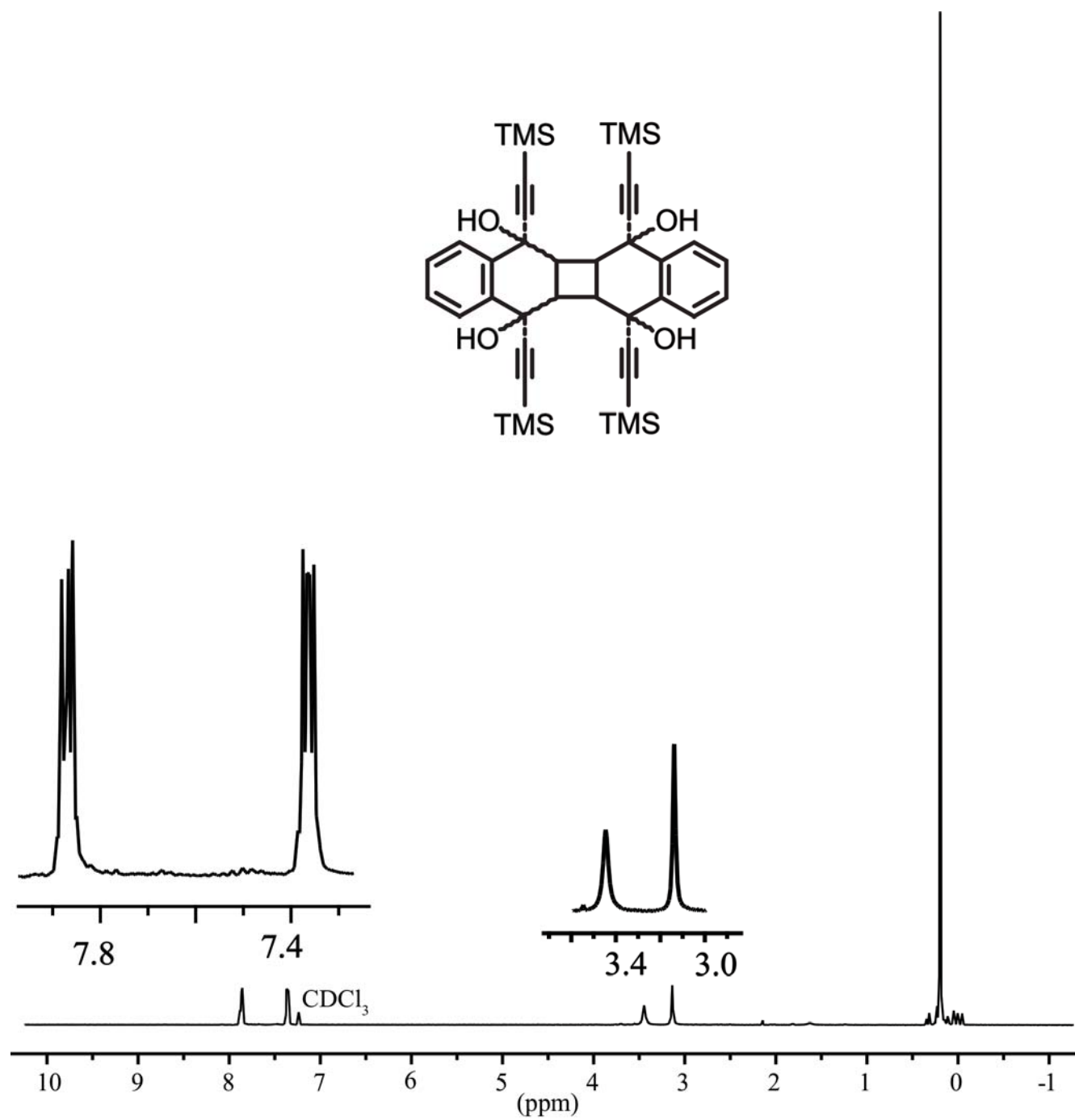
(C<sub>2c</sub>, C<sub>6a</sub>, C<sub>10c</sub>, C<sub>14a</sub>), 145.3 (C<sub>2b'</sub>, C<sub>6b'</sub>, C<sub>10b'</sub>, C<sub>14b'</sub>), 145.5 (C<sub>1</sub>, C<sub>8</sub>, C<sub>9</sub>, C<sub>16</sub>). HRMS calcd for C<sub>44</sub>H<sub>48</sub>Si<sub>4</sub> 688.2833, found 688.2890.  $\lambda_{\text{max}}$  (log  $\epsilon$ ) 323 nm (3.90), 241 nm (3.89).

References:

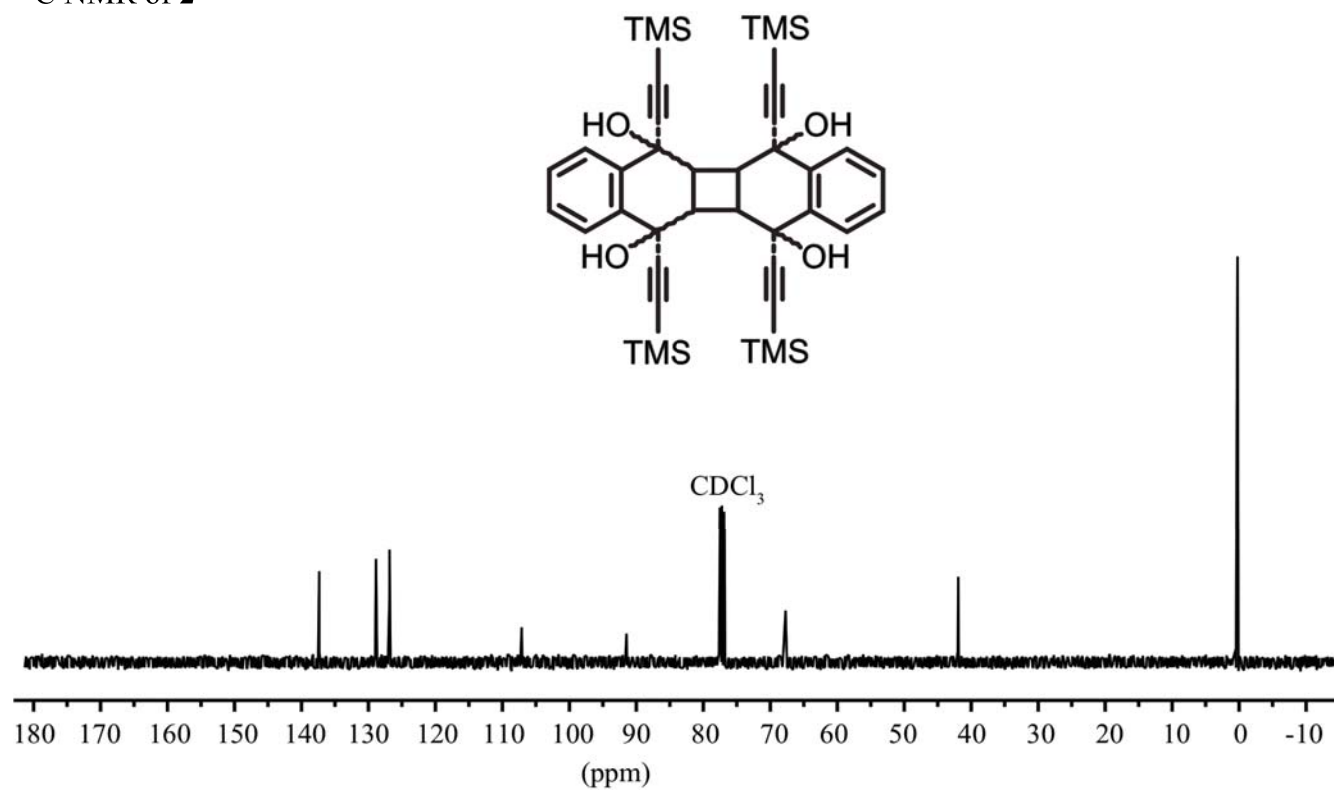
- (1) V. Dimitrov, K. Kostova, M. Genov, *Tetrahedron Lett.* **37**, 6787-6790 (1996).
- (2) Cammack, J. K.; Jalisatgi, S.; Matzger, A. J.; Negrón, A.; Vollhardt, K. P. C. *J. Org. Chem.* **1996**, *61*, 4798-4800.
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NMR spectra

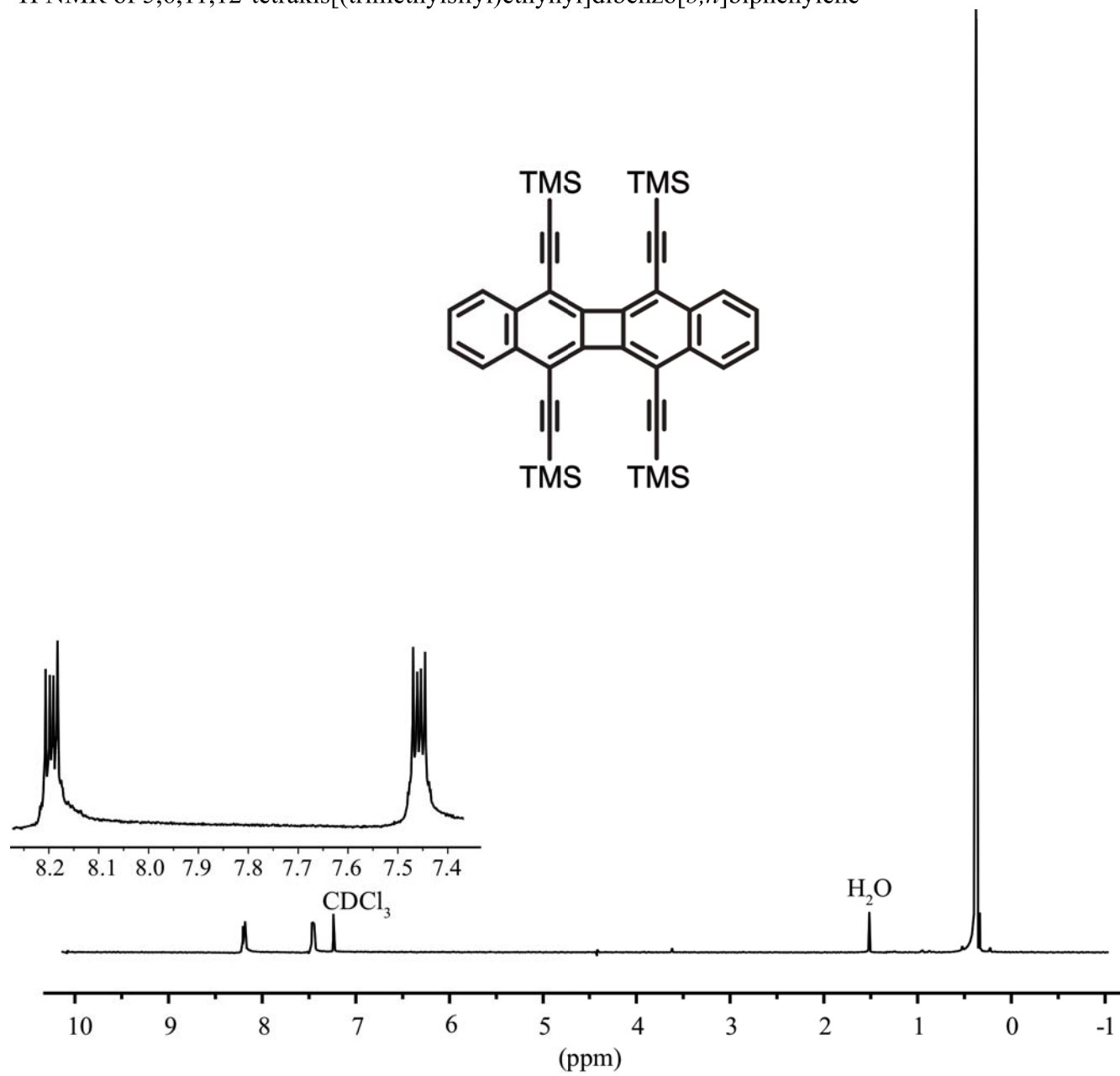
$^1\text{H}$  NMR of **2**



$^{13}\text{C}$  NMR of **2**

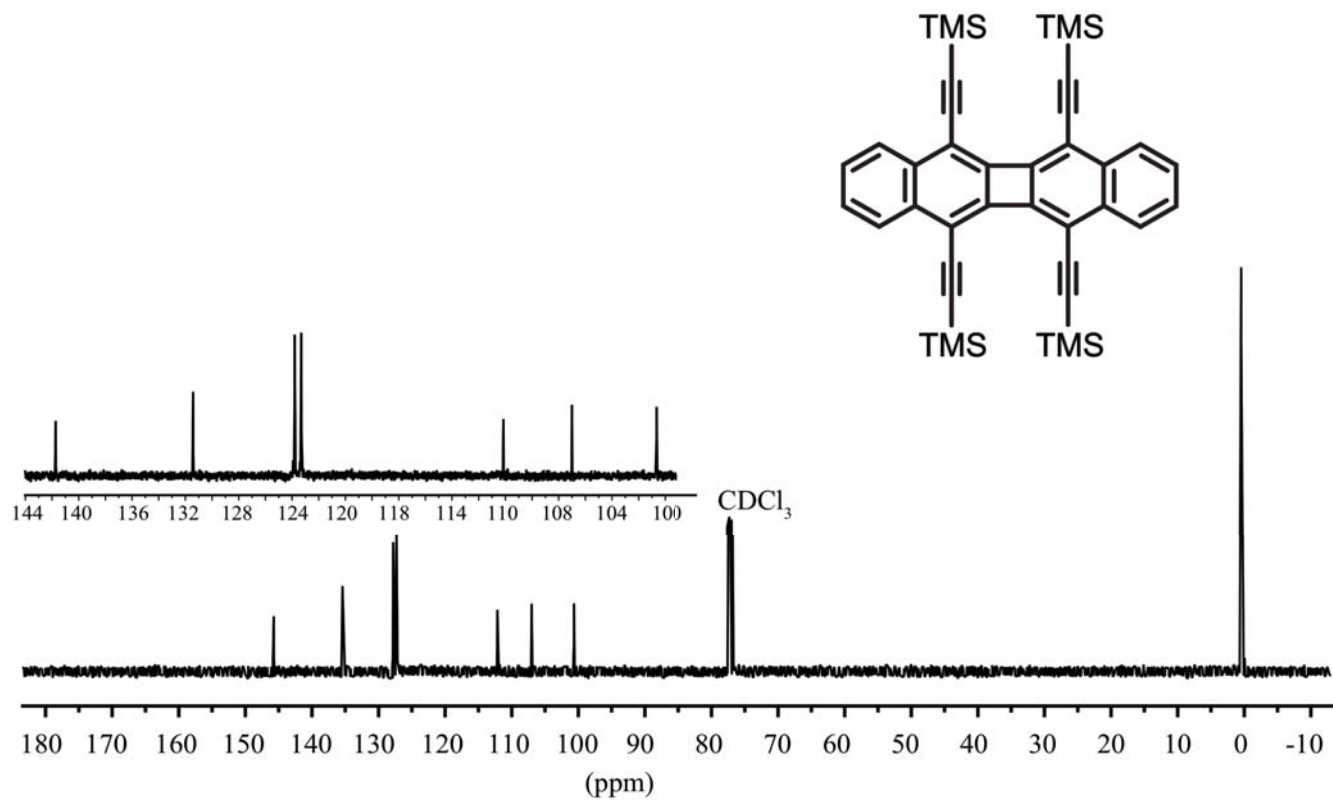


$^1\text{H}$  NMR of 5,6,11,12-tetrakis[(trimethylsilyl)ethynyl]dibenzo[*b,h*]biphenylene

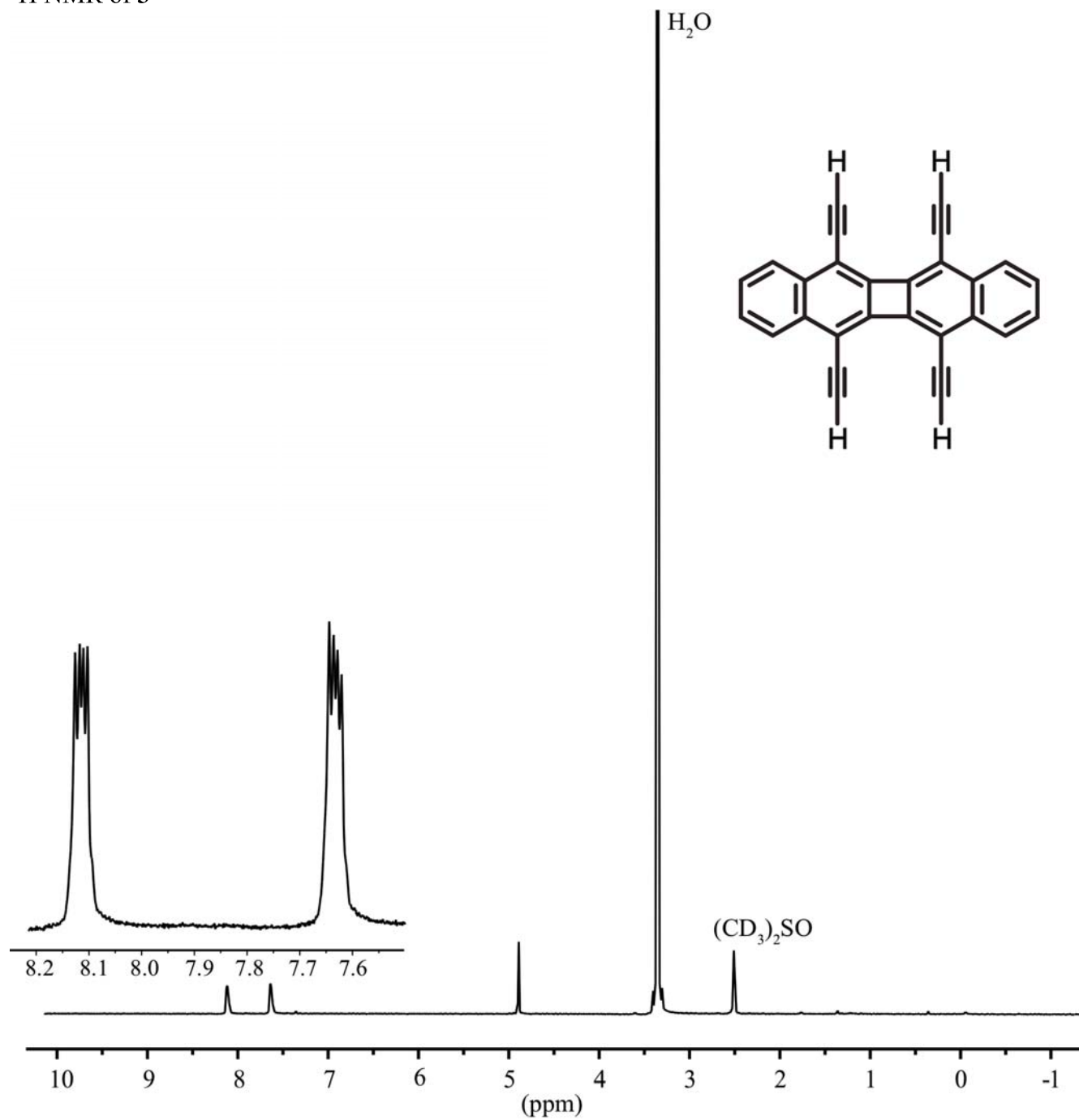




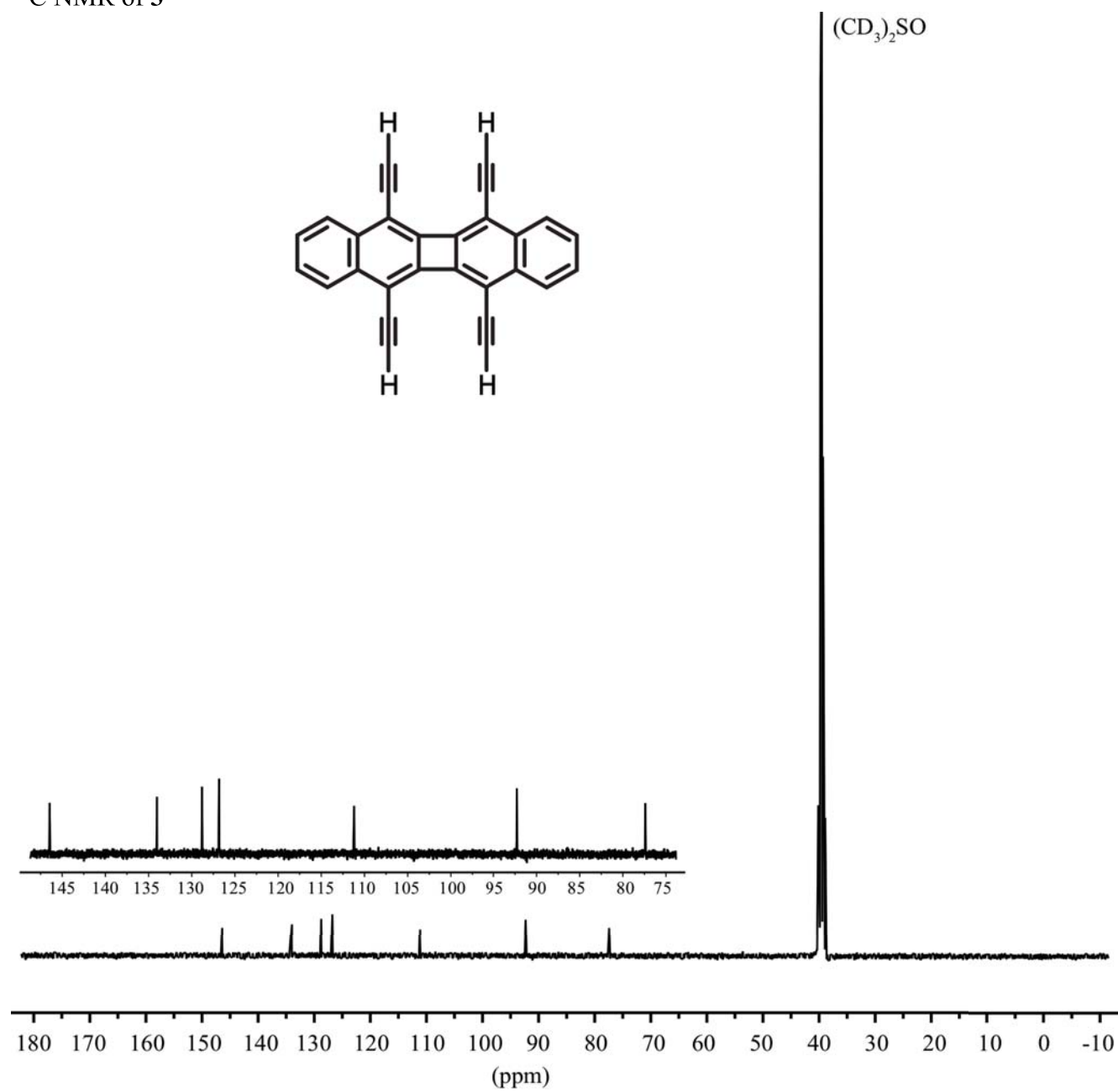
$^{13}\text{C}$  NMR of 5,6,11,12-tetrakis[(trimethylsilyl)ethynyl]dibenzo[*b,h*]biphenylene



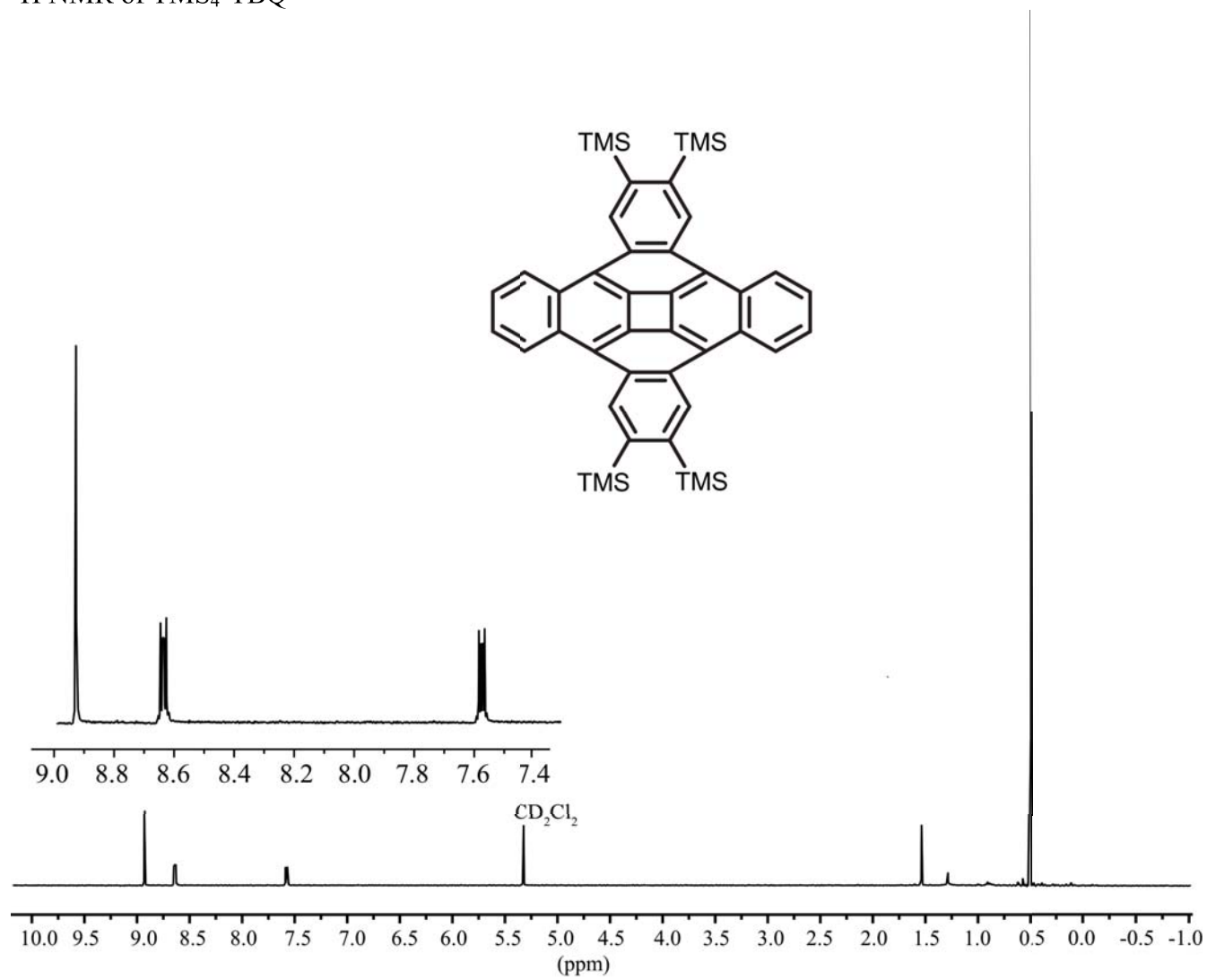
$^1\text{H}$  NMR of **3**



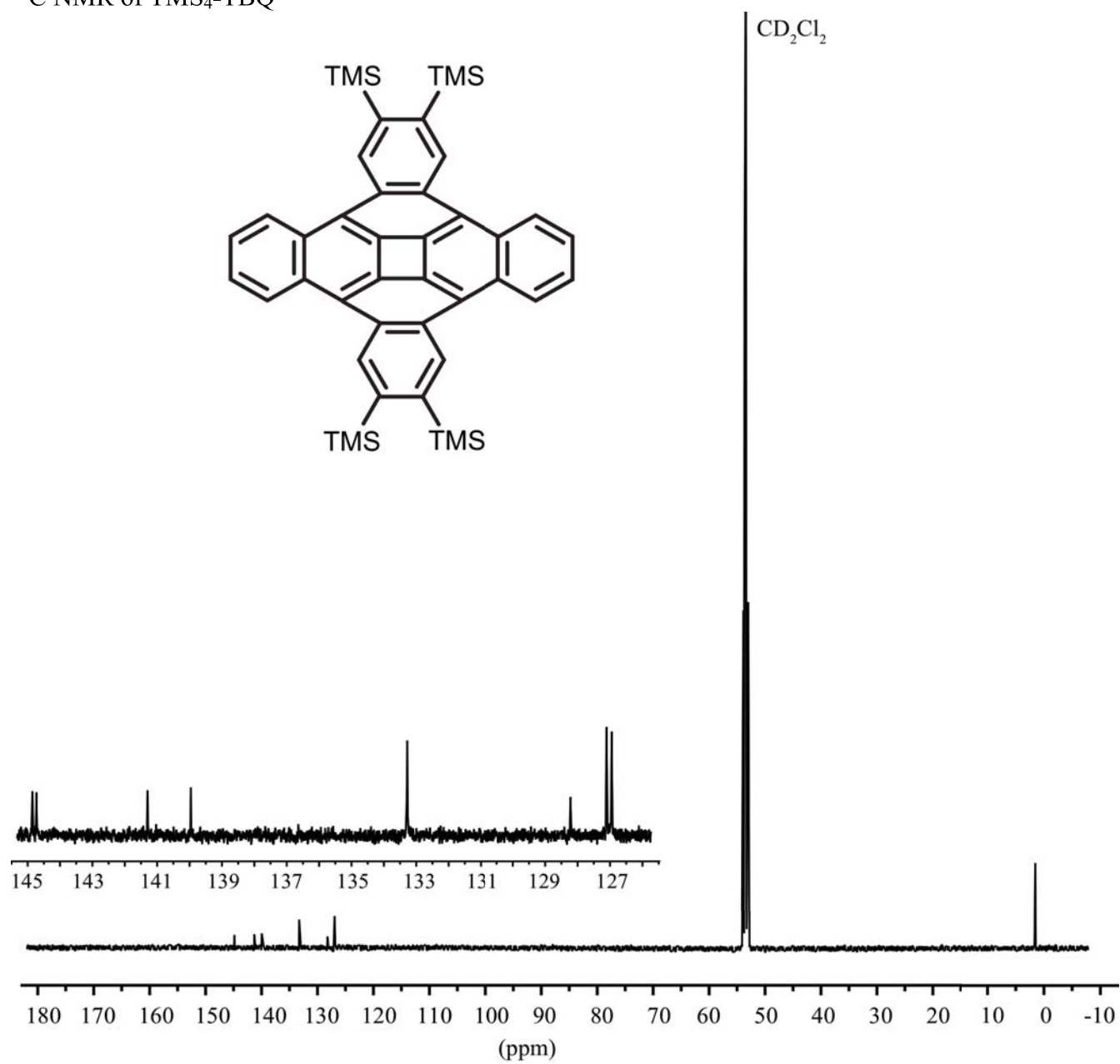
$^{13}\text{C}$  NMR of **3**



$^1\text{H}$  NMR of  $\text{TMS}_4\text{-TBQ}$

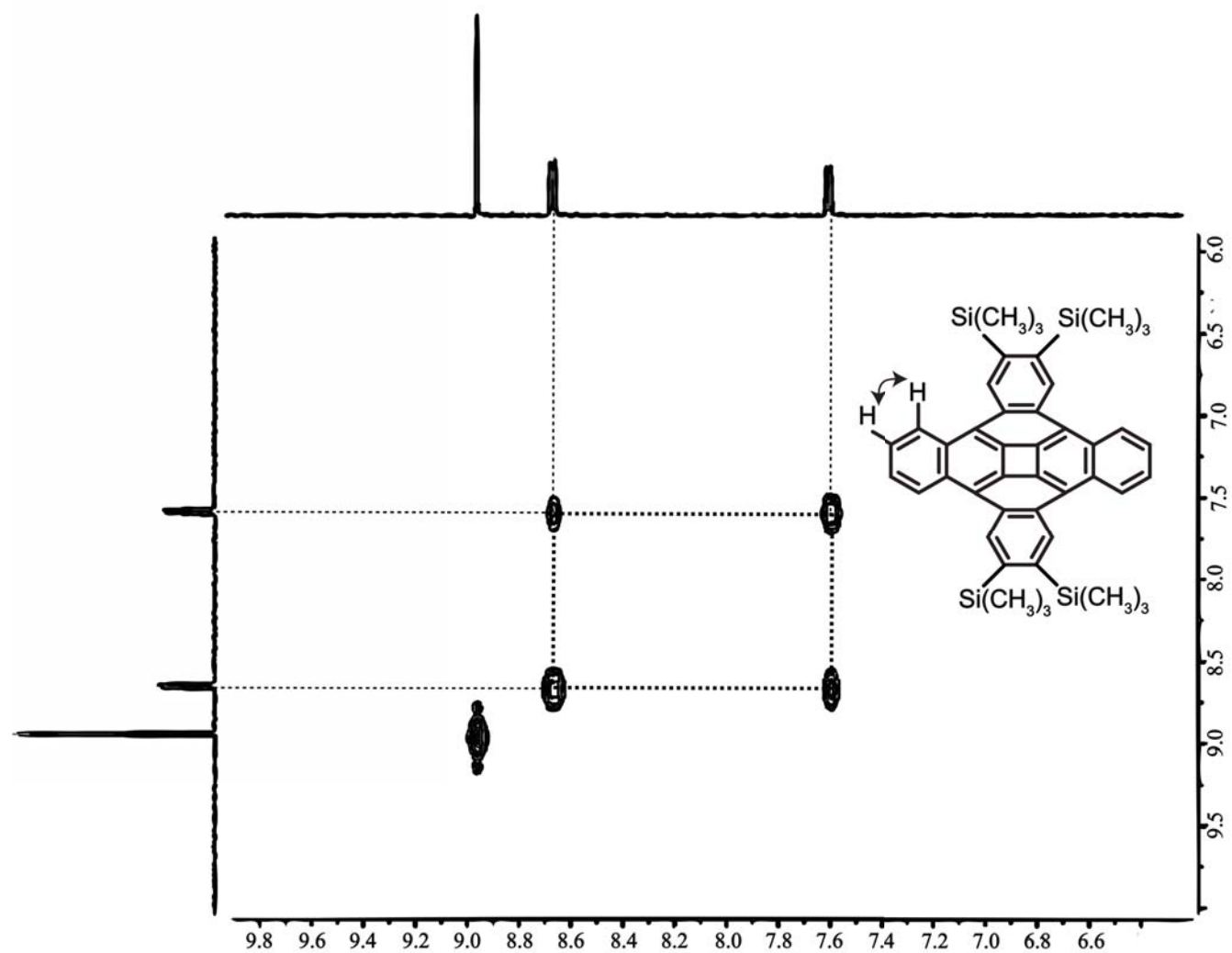


$^{13}\text{C}$  NMR of  $\text{TMS}_4\text{-TBQ}$

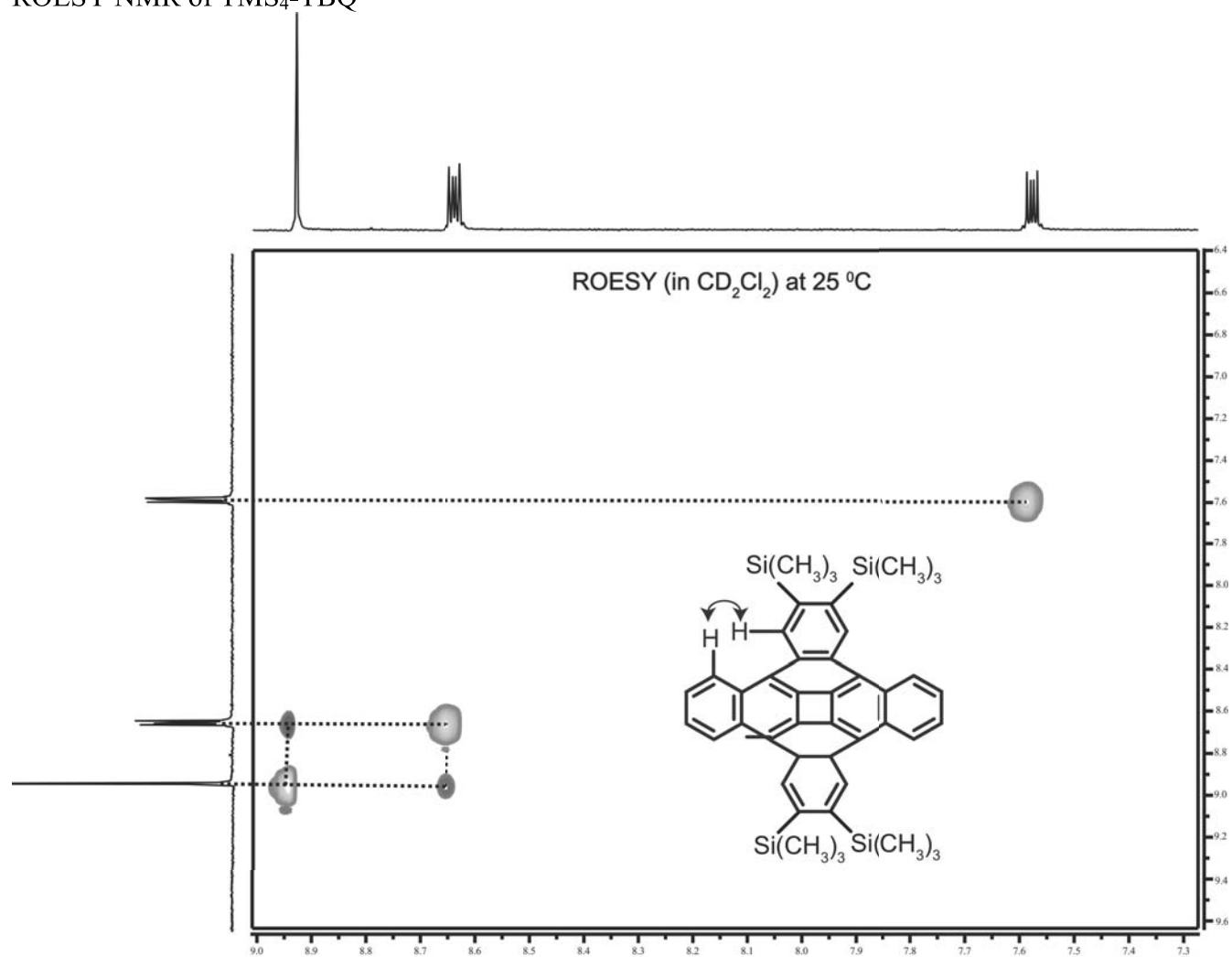


COSY NMR of TMS<sub>4</sub>-TBQ

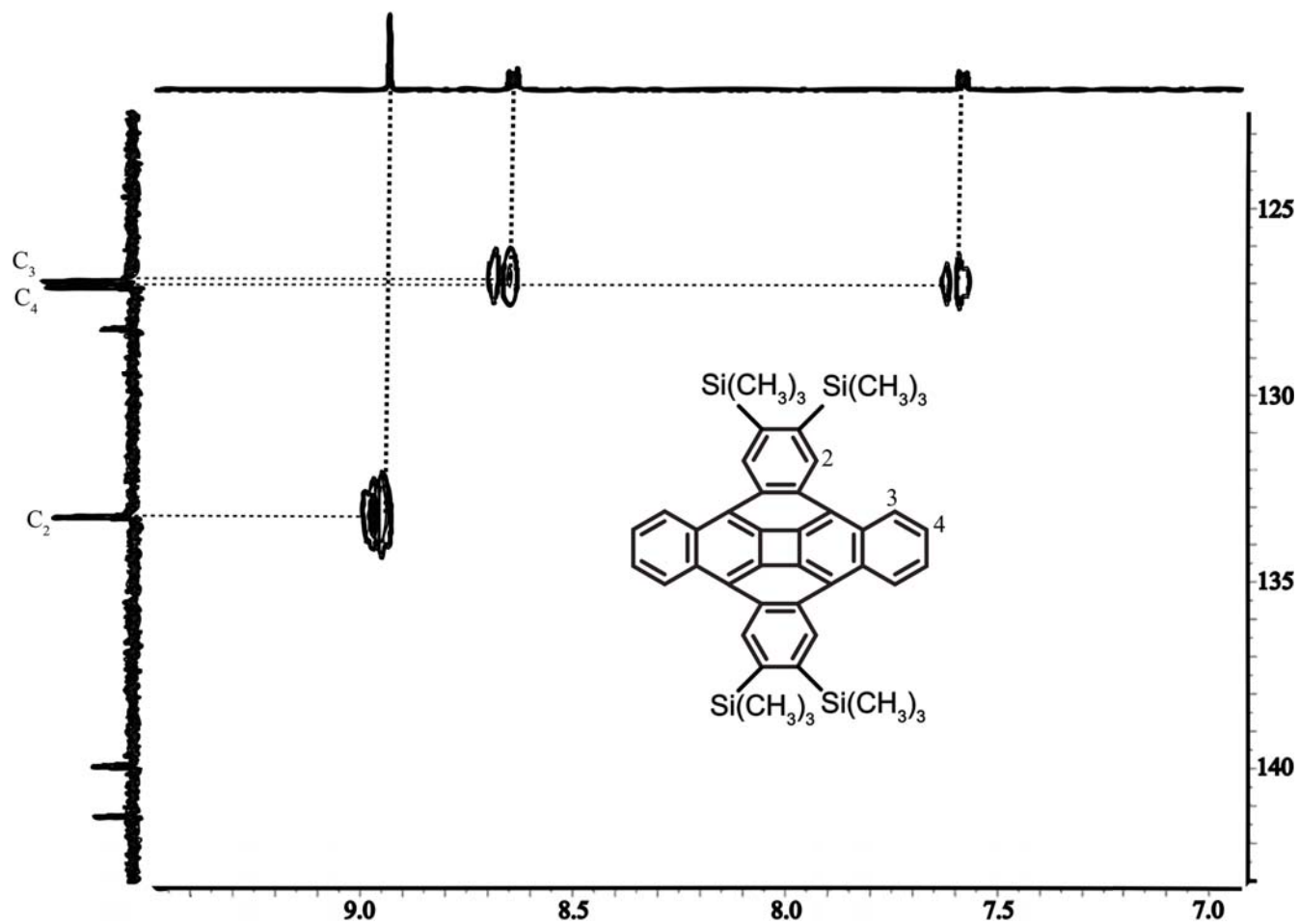
HH-COSY (in CD<sub>2</sub>Cl<sub>2</sub>) at 25 °C



# ROESY NMR of TMS<sub>4</sub>-TBQ

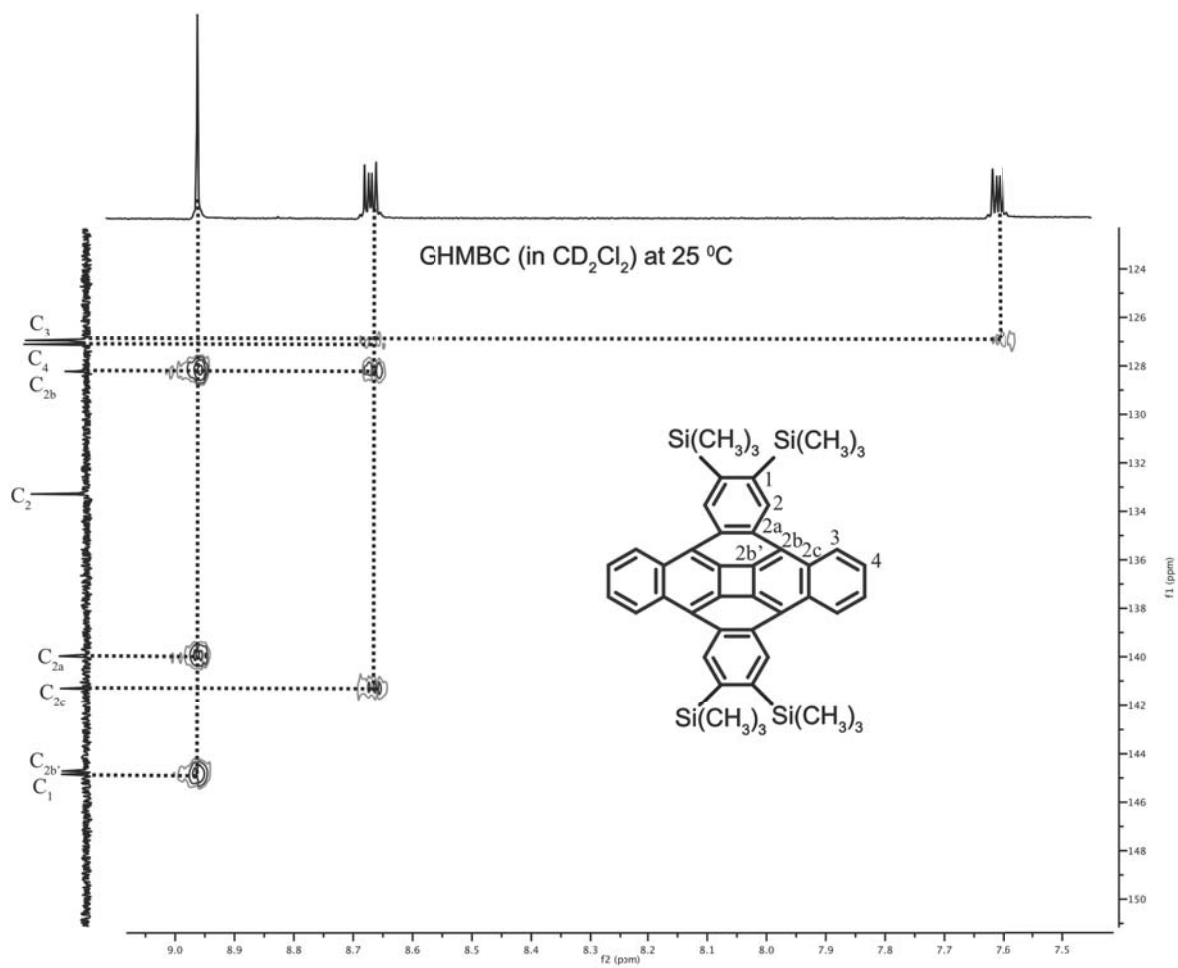


GHSQC (in CD<sub>2</sub>Cl<sub>2</sub>) at 25 °C





# HMBC NMR of TMS<sub>4</sub>-TBS



## Crystallography: **Experimental**

All measurements of the crystal were performed on an Oxford Diffraction Gemini  $\kappa$ -axis diffractometer with graphite-monochromated Enhance MoK $\alpha$  X-ray Source. The crystal was positioned at 55 mm from the CCD camera. 458 frames were measured at 0.5° intervals with a counting time of 120 sec. The data were corrected for Lorentz and polarization effects. Empirical correction for absorption was applied.<sup>[1]</sup> Data reduction and analysis were carried out with the Oxford Diffraction programs.<sup>[2]</sup>

The structure was solved by direct methods<sup>[3]</sup> and refined using WinGX<sup>[4]</sup> and SHELXL.<sup>[5]</sup> The refinement was based on  $F^2$  for all reflections except those with very negative  $F^2$ . Weighted R factors wR and all goodness-of-fit S values are based on  $F^2$ . Conventional R factors are based on F with F set to zero for negative  $F^2$ . The  $F_o^2 > 2\sigma(F_o^2)$  criterion was used only for calculating R factors and is not relevant to the choice of reflections for the refinement.

Structure contains fully disordered organic molecule occupying two possible positions with the ratio of refined occupancy equal to 0.618(3):0.382(3). In the much occupied site the following restraints were used:

DFIX 1.45 0.01 c1 c2 c2 c3 c3 c4 c4 c1 (only one geometric restraint applied for the central square ring)

DELU 0.01 c31 c32

ISOR 0.010 c1 c3 c8 c13 c15 c16 c17 c20 c27 c36 c38 c46 c47 c48

ISOR 0.005 c5 c9 c12 c24

ISOR 0.002 c11

In this residue all non-hydrogen atoms were refined with anisotropic temperature factors.

Because of lower occupancy meaning smaller charge density for the second residue more geometric restraints were used:

FLAT c5b c6b c9b c10b c11b c12b c13b c14b

FLAT c6b c7b c15b c16b c17b c18b c19b c20b

FLAT c8b c5b c27b c28b c29b c30b c31b c32b

SADI c1b c14b c2b c9b

SADI c1b c9b c2b c14b

SADI c1b c6b c2b c5b

DFIX 1.39 0.02 c15b c20b

DFIX 1.45 0.01 c1b c2b c2b c3b c3b c4b c4b c1b

SADI c1b c3b c2b c4b

SADI 0.01 c10 c13 c10b c13b

SADI 0.01 c5b c9b c5b c32b

SAME 0.02 0.02 c9b c10b c11b c12b c13b c14b

SAME 0.02 0.02 c10b c11b c12b c13b c14b c9b

SAME 0.02 0.02 c15b c16b c17b c18b c19b c20b

SAME 0.02 0.02 c16b c17b c18b c19b c20b c15b

SAME 0.02 0.02 c27b c28b c29b c30b c31b c32b

SAME 0.02 0.02 c28b c29b c30b c31b c32b c27b

Because of the above reason and also close position of some C atoms 21 of them - in the less occupied residue - were refined with isotropic temperature factors, with 12 of them fixed at  $U_{iso}=0.03$  and 2 at  $U_{iso}=0.09$ . In the case of rest non-H atoms the following restraints and constraints for temperature factors were applied:

SIMU 0.01 c16b c17b c18b

EADP c44 c44b

EADP c10 c10b

ISOR 0.010 c3b c28b c29b c30b c31b c43b c47b

ISOR 0.005 c13b

EADP c14 c14b

EADP c9 c9b

EADP si2 si2b

SIMU 0.01 si1 si1b

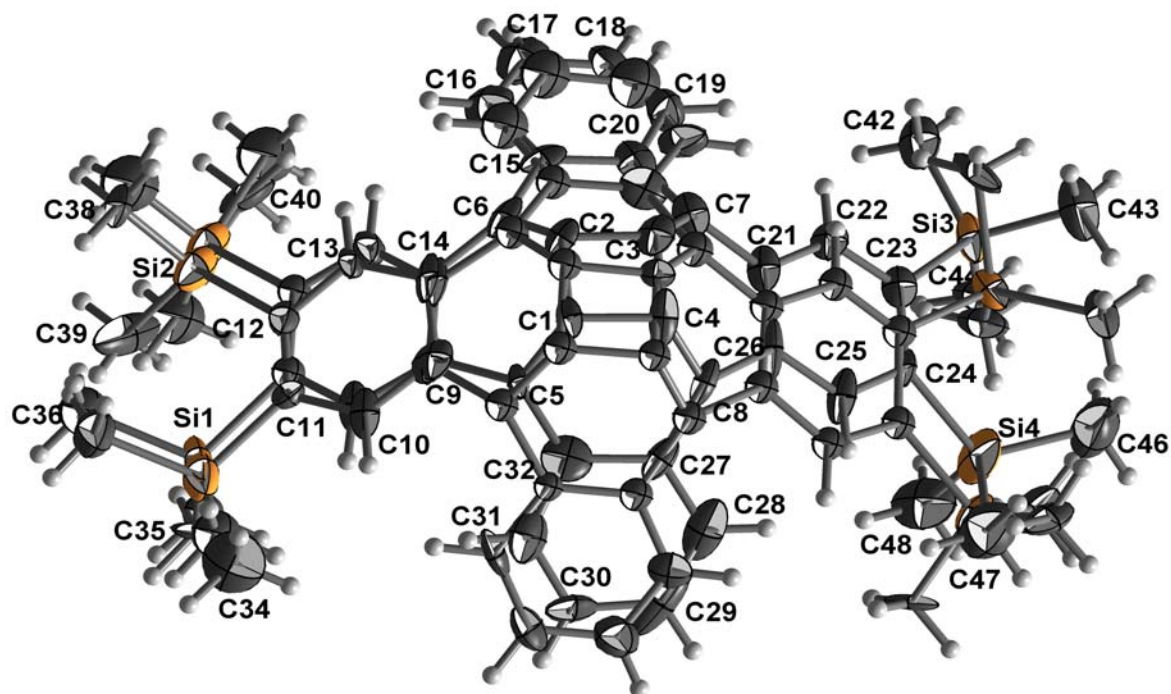
All hydrogen atoms in both residues were located geometrically and their position and temperature factors were not refined. Temperature factors for hydrogen atoms were set to be bigger than  $U_{eq}$  of corresponding C atoms of factor 1.2 and 1.5 for aromatic and methyl group H atoms respectively. Scattering factors were taken from Tables 6.1.1.4 and 4.2.4.2 in Ref. [6].

The structure is chiral. However it contains sufficiently heavy Si atoms the anomalous dispersion signal is rather weak what manifests in large error of the Flack parameter<sup>[7]</sup>. This is due to the disorder and relatively low concentration of Si atoms in the structure. Nevertheless the value of the flack parameter yields 0.11(26).

The ORTEP view of 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene with labeling of atoms in two versions **A** where both components are shown; and **B** where the component having the occupancy at 0.618 level is shown, the figures presenting crystal packing along [001], [010] and [100] directions are presented in subsequent

pages. All figures presenting the results of X-ray diffraction determination were made with use of Diamond program.<sup>[8]</sup> Details of crystal data and structure refinement, atomic coordinates and equivalent isotropic displacement parameters, bond lengths and angles, torsion angles, anisotropic displacement parameters, hydrogen coordinates and isotropic displacement parameters are presented in Tables 1-6 of this Supplementary Information. The carbon and silicon atoms labeled B refer to the fragment having 0.382(3) occupancy.

A



B

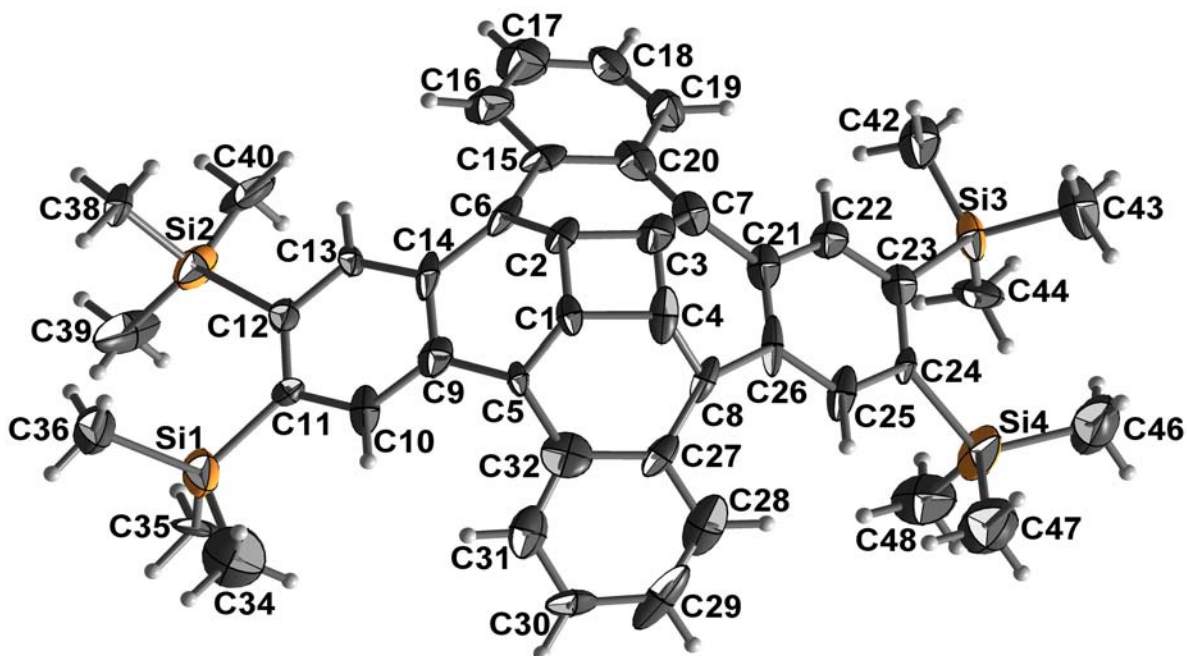


Figure 1. The ORTEP view of 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12 di[2,3]naphthalenodibenz[b,h]biphenylene with labeling of atoms (for clarity only labels of residue with higher occupancy are shown, the second residue has the same numbering scheme with the letter b added at the end). **A** – both components are shown; **B** - the component having the occupancy at 0.618 level. Displacement ellipsoids are drawn at 50% probability level.

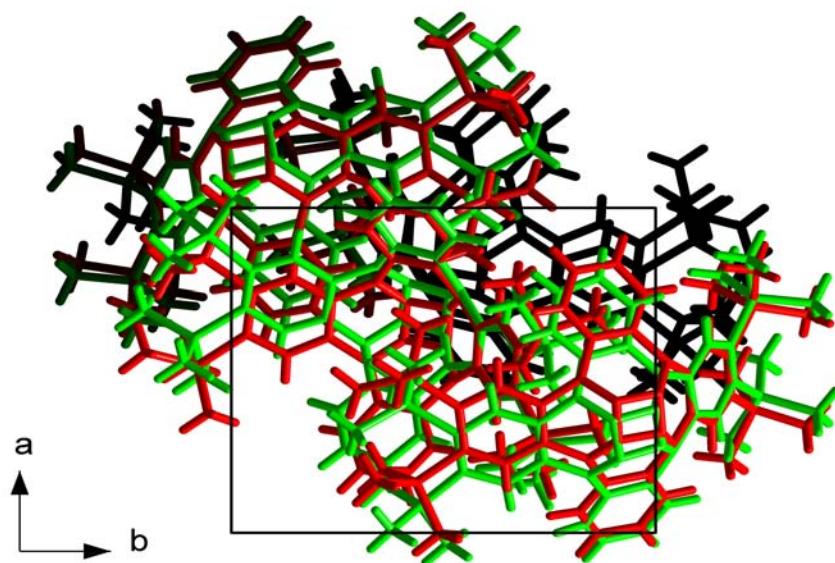


Figure 2. View of the packing of 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene along [001] direction.

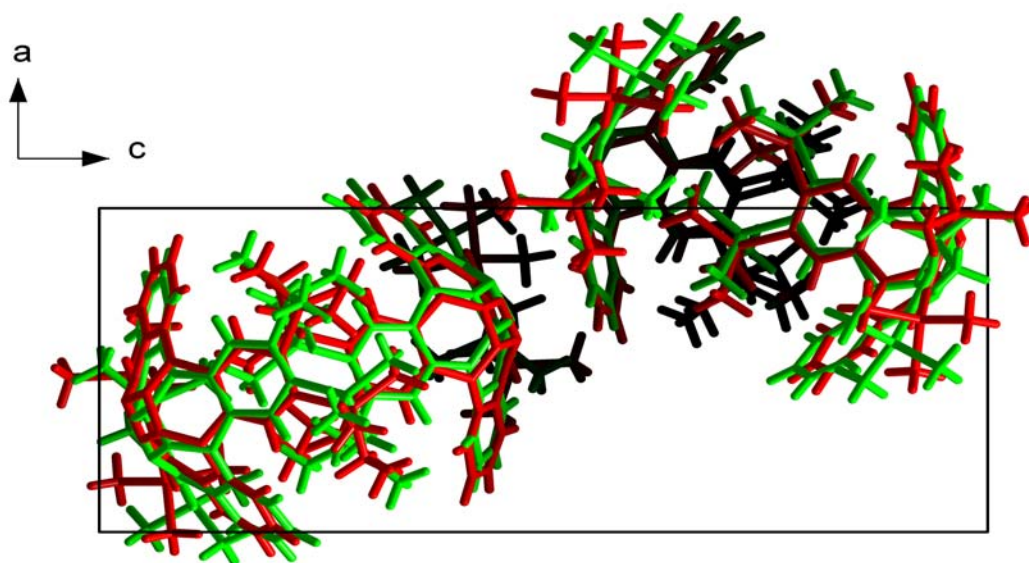


Figure 3. View of the packing of 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene along [010] direction.

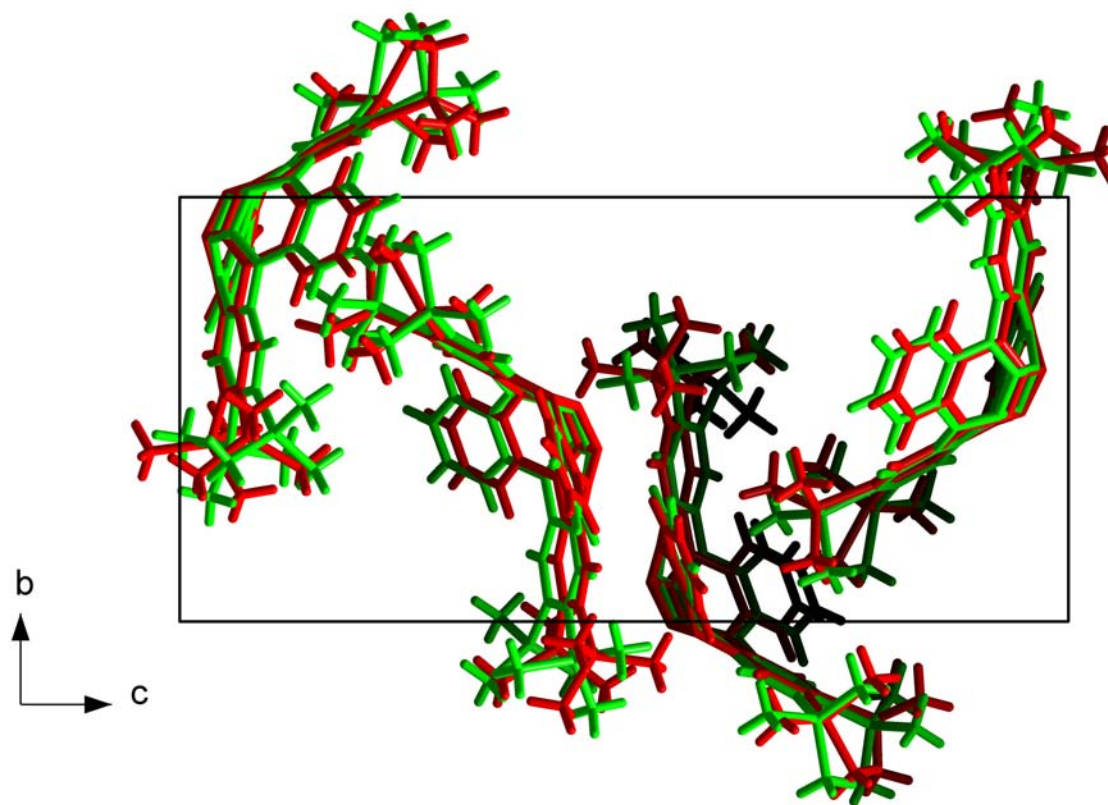


Figure 4. View of the packing of 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene along [100] direction.

Table 1. Crystal data and structure refinement for 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene

Empirical formula	C <sub>44</sub> H <sub>48</sub> Si <sub>4</sub>
Formula weight	689.18
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Unit cell dimensions	a = 11.2176(4) Å b = 12.9731(3) Å c = 27.1727(7) Å
Volume	3954.4(2) Å <sup>3</sup>
Z	4
Calculated density	1.158 Mg/m <sup>3</sup>
Absorption coefficient	0.180 mm <sup>-1</sup>
F(000)	1472
Crystal size	0.40 x 0.15 x 0.04 mm
Theta range for data collection	3.29 to 26.00 deg.
Limiting indices	-13 ≤ h ≤ 13, -15 ≤ k ≤ 16, -33 ≤ l ≤ 32
Reflections collected / unique	20645 / 7684 [R <sub>int</sub> = 0.0409]
Completeness to theta = 26.00	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.993 and 0.650
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	7684 / 297 / 687
Goodness-of-fit on F <sup>2</sup>	1.073
Final R indices [I > 2σ(I)]	R1 = 0.0909, wR2 = 0.2141
R indices (all data)	R1 = 0.1273, wR2 = 0.2267
Absolute structure parameter	0.1(3)
Largest diff. peak and hole	0.447 and -0.361 eÅ <sup>-3</sup>



Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
C(1)	6172(8)	5008(6)	4431(3)	28(2)
C(2)	7322(8)	5154(6)	4209(3)	27(2)
C(3)	7704(11)	4162(7)	4405(4)	39(3)
C(4)	6534(13)	4007(7)	4626(3)	41(3)
C(5)	5121(11)	5113(6)	4166(3)	22(2)
C(6)	7464(13)	5403(10)	3725(4)	36(3)
C(7)	8216(13)	3430(8)	4108(5)	37(3)
C(8)	5826(12)	3134(7)	4557(3)	36(3)
C(9)	5177(14)	5772(10)	3740(5)	39(2)
C(10)	4174(11)	6225(14)	3522(5)	37(2)
C(11)	4218(8)	6751(7)	3061(3)	25(2)
C(12)	5327(9)	6824(8)	2829(4)	33(2)
C(13)	6336(11)	6435(10)	3056(5)	29(3)
C(14)	6340(16)	5914(15)	3511(6)	40(2)
C(15)	8501(11)	4852(8)	3499(5)	38(3)
C(16)	9126(12)	5271(9)	3088(5)	55(3)
C(17)	9950(14)	4710(10)	2845(6)	68(4)
C(18)	10227(11)	3756(10)	3012(5)	55(3)
C(19)	9736(15)	3335(12)	3414(6)	52(3)
C(20)	8833(14)	3842(11)	3672(6)	43(4)
C(21)	7755(12)	2375(7)	4202(3)	37(2)
C(22)	8456(10)	1475(7)	4082(3)	36(2)
C(23)	8105(10)	460(7)	4149(3)	35(2)
C(24)	6947(10)	325(6)	4368(3)	26(2)
C(25)	6245(12)	1208(6)	4498(3)	43(3)
C(26)	6625(15)	2221(8)	4427(4)	47(4)
C(27)	4588(13)	3313(7)	4471(4)	38(2)

C(28)	3780(15)	2539(9)	4545(4)	66(4)
C(29)	2600(30)	2701(12)	4438(6)	74(7)
C(30)	2162(10)	3658(11)	4273(4)	44(3)
C(31)	2990(15)	4441(11)	4214(5)	54(3)
C(32)	4232(14)	4319(10)	4283(4)	48(3)
Si(1)	2749(18)	7301(18)	2834(8)	73(5)
C(34)	1571(16)	7194(15)	3381(7)	103(7)
C(35)	2082(9)	6570(11)	2349(5)	47(3)
C(36)	2923(13)	8733(9)	2720(6)	74(4)
Si(2)	5782(7)	7448(9)	2222(4)	56(2)
C(38)	6298(10)	8814(7)	2312(5)	52(3)
C(39)	4692(13)	7505(15)	1730(4)	97(7)
C(40)	7097(13)	6765(11)	1982(6)	82(5)
Si(3)	9156(3)	-547(2)	3934(1)	44(1)
C(42)	10343(11)	101(8)	3603(4)	63(3)
C(43)	9907(13)	-1220(10)	4452(5)	83(4)
C(44)	8495(13)	-1410(17)	3484(9)	58(4)
Si(4)	6018(4)	-901(2)	4437(2)	69(1)
C(46)	6867(15)	-2053(10)	4648(6)	96(5)
C(47)	4896(15)	-687(12)	4952(7)	96(5)
C(48)	5277(12)	-1117(10)	3809(5)	83(4)
C(1B)	5695(13)	5069(12)	4473(6)	30
C(2B)	6917(12)	5143(13)	4317(7)	30
C(3B)	7150(13)	4117(12)	4506(8)	27(5)
C(4B)	5947(13)	4076(11)	4702(6)	28(4)
C(5B)	4721(15)	5263(13)	4186(6)	30(5)
C(6B)	7260(20)	5400(20)	3848(9)	30
C(7B)	7719(17)	3407(16)	4246(7)	35(6)
C(8B)	5250(20)	3238(16)	4590(6)	30
C(9B)	5106(18)	5787(12)	3701(7)	39(2)
C(10B)	4254(15)	6250(20)	3398(8)	37(2)
C(11B)	4551(14)	6707(13)	2955(5)	30

C(12B)	5754(15)	6762(13)	2800(6)	30
C(13B)	6606(15)	6316(17)	3105(7)	33(7)
C(14B)	6310(20)	5840(20)	3549(8)	40(2)
C(15B)	8190(13)	4802(13)	3639(6)	31(5)
C(16B)	8864(18)	5191(15)	3248(8)	60(7)
C(17B)	9809(19)	4617(16)	3047(7)	66(6)
C(18B)	10030(20)	3614(17)	3216(9)	72(9)
C(19B)	9344(18)	3208(14)	3599(8)	49(6)
C(20B)	8451(18)	3809(14)	3823(7)	42(7)
C(21B)	7210(20)	2363(19)	4344(9)	30
C(22B)	7841(15)	1435(11)	4253(6)	30
C(23B)	7440(20)	493(15)	4321(7)	30
C(24B)	6119(14)	363(11)	4496(5)	30(3)
C(25B)	5504(15)	1299(12)	4580(6)	30
C(26B)	6026(16)	2296(16)	4494(7)	30
C(27B)	3988(13)	3481(10)	4458(4)	30
C(28B)	3061(14)	2812(14)	4523(8)	37(7)
C(29B)	1942(13)	3081(16)	4373(7)	53(7)
C(30B)	1718(14)	4047(14)	4198(6)	47(6)
C(31B)	2635(15)	4731(13)	4149(7)	42(6)
C(32B)	3763(15)	4441(11)	4275(7)	23(5)
Si(1B)	3010(30)	7290(20)	2738(12)	66(5)
C(34B)	1920(20)	7340(20)	3219(9)	63(7)
C(35B)	2410(20)	6367(17)	2200(8)	45(6)
C(36B)	3262(19)	8580(16)	2404(8)	66(6)
Si(2B)	6185(14)	7304(16)	2161(7)	56(2)
C(38B)	5170(20)	6840(20)	1666(10)	82(8)
C(39B)	6700(30)	8550(20)	2144(11)	90
C(40B)	7720(30)	6710(30)	2012(12)	90
Si(3B)	8443(4)	-644(3)	4241(2)	37(1)
C(42B)	10026(15)	-79(12)	4181(9)	69(6)
C(43B)	8444(16)	-1539(12)	4786(6)	51(4)

C(44B)	8100(30)	-1400(30)	3630(15)	58(4)
Si(4B)	5158(5)	-796(3)	4653(2)	36(1)
C(46B)	5561(18)	-2006(11)	4311(6)	54(5)
C(47B)	5232(15)	-983(13)	5328(6)	45(4)
C(48B)	3681(11)	-540(12)	4474(5)	36(4)

Table 3. Bond lengths [Å] and angles [deg] for 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene.

C(1)-C(5)	1.388(14)	C(1B)-C(5B)	1.37(2)
C(1)-C(2)	1.437(8)	C(1B)-C(2B)	1.438(10)
C(1)-C(4)	1.460(8)	C(1B)-C(4B)	1.458(10)
C(2)-C(6)	1.361(14)	C(2B)-C(6B)	1.37(2)
C(2)-C(3)	1.457(8)	C(2B)-C(3B)	1.450(10)
C(3)-C(7)	1.372(16)	C(3B)-C(7B)	1.32(3)
C(3)-C(4)	1.457(9)	C(3B)-C(4B)	1.452(10)
C(4)-C(8)	1.395(16)	C(4B)-C(8B)	1.37(3)
C(5)-C(9)	1.439(16)	C(5B)-C(32B)	1.533(17)
C(5)-C(32)	1.470(15)	C(5B)-C(9B)	1.544(18)
C(6)-C(15)	1.497(19)	C(6B)-C(15B)	1.42(3)
C(6)-C(14)	1.54(2)	C(6B)-C(14B)	1.46(4)
C(7)-C(20)	1.472(18)	C(7B)-C(21B)	1.50(3)
C(7)-C(21)	1.485(16)	C(7B)-C(20B)	1.51(2)
C(8)-C(27)	1.428(16)	C(8B)-C(27B)	1.50(2)
C(8)-C(26)	1.528(16)	C(8B)-C(26B)	1.52(3)
C(9)-C(10)	1.402(15)	C(9B)-C(10B)	1.396(14)
C(9)-C(14)	1.458(17)	C(9B)-C(14B)	1.411(16)
C(10)-C(11)	1.426(14)	C(10B)-C(11B)	1.383(14)
C(10)-H(10)	0.9500	C(10B)-H(10B)	0.9500
C(11)-C(12)	1.399(13)	C(11B)-C(12B)	1.416(14)
C(11)-Si(1)	1.90(2)	C(11B)-Si(1B)	1.98(3)
C(12)-C(13)	1.384(17)	C(12B)-C(13B)	1.391(13)
C(12)-Si(2)	1.906(14)	C(12B)-Si(2B)	1.94(2)
C(13)-C(14)	1.409(16)	C(13B)-C(14B)	1.396(14)
C(13)-H(13)	0.9500	C(13B)-H(13B)	0.9500
C(15)-C(16)	1.427(19)	C(15B)-C(16B)	1.398(15)
C(15)-C(20)	1.441(17)	C(15B)-C(20B)	1.413(13)
C(16)-C(17)	1.349(18)	C(16B)-C(17B)	1.405(15)

C(16)-H(16)	0.9500	C(16B)-H(16B)	0.9500
C(17)-C(18)	1.354(17)	C(17B)-C(18B)	1.402(15)
C(17)-H(17)	0.9500	C(17B)-H(17B)	0.9500
C(18)-C(19)	1.34(2)	C(18B)-C(19B)	1.398(15)
C(18)-H(18)	0.9500	C(18B)-H(18B)	0.9500
C(19)-C(20)	1.397(18)	C(19B)-C(20B)	1.408(15)
C(19)-H(19)	0.9500	C(19B)-H(19B)	0.9500
C(21)-C(26)	1.421(17)	C(21B)-C(26B)	1.39(3)
C(21)-C(22)	1.445(14)	C(21B)-C(22B)	1.42(3)
C(22)-C(23)	1.387(12)	C(22B)-C(23B)	1.32(2)
C(22)-H(22)	0.9500	C(22B)-H(22B)	0.9500
C(23)-C(24)	1.439(14)	C(23B)-C(24B)	1.56(2)
C(23)-Si(3)	1.853(11)	C(23B)-Si(3B)	1.87(2)
C(24)-C(25)	1.434(13)	C(24B)-C(25B)	1.41(2)
C(24)-Si(4)	1.911(10)	C(24B)-Si(4B)	1.898(15)
C(25)-C(26)	1.395(15)	C(25B)-C(26B)	1.44(3)
C(25)-H(25)	0.9500	C(25B)-H(25B)	0.9500
C(27)-C(28)	1.367(16)	C(27B)-C(28B)	1.365(14)
C(27)-C(32)	1.457(16)	C(27B)-C(32B)	1.366(14)
C(28)-C(29)	1.37(3)	C(28B)-C(29B)	1.365(16)
C(28)-H(28)	0.9500	C(28B)-H(28B)	0.9500
C(29)-C(30)	1.41(2)	C(29B)-C(30B)	1.364(14)
C(29)-H(29)	0.9500	C(29B)-H(29B)	0.9500
C(30)-C(31)	1.385(17)	C(30B)-C(31B)	1.364(15)
C(30)-H(30)	0.9500	C(30B)-H(30B)	0.9500
C(31)-C(32)	1.41(2)	C(31B)-C(32B)	1.364(14)
C(31)-H(31)	0.9500	C(31B)-H(31B)	0.9500
Si(1)-C(35)	1.79(2)	Si(1B)-C(34B)	1.79(4)
Si(1)-C(36)	1.89(3)	Si(1B)-C(36B)	1.92(4)
Si(1)-C(34)	1.99(3)	Si(1B)-C(35B)	2.01(4)
C(34)-H(34A)	0.9800	C(34B)-H(34D)	0.9800
C(34)-H(34B)	0.9800	C(34B)-H(34E)	0.9800

C(34)-H(34C)	0.9800	C(34B)-H(34F)	0.9800
C(35)-H(35A)	0.9800	C(35B)-H(35D)	0.9800
C(35)-H(35B)	0.9800	C(35B)-H(35E)	0.9800
C(35)-H(35C)	0.9800	C(35B)-H(35F)	0.9800
C(36)-H(36A)	0.9800	C(36B)-H(36D)	0.9800
C(36)-H(36B)	0.9800	C(36B)-H(36E)	0.9800
C(36)-H(36C)	0.9800	C(36B)-H(36F)	0.9800
Si(2)-C(39)	1.814(15)	Si(2B)-C(39B)	1.72(3)
Si(2)-C(40)	1.841(17)	Si(2B)-C(38B)	1.87(3)
Si(2)-C(38)	1.880(16)	Si(2B)-C(40B)	1.93(3)
C(38)-H(38A)	0.9800	C(38B)-H(38D)	0.9800
C(38)-H(38B)	0.9800	C(38B)-H(38E)	0.9800
C(38)-H(38C)	0.9800	C(38B)-H(38F)	0.9800
C(39)-H(39A)	0.9800	C(39B)-H(39D)	0.9800
C(39)-H(39B)	0.9800	C(39B)-H(39E)	0.9800
C(39)-H(39C)	0.9800	C(39B)-H(39F)	0.9800
C(40)-H(40A)	0.9800	C(40B)-H(40D)	0.9800
C(40)-H(40B)	0.9800	C(40B)-H(40E)	0.9800
C(40)-H(40C)	0.9800	C(40B)-H(40F)	0.9800
Si(3)-C(42)	1.814(13)	Si(3B)-C(43B)	1.880(16)
Si(3)-C(44)	1.82(2)	Si(3B)-C(42B)	1.929(19)
Si(3)-C(43)	1.858(12)	Si(3B)-C(44B)	1.97(4)
C(42)-H(42A)	0.9800	C(42B)-H(42D)	0.9800
C(42)-H(42B)	0.9800	C(42B)-H(42E)	0.9800
C(42)-H(42C)	0.9800	C(42B)-H(42F)	0.9800
C(43)-H(43A)	0.9800	C(43B)-H(43D)	0.9800
C(43)-H(43B)	0.9800	C(43B)-H(43E)	0.9800
C(43)-H(43C)	0.9800	C(43B)-H(43F)	0.9800
C(44)-H(44A)	0.9800	C(44B)-H(44D)	0.9800
C(44)-H(44B)	0.9800	C(44B)-H(44E)	0.9800
C(44)-H(44C)	0.9800	C(44B)-H(44F)	0.9800
Si(4)-C(46)	1.863(14)	Si(4B)-C(48B)	1.759(14)

Si(4)-C(47)	1.902(18)	Si(4B)-C(47B)	1.852(15)
Si(4)-C(48)	1.920(14)	Si(4B)-C(46B)	1.880(15)
C(46)-H(46A)	0.9800	C(46B)-H(46D)	0.9800
C(46)-H(46B)	0.9800	C(46B)-H(46E)	0.9800
C(46)-H(46C)	0.9800	C(46B)-H(46F)	0.9800
C(47)-H(47A)	0.9800	C(47B)-H(47D)	0.9800
C(47)-H(47B)	0.9800	C(47B)-H(47E)	0.9800
C(47)-H(47C)	0.9800	C(47B)-H(47F)	0.9800
C(48)-H(48A)	0.9800	C(48B)-H(48D)	0.9800
C(48)-H(48B)	0.9800	C(48B)-H(48E)	0.9800
C(48)-H(48C)	0.9800	C(48B)-H(48F)	0.9800
C(5)-C(1)-C(2)	122.1(8)	C(5B)-C(1B)-C(2B)	125.6(10)
C(5)-C(1)-C(4)	120.8(9)	C(5B)-C(1B)-C(4B)	124.2(16)
C(2)-C(1)-C(4)	91.1(8)	C(2B)-C(1B)-C(4B)	90.0(6)
C(6)-C(2)-C(1)	122.8(10)	C(6B)-C(2B)-C(1B)	123.8(13)
C(6)-C(2)-C(3)	121.8(9)	C(6B)-C(2B)-C(3B)	120(2)
C(1)-C(2)-C(3)	89.7(7)	C(1B)-C(2B)-C(3B)	90.3(7)
C(7)-C(3)-C(2)	121.3(9)	C(7B)-C(3B)-C(2B)	122.4(18)
C(7)-C(3)-C(4)	121.6(11)	C(7B)-C(3B)-C(4B)	128.2(18)
C(2)-C(3)-C(4)	90.5(8)	C(2B)-C(3B)-C(4B)	89.8(7)
C(8)-C(4)-C(3)	124.7(10)	C(8B)-C(4B)-C(3B)	118.3(16)
C(8)-C(4)-C(1)	121.0(10)	C(8B)-C(4B)-C(1B)	119.8(17)
C(3)-C(4)-C(1)	88.8(8)	C(3B)-C(4B)-C(1B)	89.5(7)
C(1)-C(5)-C(9)	116.0(10)	C(1B)-C(5B)-C(32B)	110.0(14)
C(1)-C(5)-C(32)	113.2(8)	C(1B)-C(5B)-C(9B)	110.2(13)
C(9)-C(5)-C(32)	128.3(10)	C(32B)-C(5B)-C(9B)	129.6(12)
C(2)-C(6)-C(15)	112.0(12)	C(2B)-C(6B)-C(15B)	117(2)
C(2)-C(6)-C(14)	111.8(10)	C(2B)-C(6B)-C(14B)	114.0(17)
C(15)-C(6)-C(14)	133.3(10)	C(15B)-C(6B)-C(14B)	122.0(16)
C(3)-C(7)-C(20)	114.7(11)	C(3B)-C(7B)-C(21B)	110.5(17)
C(3)-C(7)-C(21)	113.0(13)	C(3B)-C(7B)-C(20B)	115.4(17)
C(20)-C(7)-C(21)	129.5(10)	C(21B)-C(7B)-C(20B)	131.2(18)



C(4)-C(8)-C(27)	116.4(9)	C(4B)-C(8B)-C(27B)	115.1(16)
C(4)-C(8)-C(26)	109.1(11)	C(4B)-C(8B)-C(26B)	110.7(18)
C(27)-C(8)-C(26)	131.2(9)	C(27B)-C(8B)-C(26B)	131.9(16)
C(10)-C(9)-C(5)	123.7(13)	C(10B)-C(9B)-C(14B)	117.4(9)
C(10)-C(9)-C(14)	118.9(10)	C(10B)-C(9B)-C(5B)	120.0(13)
C(5)-C(9)-C(14)	117.2(11)	C(14B)-C(9B)-C(5B)	122.6(11)
C(9)-C(10)-C(11)	123.0(10)	C(11B)-C(10B)-C(9B)	122.2(9)
C(9)-C(10)-H(10)	118.5	C(11B)-C(10B)-H(10B)	118.9
C(11)-C(10)-H(10)	118.5	C(9B)-C(10B)-H(10B)	118.9
C(12)-C(11)-C(10)	117.4(9)	C(10B)-C(11B)-C(12B)	120.6(10)
C(12)-C(11)-Si(1)	126.8(9)	C(10B)-C(11B)-Si(1B)	102.4(15)
C(10)-C(11)-Si(1)	115.8(10)	C(12B)-C(11B)-Si(1B)	136.5(14)
C(13)-C(12)-C(11)	120.1(9)	C(13B)-C(12B)-C(11B)	117.2(9)
C(13)-C(12)-Si(2)	108.8(8)	C(13B)-C(12B)-Si(2B)	121.0(11)
C(11)-C(12)-Si(2)	131.1(7)	C(11B)-C(12B)-Si(2B)	121.5(11)
C(12)-C(13)-C(14)	124.7(11)	C(12B)-C(13B)-C(14B)	122.3(10)
C(12)-C(13)-H(13)	117.7	C(12B)-C(13B)-H(13B)	118.9
C(14)-C(13)-H(13)	117.7	C(14B)-C(13B)-H(13B)	118.9
C(13)-C(14)-C(9)	115.7(11)	C(13B)-C(14B)-C(9B)	120.2(10)
C(13)-C(14)-C(6)	122.8(12)	C(13B)-C(14B)-C(6B)	118.6(15)
C(9)-C(14)-C(6)	121.1(9)	C(9B)-C(14B)-C(6B)	121.2(12)
C(16)-C(15)-C(20)	118.4(13)	C(16B)-C(15B)-C(20B)	119.1(10)
C(16)-C(15)-C(6)	121.4(10)	C(16B)-C(15B)-C(6B)	120.5(17)
C(20)-C(15)-C(6)	120.0(13)	C(20B)-C(15B)-C(6B)	120.5(17)
C(17)-C(16)-C(15)	120.9(12)	C(15B)-C(16B)-C(17B)	120.8(10)
C(17)-C(16)-H(16)	119.6	C(15B)-C(16B)-H(16B)	119.6
C(15)-C(16)-H(16)	119.6	C(17B)-C(16B)-H(16B)	119.6
C(16)-C(17)-C(18)	119.2(14)	C(18B)-C(17B)-C(16B)	119.9(10)
C(16)-C(17)-H(17)	120.4	C(18B)-C(17B)-H(17B)	120.1
C(18)-C(17)-H(17)	120.4	C(16B)-C(17B)-H(17B)	120.1
C(19)-C(18)-C(17)	123.4(13)	C(19B)-C(18B)-C(17B)	119.7(10)
C(19)-C(18)-H(18)	118.3	C(19B)-C(18B)-H(18B)	120.2

C(17)-C(18)-H(18)	118.3	C(17B)-C(18B)-H(18B)	120.2
C(18)-C(19)-C(20)	121.0(12)	C(18B)-C(19B)-C(20B)	120.4(10)
C(18)-C(19)-H(19)	119.5	C(18B)-C(19B)-H(19B)	119.8
C(20)-C(19)-H(19)	119.5	C(20B)-C(19B)-H(19B)	119.8
C(19)-C(20)-C(15)	116.9(14)	C(19B)-C(20B)-C(15B)	119.9(10)
C(19)-C(20)-C(7)	125.0(12)	C(19B)-C(20B)-C(7B)	121.8(15)
C(15)-C(20)-C(7)	118.1(13)	C(15B)-C(20B)-C(7B)	118.2(15)
C(26)-C(21)-C(22)	118.0(8)	C(26B)-C(21B)-C(22B)	118(2)
C(26)-C(21)-C(7)	121.0(10)	C(26B)-C(21B)-C(7B)	118(2)
C(22)-C(21)-C(7)	121.1(11)	C(22B)-C(21B)-C(7B)	123.0(18)
C(23)-C(22)-C(21)	125.6(10)	C(23B)-C(22B)-C(21B)	126.1(18)
C(23)-C(22)-H(22)	117.2	C(23B)-C(22B)-H(22B)	117.0
C(21)-C(22)-H(22)	117.2	C(21B)-C(22B)-H(22B)	117.0
C(22)-C(23)-C(24)	115.2(9)	C(22B)-C(23B)-C(24B)	118.1(17)
C(22)-C(23)-Si(3)	116.6(9)	C(22B)-C(23B)-Si(3B)	120.4(17)
C(24)-C(23)-Si(3)	128.2(6)	C(24B)-C(23B)-Si(3B)	121.4(13)
C(25)-C(24)-C(23)	120.1(8)	C(25B)-C(24B)-C(23B)	114.6(14)
C(25)-C(24)-Si(4)	109.9(8)	C(25B)-C(24B)-Si(4B)	111.6(11)
C(23)-C(24)-Si(4)	129.3(6)	C(23B)-C(24B)-Si(4B)	133.8(12)
C(26)-C(25)-C(24)	123.3(12)	C(24B)-C(25B)-C(26B)	123.2(15)
C(26)-C(25)-H(25)	118.3	C(24B)-C(25B)-H(25B)	118.4
C(24)-C(25)-H(25)	118.3	C(26B)-C(25B)-H(25B)	118.4
C(25)-C(26)-C(21)	117.7(10)	C(21B)-C(26B)-C(25B)	119(2)
C(25)-C(26)-C(8)	121.3(13)	C(21B)-C(26B)-C(8B)	123(2)
C(21)-C(26)-C(8)	120.9(10)	C(25B)-C(26B)-C(8B)	117.6(15)
C(28)-C(27)-C(8)	120.1(10)	C(28B)-C(27B)-C(32B)	119.1(10)
C(28)-C(27)-C(32)	121.8(13)	C(28B)-C(27B)-C(8B)	123.9(13)
C(8)-C(27)-C(32)	118.0(9)	C(32B)-C(27B)-C(8B)	117.0(14)
C(27)-C(28)-C(29)	119.7(13)	C(27B)-C(28B)-C(29B)	120.0(10)
C(27)-C(28)-H(28)	120.1	C(27B)-C(28B)-H(28B)	120.0
C(29)-C(28)-H(28)	120.1	C(29B)-C(28B)-H(28B)	120.0
C(28)-C(29)-C(30)	122.5(17)	C(30B)-C(29B)-C(28B)	120.5(10)

C(28)-C(29)-H(29)	118.7	C(30B)-C(29B)-H(29B)	119.7
C(30)-C(29)-H(29)	118.7	C(28B)-C(29B)-H(29B)	119.7
C(31)-C(30)-C(29)	116.8(15)	C(29B)-C(30B)-C(31B)	119.5(10)
C(31)-C(30)-H(30)	121.6	C(29B)-C(30B)-H(30B)	120.2
C(29)-C(30)-H(30)	121.6	C(31B)-C(30B)-H(30B)	120.2
C(30)-C(31)-C(32)	124.3(14)	C(30B)-C(31B)-C(32B)	119.7(10)
C(30)-C(31)-H(31)	117.9	C(30B)-C(31B)-H(31B)	120.1
C(32)-C(31)-H(31)	117.9	C(32B)-C(31B)-H(31B)	120.1
C(31)-C(32)-C(27)	114.6(11)	C(31B)-C(32B)-C(27B)	120.9(10)
C(31)-C(32)-C(5)	124.2(12)	C(31B)-C(32B)-C(5B)	114.8(13)
C(27)-C(32)-C(5)	121.2(12)	C(27B)-C(32B)-C(5B)	124.3(13)
C(35)-Si(1)-C(36)	116.3(12)	C(34B)-Si(1B)-C(36B)	115(2)
C(35)-Si(1)-C(11)	113.8(13)	C(34B)-Si(1B)-C(11B)	113.1(18)
C(36)-Si(1)-C(11)	109.4(11)	C(36B)-Si(1B)-C(11B)	110.2(17)
C(35)-Si(1)-C(34)	103.6(12)	C(34B)-Si(1B)-C(35B)	109.0(19)
C(36)-Si(1)-C(34)	105.0(14)	C(36B)-Si(1B)-C(35B)	103.0(17)
C(11)-Si(1)-C(34)	107.8(12)	C(11B)-Si(1B)-C(35B)	106.1(18)
Si(1)-C(34)-H(34A)	109.5	Si(1B)-C(34B)-H(34D)	109.5
Si(1)-C(34)-H(34B)	109.5	Si(1B)-C(34B)-H(34E)	109.5
H(34A)-C(34)-H(34B)	109.5	H(34D)-C(34B)-H(34E)	109.5
Si(1)-C(34)-H(34C)	109.5	Si(1B)-C(34B)-H(34F)	109.5
H(34A)-C(34)-H(34C)	109.5	H(34D)-C(34B)-H(34F)	109.5
H(34B)-C(34)-H(34C)	109.5	H(34E)-C(34B)-H(34F)	109.5
Si(1)-C(35)-H(35A)	109.5	Si(1B)-C(35B)-H(35D)	109.5
Si(1)-C(35)-H(35B)	109.5	Si(1B)-C(35B)-H(35E)	109.5
H(35A)-C(35)-H(35B)	109.5	H(35D)-C(35B)-H(35E)	109.5
Si(1)-C(35)-H(35C)	109.5	Si(1B)-C(35B)-H(35F)	109.5
H(35A)-C(35)-H(35C)	109.5	H(35D)-C(35B)-H(35F)	109.5
H(35B)-C(35)-H(35C)	109.5	H(35E)-C(35B)-H(35F)	109.5
Si(1)-C(36)-H(36A)	109.5	Si(1B)-C(36B)-H(36D)	109.5
Si(1)-C(36)-H(36B)	109.5	Si(1B)-C(36B)-H(36E)	109.5
H(36A)-C(36)-H(36B)	109.5	H(36D)-C(36B)-H(36E)	109.5

Si(1)-C(36)-H(36C)	109.5	Si(1B)-C(36B)-H(36F)	109.5
H(36A)-C(36)-H(36C)	109.5	H(36D)-C(36B)-H(36F)	109.5
H(36B)-C(36)-H(36C)	109.5	H(36E)-C(36B)-H(36F)	109.5
C(39)-Si(2)-C(40)	107.4(10)	C(39B)-Si(2B)-C(38B)	119.6(17)
C(39)-Si(2)-C(38)	105.4(9)	C(39B)-Si(2B)-C(40B)	93.8(16)
C(40)-Si(2)-C(38)	104.7(7)	C(38B)-Si(2B)-C(40B)	105.6(15)
C(39)-Si(2)-C(12)	118.4(7)	C(39B)-Si(2B)-C(12B)	116.7(15)
C(40)-Si(2)-C(12)	108.4(8)	C(38B)-Si(2B)-C(12B)	112.1(14)
C(38)-Si(2)-C(12)	111.7(7)	C(40B)-Si(2B)-C(12B)	105.5(14)
Si(2)-C(38)-H(38A)	109.5	Si(2B)-C(38B)-H(38D)	109.5
Si(2)-C(38)-H(38B)	109.5	Si(2B)-C(38B)-H(38E)	109.5
H(38A)-C(38)-H(38B)	109.5	H(38D)-C(38B)-H(38E)	109.5
Si(2)-C(38)-H(38C)	109.5	Si(2B)-C(38B)-H(38F)	109.5
H(38A)-C(38)-H(38C)	109.5	H(38D)-C(38B)-H(38F)	109.5
H(38B)-C(38)-H(38C)	109.5	H(38E)-C(38B)-H(38F)	109.5
Si(2)-C(39)-H(39A)	109.5	Si(2B)-C(39B)-H(39D)	109.5
Si(2)-C(39)-H(39B)	109.5	Si(2B)-C(39B)-H(39E)	109.5
H(39A)-C(39)-H(39B)	109.5	H(39D)-C(39B)-H(39E)	109.5
Si(2)-C(39)-H(39C)	109.5	Si(2B)-C(39B)-H(39F)	109.5
H(39A)-C(39)-H(39C)	109.5	H(39D)-C(39B)-H(39F)	109.5
H(39B)-C(39)-H(39C)	109.5	H(39E)-C(39B)-H(39F)	109.5
Si(2)-C(40)-H(40A)	109.5	Si(2B)-C(40B)-H(40D)	109.5
Si(2)-C(40)-H(40B)	109.5	Si(2B)-C(40B)-H(40E)	109.5
H(40A)-C(40)-H(40B)	109.5	H(40D)-C(40B)-H(40E)	109.5
Si(2)-C(40)-H(40C)	109.5	Si(2B)-C(40B)-H(40F)	109.5
H(40A)-C(40)-H(40C)	109.5	H(40D)-C(40B)-H(40F)	109.5
H(40B)-C(40)-H(40C)	109.5	H(40E)-C(40B)-H(40F)	109.5
C(42)-Si(3)-C(44)	104.5(6)	C(23B)-Si(3B)-C(43B)	113.3(9)
C(42)-Si(3)-C(23)	107.3(5)	C(23B)-Si(3B)-C(42B)	105.4(8)
C(44)-Si(3)-C(23)	112.7(6)	C(43B)-Si(3B)-C(42B)	107.5(9)
C(42)-Si(3)-C(43)	105.2(6)	C(23B)-Si(3B)-C(44B)	111.9(13)
C(44)-Si(3)-C(43)	113.9(9)	C(43B)-Si(3B)-C(44B)	110.9(13)

C(23)-Si(3)-C(43)	112.4(5)	C(42B)-Si(3B)-C(44B)	107.4(10)
Si(3)-C(42)-H(42A)	109.5	Si(3B)-C(42B)-H(42D)	109.5
Si(3)-C(42)-H(42B)	109.5	Si(3B)-C(42B)-H(42E)	109.5
H(42A)-C(42)-H(42B)	109.5	H(42D)-C(42B)-H(42E)	109.5
Si(3)-C(42)-H(42C)	109.5	Si(3B)-C(42B)-H(42F)	109.5
H(42A)-C(42)-H(42C)	109.5	H(42D)-C(42B)-H(42F)	109.5
H(42B)-C(42)-H(42C)	109.5	H(42E)-C(42B)-H(42F)	109.5
Si(3)-C(43)-H(43A)	109.5	Si(3B)-C(43B)-H(43D)	109.5
Si(3)-C(43)-H(43B)	109.5	Si(3B)-C(43B)-H(43E)	109.5
H(43A)-C(43)-H(43B)	109.5	H(43D)-C(43B)-H(43E)	109.5
Si(3)-C(43)-H(43C)	109.5	Si(3B)-C(43B)-H(43F)	109.5
H(43A)-C(43)-H(43C)	109.5	H(43D)-C(43B)-H(43F)	109.5
H(43B)-C(43)-H(43C)	109.5	H(43E)-C(43B)-H(43F)	109.5
Si(3)-C(44)-H(44A)	109.5	Si(3B)-C(44B)-H(44D)	109.5
Si(3)-C(44)-H(44B)	109.5	Si(3B)-C(44B)-H(44E)	109.5
H(44A)-C(44)-H(44B)	109.5	H(44D)-C(44B)-H(44E)	109.5
Si(3)-C(44)-H(44C)	109.5	Si(3B)-C(44B)-H(44F)	109.5
H(44A)-C(44)-H(44C)	109.5	H(44D)-C(44B)-H(44F)	109.5
H(44B)-C(44)-H(44C)	109.5	H(44E)-C(44B)-H(44F)	109.5
C(46)-Si(4)-C(47)	103.3(7)	C(48B)-Si(4B)-C(47B)	110.0(8)
C(46)-Si(4)-C(24)	114.8(6)	C(48B)-Si(4B)-C(46B)	104.3(8)
C(47)-Si(4)-C(24)	108.2(6)	C(47B)-Si(4B)-C(46B)	111.7(8)
C(46)-Si(4)-C(48)	112.2(7)	C(48B)-Si(4B)-C(24B)	108.9(7)
C(47)-Si(4)-C(48)	112.9(7)	C(47B)-Si(4B)-C(24B)	107.5(6)
C(24)-Si(4)-C(48)	105.6(5)	C(46B)-Si(4B)-C(24B)	114.5(7)
Si(4)-C(46)-H(46A)	109.5	Si(4B)-C(46B)-H(46D)	109.5
Si(4)-C(46)-H(46B)	109.5	Si(4B)-C(46B)-H(46E)	109.5
H(46A)-C(46)-H(46B)	109.5	H(46D)-C(46B)-H(46E)	109.5
Si(4)-C(46)-H(46C)	109.5	Si(4B)-C(46B)-H(46F)	109.5
H(46A)-C(46)-H(46C)	109.5	H(46D)-C(46B)-H(46F)	109.5
H(46B)-C(46)-H(46C)	109.5	H(46E)-C(46B)-H(46F)	109.5
Si(4)-C(47)-H(47A)	109.5	Si(4B)-C(47B)-H(47D)	109.5

Si(4)-C(47)-H(47B)	109.5	Si(4B)-C(47B)-H(47E)	109.5
H(47A)-C(47)-H(47B)	109.5	H(47D)-C(47B)-H(47E)	109.5
Si(4)-C(47)-H(47C)	109.5	Si(4B)-C(47B)-H(47F)	109.5
H(47A)-C(47)-H(47C)	109.5	H(47D)-C(47B)-H(47F)	109.5
H(47B)-C(47)-H(47C)	109.5	H(47E)-C(47B)-H(47F)	109.5
Si(4)-C(48)-H(48A)	109.5	Si(4B)-C(48B)-H(48D)	109.5
Si(4)-C(48)-H(48B)	109.5	Si(4B)-C(48B)-H(48E)	109.5
H(48A)-C(48)-H(48B)	109.5	H(48D)-C(48B)-H(48E)	109.5
Si(4)-C(48)-H(48C)	109.5	Si(4B)-C(48B)-H(48F)	109.5
H(48A)-C(48)-H(48C)	109.5	H(48D)-C(48B)-H(48F)	109.5
H(48B)-C(48)-H(48C)	109.5	H(48E)-C(48B)-H(48F)	109.5

Table 4. Torsion angles [deg] for 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene.

C(5)-C(1)-C(2)-C(6)	-0.1(13)	C(5B)-C(1B)-C(2B)-C(6B)	-2(3)
C(4)-C(1)-C(2)-C(6)	128.0(10)	C(4B)-C(1B)-C(2B)-C(6B)	132(2)
C(5)-C(1)-C(2)-C(3)	-128.7(9)	C(5B)-C(1B)-C(2B)-C(3B)	-129.1(19)
C(4)-C(1)-C(2)-C(3)	-0.6(8)	C(4B)-C(1B)-C(2B)-C(3B)	4.6(16)
C(6)-C(2)-C(3)-C(7)	-0.6(18)	C(6B)-C(2B)-C(3B)-C(7B)	2(2)
C(1)-C(2)-C(3)-C(7)	128.8(12)	C(1B)-C(2B)-C(3B)-C(7B)	132.2(19)
C(6)-C(2)-C(3)-C(4)	-128.8(11)	C(6B)-C(2B)-C(3B)-C(4B)	-134.9(17)
C(1)-C(2)-C(3)-C(4)	0.6(8)	C(1B)-C(2B)-C(3B)-C(4B)	-4.6(16)
C(7)-C(3)-C(4)-C(8)	-0.9(16)	C(7B)-C(3B)-C(4B)-C(8B)	-4(3)
C(2)-C(3)-C(4)-C(8)	127.1(10)	C(2B)-C(3B)-C(4B)-C(8B)	128.6(15)
C(7)-C(3)-C(4)-C(1)	-128.6(10)	C(7B)-C(3B)-C(4B)-C(1B)	-128.1(19)
C(2)-C(3)-C(4)-C(1)	-0.6(8)	C(2B)-C(3B)-C(4B)-C(1B)	4.6(16)
C(5)-C(1)-C(4)-C(8)	-1.0(14)	C(5B)-C(1B)-C(4B)-C(8B)	7(2)
C(2)-C(1)-C(4)-C(8)	-130.0(10)	C(2B)-C(1B)-C(4B)-C(8B)	-127.4(17)
C(5)-C(1)-C(4)-C(3)	129.6(10)	C(5B)-C(1B)-C(4B)-C(3B)	130.1(17)
C(2)-C(1)-C(4)-C(3)	0.6(8)	C(2B)-C(1B)-C(4B)-C(3B)	-4.6(16)
C(2)-C(1)-C(5)-C(9)	-25.4(12)	C(2B)-C(1B)-C(5B)-C(32B)	137.4(17)
C(4)-C(1)-C(5)-C(9)	-139.0(9)	C(4B)-C(1B)-C(5B)-C(32B)	18(2)
C(2)-C(1)-C(5)-C(32)	138.6(9)	C(2B)-C(1B)-C(5B)-C(9B)	-12(2)
C(4)-C(1)-C(5)-C(32)	24.9(13)	C(4B)-C(1B)-C(5B)-C(9B)	-130.6(11)
C(1)-C(2)-C(6)-C(15)	-140.9(8)	C(1B)-C(2B)-C(6B)-C(15B)	-136.1(16)
C(3)-C(2)-C(6)-C(15)	-27.8(14)	C(3B)-C(2B)-C(6B)-C(15B)	-23(2)
C(1)-C(2)-C(6)-C(14)	22.6(14)	C(1B)-C(2B)-C(6B)-C(14B)	15(3)
C(3)-C(2)-C(6)-C(14)	135.6(12)	C(3B)-C(2B)-C(6B)-C(14B)	128.0(18)
C(2)-C(3)-C(7)-C(20)	26.6(17)	C(2B)-C(3B)-C(7B)-C(21B)	-143.7(18)
C(4)-C(3)-C(7)-C(20)	139.3(11)	C(4B)-C(3B)-C(7B)-C(21B)	-24(3)
C(2)-C(3)-C(7)-C(21)	-136.6(11)	C(2B)-C(3B)-C(7B)-C(20B)	19(2)
C(4)-C(3)-C(7)-C(21)	-23.9(14)	C(4B)-C(3B)-C(7B)-C(20B)	138.8(19)
C(3)-C(4)-C(8)-C(27)	-136.4(10)	C(3B)-C(4B)-C(8B)-C(27B)	-137.3(14)

C(1)-C(4)-C(8)-C(27)	-23.7(14)	C(1B)-C(4B)-C(8B)-C(27B)	-30.0(18)
C(3)-C(4)-C(8)-C(26)	25.3(13)	C(3B)-C(4B)-C(8B)-C(26B)	28(2)
C(1)-C(4)-C(8)-C(26)	137.9(9)	C(1B)-C(4B)-C(8B)-C(26B)	134.8(15)
C(1)-C(5)-C(9)-C(10)	-159.4(11)	C(1B)-C(5B)-C(9B)-C(10B)	-166.8(17)
C(32)-C(5)-C(9)-C(10)	39.6(18)	C(32B)-C(5B)-C(9B)-C(10B)	52(2)
C(1)-C(5)-C(9)-C(14)	24.6(14)	C(1B)-C(5B)-C(9B)-C(14B)	12.2(18)
C(32)-C(5)-C(9)-C(14)	-136.5(14)	C(32B)-C(5B)-C(9B)-C(14B)	-129(2)
C(5)-C(9)-C(10)-C(11)	-170.6(12)	C(14B)-C(9B)-C(10B)-C(11B)	2(3)
C(14)-C(9)-C(10)-C(11)	5(2)	C(5B)-C(9B)-C(10B)-C(11B)	-178.6(16)
C(9)-C(10)-C(11)-C(12)	-1.2(19)	C(9B)-C(10B)-C(11B)-C(12B)	-2(3)
C(9)-C(10)-C(11)-Si(1)	179.8(13)	C(9B)-C(10B)-C(11B)-Si(1B)	-176(2)
C(10)-C(11)-C(12)-C(13)	-2.8(16)	C(10B)-C(11B)-C(12B)-C(13B)	2(3)
Si(1)-C(11)-C(12)-C(13)	176.1(12)	Si(1B)-C(11B)-C(12B)-C(13B)	172(2)
C(10)-C(11)-C(12)-Si(2)	-180.0(11)	C(10B)-C(11B)-C(12B)-Si(2B)	175.2(18)
Si(1)-C(11)-C(12)-Si(2)	-1.1(17)	Si(1B)-C(11B)-C(12B)-Si(2B)	-15(3)
C(11)-C(12)-C(13)-C(14)	2.6(19)	C(11B)-C(12B)-C(13B)-C(14B)	-1(3)
Si(2)-C(12)-C(13)-C(14)	-179.6(13)	Si(2B)-C(12B)-C(13B)-C(14B)	-174(2)
C(12)-C(13)-C(14)-C(9)	2(2)	C(12B)-C(13B)-C(14B)-C(9B)	1(3)
C(12)-C(13)-C(14)-C(6)	173.9(12)	C(12B)-C(13B)-C(14B)-C(6B)	-179.6(18)
C(10)-C(9)-C(14)-C(13)	-5(2)	C(10B)-C(9B)-C(14B)-C(13B)	-2(3)
C(5)-C(9)-C(14)-C(13)	170.9(12)	C(5B)-C(9B)-C(14B)-C(13B)	179.5(16)
C(10)-C(9)-C(14)-C(6)	-177.8(12)	C(10B)-C(9B)-C(14B)-C(6B)	178.8(18)
C(5)-C(9)-C(14)-C(6)	-1.6(18)	C(5B)-C(9B)-C(14B)-C(6B)	0(3)
C(2)-C(6)-C(14)-C(13)	166.4(14)	C(2B)-C(6B)-C(14B)-C(13B)	167(2)
C(15)-C(6)-C(14)-C(13)	-35(2)	C(15B)-C(6B)-C(14B)-C(13B)	-44(3)
C(2)-C(6)-C(14)-C(9)	-21.6(17)	C(2B)-C(6B)-C(14B)-C(9B)	-13(3)
C(15)-C(6)-C(14)-C(9)	137.1(14)	C(15B)-C(6B)-C(14B)-C(9B)	136(2)
C(2)-C(6)-C(15)-C(16)	-153.5(10)	C(2B)-C(6B)-C(15B)-C(16B)	-158.5(18)
C(14)-C(6)-C(15)-C(16)	47.8(16)	C(14B)-C(6B)-C(15B)-C(16B)	53(2)
C(2)-C(6)-C(15)-C(20)	31.1(13)	C(2B)-C(6B)-C(15B)-C(20B)	21.3(17)
C(14)-C(6)-C(15)-C(20)	-127.5(14)	C(14B)-C(6B)-C(15B)-C(20B)	-127(2)
C(20)-C(15)-C(16)-C(17)	4.5(17)	C(20B)-C(15B)-C(16B)-C(17B)	-2(2)



C(6)-C(15)-C(16)-C(17)	-170.9(11)	C(6B)-C(15B)-C(16B)-C(17B)	178.3(14)
C(15)-C(16)-C(17)-C(18)	-3.4(19)	C(15B)-C(16B)-C(17B)-C(18B)	4(3)
C(16)-C(17)-C(18)-C(19)	-1(2)	C(16B)-C(17B)-C(18B)-C(19B)	-3(3)
C(17)-C(18)-C(19)-C(20)	4(2)	C(17B)-C(18B)-C(19B)-C(20B)	-2(4)
C(18)-C(19)-C(20)-C(15)	-3(2)	C(18B)-C(19B)-C(20B)-C(15B)	4(3)
C(18)-C(19)-C(20)-C(7)	178.1(13)	C(18B)-C(19B)-C(20B)-C(7B)	-178.2(19)
C(16)-C(15)-C(20)-C(19)	-1.2(17)	C(16B)-C(15B)-C(20B)-C(19B)	-3(2)
C(6)-C(15)-C(20)-C(19)	174.2(11)	C(6B)-C(15B)-C(20B)-C(19B)	177.3(14)
C(16)-C(15)-C(20)-C(7)	177.8(11)	C(16B)-C(15B)-C(20B)-C(7B)	179.6(14)
C(6)-C(15)-C(20)-C(7)	-6.8(16)	C(6B)-C(15B)-C(20B)-C(7B)	-0.2(19)
C(3)-C(7)-C(20)-C(19)	157.0(14)	C(3B)-C(7B)-C(20B)-C(19B)	162.6(19)
C(21)-C(7)-C(20)-C(19)	-43(2)	C(21B)-C(7B)-C(20B)-C(19B)	-39(3)
C(3)-C(7)-C(20)-C(15)	-21.9(17)	C(3B)-C(7B)-C(20B)-C(15B)	-20(2)
C(21)-C(7)-C(20)-C(15)	137.8(12)	C(21B)-C(7B)-C(20B)-C(15B)	139(2)
C(3)-C(7)-C(21)-C(26)	22.4(13)	C(3B)-C(7B)-C(21B)-C(26B)	26(3)
C(20)-C(7)-C(21)-C(26)	-137.6(13)	C(20B)-C(7B)-C(21B)-C(26B)	-133(2)
C(3)-C(7)-C(21)-C(22)	-155.7(9)	C(3B)-C(7B)-C(21B)-C(22B)	-159(2)
C(20)-C(7)-C(21)-C(22)	44.3(16)	C(20B)-C(7B)-C(21B)-C(22B)	42(3)
C(26)-C(21)-C(22)-C(23)	2.7(13)	C(26B)-C(21B)-C(22B)-C(23B)	-4(4)
C(7)-C(21)-C(22)-C(23)	-179.1(9)	C(7B)-C(21B)-C(22B)-C(23B)	-178.6(19)
C(21)-C(22)-C(23)-C(24)	-1.5(13)	C(21B)-C(22B)-C(23B)-C(24B)	3(3)
C(21)-C(22)-C(23)-Si(3)	177.2(7)	C(21B)-C(22B)-C(23B)-Si(3B)	-173.9(17)
C(22)-C(23)-C(24)-C(25)	0.3(12)	C(22B)-C(23B)-C(24B)-C(25B)	-2(2)
Si(3)-C(23)-C(24)-C(25)	-178.2(7)	Si(3B)-C(23B)-C(24B)-C(25B)	174.8(11)
C(22)-C(23)-C(24)-Si(4)	169.8(7)	C(22B)-C(23B)-C(24B)-Si(4B)	-178.7(12)
Si(3)-C(23)-C(24)-Si(4)	-8.7(12)	Si(3B)-C(23B)-C(24B)-Si(4B)	-2(2)
C(23)-C(24)-C(25)-C(26)	-0.4(14)	C(23B)-C(24B)-C(25B)-C(26B)	2(2)
Si(4)-C(24)-C(25)-C(26)	-171.8(8)	Si(4B)-C(24B)-C(25B)-C(26B)	179.6(13)
C(24)-C(25)-C(26)-C(21)	1.7(14)	C(22B)-C(21B)-C(26B)-C(25B)	4(4)
C(24)-C(25)-C(26)-C(8)	178.0(9)	C(7B)-C(21B)-C(26B)-C(25B)	178.6(15)
C(22)-C(21)-C(26)-C(25)	-2.6(12)	C(22B)-C(21B)-C(26B)-C(8B)	-178.5(16)
C(7)-C(21)-C(26)-C(25)	179.2(9)	C(7B)-C(21B)-C(26B)-C(8B)	-4(4)

C(22)-C(21)-C(26)-C(8)	-179.0(9)	C(24B)-C(25B)-C(26B)-C(21B)	-3(3)
C(7)-C(21)-C(26)-C(8)	2.8(13)	C(24B)-C(25B)-C(26B)-C(8B)	178.9(15)
C(4)-C(8)-C(26)-C(25)	158.2(9)	C(4B)-C(8B)-C(26B)-C(21B)	-24(3)
C(27)-C(8)-C(26)-C(25)	-43.8(14)	C(27B)-C(8B)-C(26B)-C(21B)	137(2)
C(4)-C(8)-C(26)-C(21)	-25.5(12)	C(4B)-C(8B)-C(26B)-C(25B)	153.8(16)
C(27)-C(8)-C(26)-C(21)	132.5(11)	C(27B)-C(8B)-C(26B)-C(25B)	-45(3)
C(4)-C(8)-C(27)-C(28)	-160.4(9)	C(4B)-C(8B)-C(27B)-C(28B)	-153.1(16)
C(26)-C(8)-C(27)-C(28)	42.8(15)	C(26B)-C(8B)-C(27B)-C(28B)	46(2)
C(4)-C(8)-C(27)-C(32)	22.2(13)	C(4B)-C(8B)-C(27B)-C(32B)	25.2(15)
C(26)-C(8)-C(27)-C(32)	-134.6(10)	C(26B)-C(8B)-C(27B)-C(32B)	-136(2)
C(8)-C(27)-C(28)-C(29)	-176.8(11)	C(32B)-C(27B)-C(28B)-C(29B)	5(2)
C(32)-C(27)-C(28)-C(29)	0.5(17)	C(8B)-C(27B)-C(28B)-C(29B)	-177.1(14)
C(27)-C(28)-C(29)-C(30)	-3(2)	C(27B)-C(28B)-C(29B)-C(30B)	-6(3)
C(28)-C(29)-C(30)-C(31)	1(2)	C(28B)-C(29B)-C(30B)-C(31B)	3(3)
C(29)-C(30)-C(31)-C(32)	3.4(19)	C(29B)-C(30B)-C(31B)-C(32B)	0(3)
C(30)-C(31)-C(32)-C(27)	-5.6(17)	C(30B)-C(31B)-C(32B)-C(27B)	-1(3)
C(30)-C(31)-C(32)-C(5)	172.6(11)	C(30B)-C(31B)-C(32B)-C(5B)	177.8(15)
C(28)-C(27)-C(32)-C(31)	3.5(15)	C(28B)-C(27B)-C(32B)-C(31B)	-1(2)
C(8)-C(27)-C(32)-C(31)	-179.1(9)	C(8B)-C(27B)-C(32B)-C(31B)	-179.5(15)
C(28)-C(27)-C(32)-C(5)	-174.7(9)	C(28B)-C(27B)-C(32B)-C(5B)	179.9(14)
C(8)-C(27)-C(32)-C(5)	2.6(14)	C(8B)-C(27B)-C(32B)-C(5B)	1.5(18)
C(1)-C(5)-C(32)-C(31)	156.0(10)	C(1B)-C(5B)-C(32B)-C(31B)	158.4(17)
C(9)-C(5)-C(32)-C(31)	-42.5(18)	C(9B)-C(5B)-C(32B)-C(31B)	-61(2)
C(1)-C(5)-C(32)-C(27)	-25.9(13)	C(1B)-C(5B)-C(32B)-C(27B)	-23(2)
C(9)-C(5)-C(32)-C(27)	135.6(12)	C(9B)-C(5B)-C(32B)-C(27B)	118.3(18)
C(12)-C(11)-Si(1)-C(35)	76.9(16)	C(10B)-C(11B)-Si(1B)-C(34B)	15(2)
C(10)-C(11)-Si(1)-C(35)	-104.2(14)	C(12B)-C(11B)-Si(1B)-C(34B)	-157(2)
C(12)-C(11)-Si(1)-C(36)	-55.1(17)	C(10B)-C(11B)-Si(1B)-C(36B)	145(2)
C(10)-C(11)-Si(1)-C(36)	123.8(13)	C(12B)-C(11B)-Si(1B)-C(36B)	-27(3)
C(12)-C(11)-Si(1)-C(34)	-168.8(10)	C(10B)-C(11B)-Si(1B)-C(35B)	-105(2)
C(10)-C(11)-Si(1)-C(34)	10.1(17)	C(12B)-C(11B)-Si(1B)-C(35B)	84(2)
C(13)-C(12)-Si(2)-C(39)	152.9(11)	C(13B)-C(12B)-Si(2B)-C(39B)	-86(2)

C(11)-C(12)-Si(2)-C(39)	-29.7(16)	C(11B)-C(12B)-Si(2B)-C(39B)	100.8(19)
C(13)-C(12)-Si(2)-C(40)	30.4(12)	C(13B)-C(12B)-Si(2B)-C(38B)	131.0(18)
C(11)-C(12)-Si(2)-C(40)	-152.2(10)	C(11B)-C(12B)-Si(2B)-C(38B)	-42(2)
C(13)-C(12)-Si(2)-C(38)	-84.5(9)	C(13B)-C(12B)-Si(2B)-C(40B)	17(2)
C(11)-C(12)-Si(2)-C(38)	93.0(11)	C(11B)-C(12B)-Si(2B)-C(40B)	-156.7(17)
C(22)-C(23)-Si(3)-C(42)	-7.8(8)	C(22B)-C(23B)-Si(3B)-C(43B)	127.6(15)
C(24)-C(23)-Si(3)-C(42)	170.7(8)	C(24B)-C(23B)-Si(3B)-C(43B)	-49.2(16)
C(22)-C(23)-Si(3)-C(44)	-122.3(9)	C(22B)-C(23B)-Si(3B)-C(42B)	10.3(18)
C(24)-C(23)-Si(3)-C(44)	56.2(11)	C(24B)-C(23B)-Si(3B)-C(42B)	-166.5(14)
C(22)-C(23)-Si(3)-C(43)	107.3(8)	C(22B)-C(23B)-Si(3B)-C(44B)	-106.2(18)
C(24)-C(23)-Si(3)-C(43)	-74.2(9)	C(24B)-C(23B)-Si(3B)-C(44B)	77.1(17)
C(25)-C(24)-Si(4)-C(46)	-145.5(8)	C(25B)-C(24B)-Si(4B)-C(48B)	37.8(12)
C(23)-C(24)-Si(4)-C(46)	44.2(11)	C(23B)-C(24B)-Si(4B)-C(48B)	-145.4(14)
C(25)-C(24)-Si(4)-C(47)	-30.7(9)	C(25B)-C(24B)-Si(4B)-C(47B)	-81.3(12)
C(23)-C(24)-Si(4)-C(47)	158.9(9)	C(23B)-C(24B)-Si(4B)-C(47B)	95.5(16)
C(25)-C(24)-Si(4)-C(48)	90.4(7)	C(25B)-C(24B)-Si(4B)-C(46B)	154.0(11)
C(23)-C(24)-Si(4)-C(48)	-79.9(9)	C(23B)-C(24B)-Si(4B)-C(46B)	-29.2(17)

Table 5. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene. The anisotropic displacement factor exponent takes the form:  $-2 \pi^2 [h^2 a^{*2} U_{11} + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	43(6)	14(4)	28(4)	-7(3)	-4(4)	11(4)
C(2)	44(6)	13(4)	24(5)	-9(3)	3(4)	-6(4)
C(3)	54(7)	27(5)	37(6)	-6(4)	-7(5)	-9(5)
C(4)	91(13)	21(5)	13(5)	-5(3)	1(7)	16(7)
C(5)	32(4)	10(3)	24(4)	-3(3)	-7(3)	6(3)
C(6)	60(9)	19(4)	29(7)	-1(5)	-4(5)	-21(5)
C(7)	53(9)	28(5)	29(6)	-13(5)	-13(6)	7(6)
C(8)	68(7)	15(4)	25(4)	3(3)	6(5)	-4(5)
C(9)	56(3)	23(2)	39(3)	-2(2)	-13(3)	-11(3)
C(10)	73(5)	16(2)	23(7)	-8(5)	-21(4)	2(3)
C(11)	26(3)	22(2)	26(3)	0(2)	2(2)	-5(2)
C(12)	40(5)	25(3)	34(4)	5(3)	-11(4)	-5(4)
C(13)	32(6)	19(5)	35(5)	4(4)	-22(5)	-5(5)
C(14)	74(5)	8(3)	38(4)	2(3)	-24(3)	-7(3)
C(15)	38(5)	37(5)	38(5)	-9(4)	-2(5)	-23(5)
C(16)	54(7)	38(5)	74(7)	-11(5)	4(6)	-12(5)
C(17)	75(7)	59(6)	70(7)	-6(6)	-8(6)	-17(6)
C(18)	37(7)	59(8)	68(9)	3(7)	-10(6)	14(6)
C(19)	49(10)	42(7)	64(10)	8(7)	8(7)	16(7)
C(20)	47(7)	36(6)	47(7)	-11(5)	-16(6)	6(6)
C(21)	61(8)	19(4)	29(5)	-10(4)	-16(5)	2(5)
C(22)	45(6)	29(5)	34(5)	-5(4)	-7(4)	-4(5)
C(23)	50(7)	26(4)	30(5)	-7(4)	-14(5)	0(5)
C(24)	40(5)	8(3)	30(4)	1(3)	-3(4)	2(3)
C(25)	91(9)	13(4)	26(4)	-6(3)	-7(5)	3(5)
C(26)	102(12)	16(4)	25(6)	0(4)	-16(8)	17(8)
C(27)	66(7)	20(4)	28(4)	-5(3)	10(5)	-13(5)

C(28)	111(12)	35(6)	52(7)	1(5)	47(8)	14(7)
C(29)	150(20)	29(7)	45(9)	-13(7)	60(12)	-24(12)
C(30)	29(7)	65(9)	37(6)	-2(6)	13(5)	-14(7)
C(31)	85(10)	47(8)	31(6)	6(6)	-1(7)	0(9)
C(32)	61(8)	55(7)	28(5)	-20(5)	-7(6)	-4(7)
Si(1)	75(9)	34(3)	111(7)	19(4)	-39(5)	-8(4)
C(34)	103(14)	90(12)	115(14)	-5(11)	57(11)	36(10)
C(35)	10(5)	77(9)	54(7)	5(7)	-8(5)	-11(6)
C(36)	79(7)	41(5)	101(8)	17(6)	-22(7)	-11(6)
Si(2)	72(6)	59(4)	36(3)	16(2)	-9(3)	-22(4)
C(38)	56(6)	22(4)	76(7)	19(4)	2(5)	1(4)
C(39)	83(10)	169(18)	38(6)	47(9)	-27(6)	-70(12)
C(40)	72(10)	68(9)	107(11)	24(8)	8(10)	-46(10)
Si(3)	65(2)	23(1)	43(2)	-5(1)	-18(2)	14(1)
C(42)	88(9)	35(5)	65(7)	-3(5)	-29(6)	-6(6)
C(43)	107(8)	68(7)	74(7)	13(6)	-25(6)	28(7)
C(44)	25(11)	49(4)	99(15)	-12(8)	-1(8)	0(8)
Si(4)	93(3)	15(1)	100(3)	-5(2)	16(3)	3(2)
C(46)	116(9)	57(7)	116(8)	23(6)	19(7)	0(7)
C(47)	103(9)	70(8)	115(9)	0(8)	14(8)	-5(7)
C(48)	81(7)	61(6)	107(8)	-34(6)	7(6)	-8(6)
C(3B)	24(9)	28(7)	29(8)	-3(6)	0(7)	-1(7)
C(9B)	56(3)	23(2)	39(3)	-2(2)	-13(3)	-11(3)
C(10B)	73(5)	16(2)	23(7)	-8(5)	-21(4)	2(3)
C(13B)	34(8)	29(8)	35(8)	2(5)	-16(5)	0(5)
C(14B)	74(5)	8(3)	38(4)	2(3)	-24(3)	-7(3)
C(19B)	37(13)	37(11)	73(17)	-13(11)	22(10)	-1(10)
C(20B)	48(15)	54(14)	23(12)	-16(10)	3(10)	3(12)
C(28B)	35(10)	43(11)	34(9)	-10(7)	12(7)	7(8)
C(29B)	47(10)	61(10)	51(9)	1(8)	-9(7)	-1(8)
C(30B)	49(10)	58(9)	35(7)	5(7)	-15(7)	16(8)
C(31B)	50(10)	48(10)	28(8)	9(7)	-8(6)	30(7)

Si(1B)	64(10)	21(4)	114(11)	17(6)	-63(10)	-10(6)
Si(2B)	72(6)	59(4)	36(3)	16(2)	-9(3)	-22(4)
Si(3B)	39(3)	31(2)	39(2)	-14(2)	-14(2)	11(2)
C(42B)	34(10)	31(9)	141(19)	-22(11)	-35(11)	19(8)
C(43B)	63(8)	35(7)	54(7)	0(6)	-22(7)	14(7)
C(44B)	25(11)	49(4)	99(15)	-12(8)	-1(8)	0(8)
Si(4B)	54(4)	20(2)	35(2)	-4(2)	-1(2)	-18(2)
C(46B)	78(13)	29(8)	53(10)	-17(7)	7(9)	-17(9)
C(47B)	49(8)	50(7)	38(7)	-5(6)	-3(6)	-28(6)
C(48B)	8(7)	49(9)	51(8)	-25(7)	4(6)	-9(6)

Table 6. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene.

	x	y	z	U(eq)
H(10B)	3443	6245	3499	45
H(13B)	7419	6336	3008	39
H(16B)	8682	5851	3116	72
H(17B)	10296	4908	2797	79
H(18B)	10647	3212	3071	86
H(19B)	9480	2523	3708	59
H(22B)	8631	1499	4131	36
H(25B)	4708	1268	4698	36
H(28B)	3195	2161	4672	45
H(29B)	1314	2591	4390	63
H(30B)	930	4242	4110	57
H(31B)	2487	5406	4028	51
H(34D)	1839	6656	3368	95
H(34E)	1149	7554	3082	95
H(34F)	2170	7837	3470	95
H(35D)	3012	6328	1938	67
H(35E)	1669	6646	2066	67
H(35F)	2269	5677	2333	67
H(36D)	3859	8486	2144	99
H(36E)	3546	9096	2640	99
H(36F)	2511	8814	2258	99
H(38D)	5080	6087	1691	123
H(38E)	5498	7015	1344	123
H(38F)	4383	7163	1704	123
H(39D)	6094	9018	2277	135
H(39E)	6883	8746	1804	135
H(39F)	7429	8607	2344	135
H(40D)	7627	5986	1923	135

H(40E)	8243	6768	2301	135
H(40F)	8085	7087	1736	135
H(42D)	10210	334	4474	103
H(42E)	10068	359	3888	103
H(42F)	10605	-641	4152	103
H(43D)	8578	-1141	5087	76
H(43E)	9080	-2049	4747	76
H(43F)	7673	-1892	4806	76
H(44D)	8091	-920	3352	86
H(44E)	7318	-1736	3657	86
H(44F)	8714	-1925	3576	86
H(46D)	5506	-1881	3956	80
H(46E)	5010	-2559	4403	80
H(46F)	6378	-2209	4395	80
H(47D)	6060	-1108	5426	68
H(47E)	4740	-1576	5421	68
H(47F)	4935	-363	5494	68
H(48D)	3650	-437	4116	54
H(48E)	3397	83	4640	54
H(48F)	3172	-1125	4564	54
H(10)	3431	6179	3688	45
H(13)	7078	6525	2893	34
H(16)	8959	5955	2983	66
H(17)	10331	4980	2561	82
H(18)	10799	3365	2834	66
H(19)	10008	2682	3526	62
H(22)	9224	1589	3945	43
H(25)	5482	1097	4640	52
H(28)	4035	1891	4669	79
H(29)	2053	2146	4476	89
H(30)	1340	3763	4206	52
H(31)	2705	5102	4121	65



H(34A)	1868	7572	3668	154
H(34B)	1457	6468	3468	154
H(34C)	809	7490	3276	154
H(35A)	2594	6595	2057	71
H(35B)	1300	6862	2269	71
H(35C)	1985	5853	2455	71
H(36A)	3286	9057	3009	111
H(36B)	2139	9039	2659	111
H(36C)	3436	8842	2432	111
H(38A)	6912	8834	2569	77
H(38B)	5621	9244	2412	77
H(38C)	6629	9078	2003	77
H(39A)	3976	7863	1846	145
H(39B)	4481	6804	1628	145
H(39C)	5030	7879	1449	145
H(40A)	7700	6709	2242	123
H(40B)	7427	7147	1703	123
H(40C)	6863	6073	1874	123
H(42A)	10004	490	3327	94
H(42B)	10908	-411	3477	94
H(42C)	10758	576	3825	94
H(43A)	9313	-1598	4646	125
H(43B)	10306	-713	4663	125
H(43C)	10498	-1705	4322	125
H(44A)	7841	-1795	3638	86
H(44B)	9101	-1893	3365	86
H(44C)	8185	-1007	3207	86
H(46A)	7210	-1917	4973	144
H(46B)	7508	-2202	4413	144
H(46C)	6329	-2647	4668	144
H(47A)	5320	-590	5264	144
H(47B)	4370	-1288	4977	144

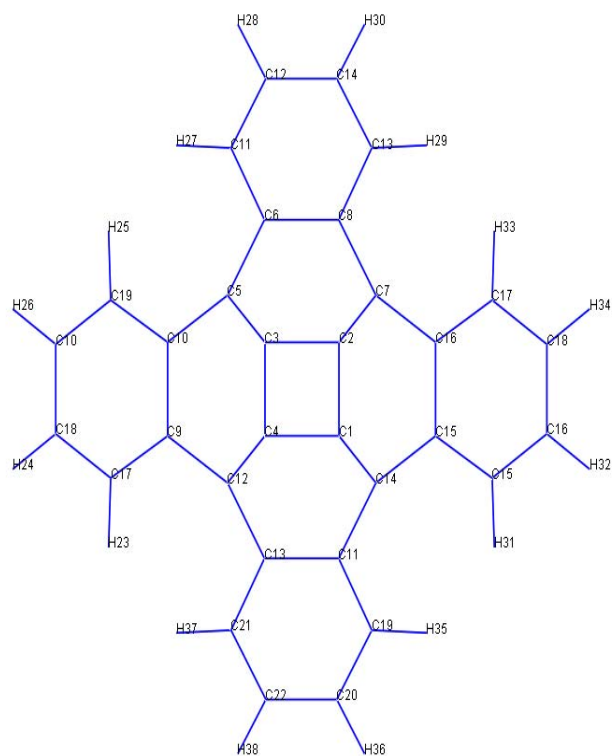
H(47C)	4419	-72	4880	144
H(48A)	4812	-506	3719	125
H(48B)	4749	-1717	3827	125
H(48C)	5893	-1238	3559	125

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## Calculations

The molecular geometry of 5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene was computed at the B3LYP/6-311G\*\* level of theory using Gaussian03 (1) starting from 4 geometries having  $C_2$ ,  $C_s$ ,  $C_{2v}$  or  $C_{4v}$  symmetry. All of them converged to  $C_{4v}$  symmetry, which corresponds to the real minimum at the B3LYP/6-311G\*\* level, with no imaginary frequencies. The molecular geometry of 1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene were started from two geometries having  $C_2$  or  $C_s$  symmetry. The optimized geometries (at B3LYP/6-311G\*\* level of theory) converged to similar points, both with no imaginary frequencies. Although nominally the  $C_2$  system is of lower energy, the difference in energy is insignificant (0.004 kJ/mol). The B3LYP/6-311G\*\* level of theory has been chosen as it gives very good agreement between optimized and experimental geometry obtained from single crystal X-ray diffraction for highly non-planar systems (2).



# 5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene

Level of theory: B3LYP/6-311G\*\*

Point group:  $C_{4v}$

Total Energy [Hartree]: -1229.2125896

C1	0.727119	-0.727119	1.646095
C2	0.727119	0.727119	1.646095
C3	-0.727119	0.727119	1.646095
C4	-0.727119	-0.727119	1.646095
C5	-1.458379	1.458379	0.767899
C6	-0.729661	2.633339	0.235832
C7	1.458379	1.458379	0.767899
C8	0.729661	2.633339	0.235832
C9	-2.633339	-0.729661	0.235832
C10	-2.633339	0.729661	0.235832
C11	0.729661	-2.633339	0.235832
C12	-1.458379	-1.458379	0.767899

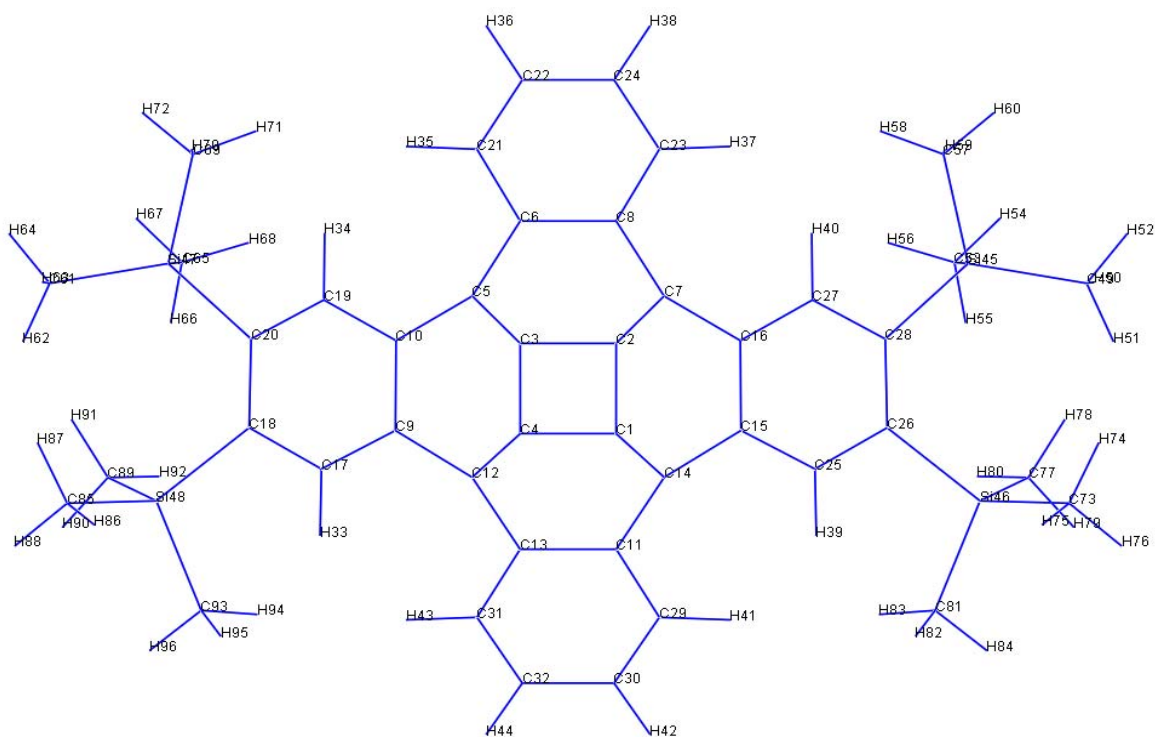
C13	-0.729661	-2.633339	0.235832
C14	1.458379	-1.458379	0.767899
C15	2.633339	-0.729661	0.235832
C16	2.633339	0.729661	0.235832
C17	-3.749773	-1.383677	-0.312944
C18	-4.827425	-0.696719	-0.847188
C19	-3.749773	1.383677	-0.312944
C10	-4.827425	0.696719	-0.847188
C11	-1.383677	3.749773	-0.312944
C12	-0.696719	4.827425	-0.847188
C13	1.383677	3.749773	-0.312944
C14	0.696719	4.827425	-0.847188
C15	3.749773	-1.383677	-0.312944
C16	4.827425	-0.696719	-0.847188
C17	3.749773	1.383677	-0.312944
C18	4.827425	0.696719	-0.847188
C19	1.383677	-3.749773	-0.312944
C20	0.696719	-4.827425	-0.847188
C21	-1.383677	-3.749773	-0.312944
C22	-0.696719	-4.827425	-0.847188
H23	-3.791470	-2.462255	-0.292973
H24	-5.670899	-1.245934	-1.249724
H25	-3.791470	2.462255	-0.292973
H26	-5.670899	1.245934	-1.249724
H27	-2.462255	3.791470	-0.292973
H28	-1.245934	5.670899	-1.249724
H29	2.462255	3.791470	-0.292973
H30	1.245934	5.670899	-1.249724
H31	3.791470	-2.462255	-0.292973
H32	5.670899	-1.245934	-1.249724
H33	3.791470	2.462255	-0.292973
H34	5.670899	1.245934	-1.249724

H35	2.462255	-3.791470	-0.292973
H36	1.245934	-5.670899	-1.249724
H37	-2.462255	-3.791470	-0.292973
H38	-1.245934	-5.670899	-1.249724

Bond lengths [Å] and bonds angles [deg]

Parameter	Value	Parameter	Value	Parameter	Value	Parameter	Value
R(1,2)	1.4542	R(22,38)	1.084	A(8,7,16)	130.6381	A(18,20,36)	120.4404
R(1,4)	1.4542	R(23,24)	1.3852	A(6,8,7)	119.4655	A(19,20,36)	119.8222
R(1,14)	1.3567	R(23,39)	1.0796	A(6,8,23)	117.7322	A(6,21,22)	122.5356
R(2,3)	1.4542	R(24,40)	1.084	A(7,8,23)	122.776	A(6,21,37)	119.2336
R(2,7)	1.3567	R(25,26)	1.3852	A(10,9,12)	119.4655	A(22,21,37)	118.2014
R(3,4)	1.4542	R(25,41)	1.0796	A(10,9,17)	117.7322	A(21,22,24)	119.7319
R(3,5)	1.3567	R(26,28)	1.3934	A(12,9,17)	122.776	A(21,22,38)	119.8222
R(4,12)	1.3567	R(26,42)	1.084	A(5,10,9)	119.4655	A(24,22,38)	120.4404
R(5,6)	1.4814	R(27,28)	1.3852	A(5,10,19)	122.776	A(8,23,24)	122.5356
R(5,10)	1.4814	R(27,43)	1.0796	A(9,10,19)	117.7322	A(8,23,39)	119.2336
R(6,8)	1.4593	R(28,44)	1.084	A(13,11,14)	119.4655	A(24,23,39)	118.2014
R(6,21)	1.4055	R(29,30)	1.3852	A(13,11,29)	117.7322	A(22,24,23)	119.7319
R(7,8)	1.4814	R(29,45)	1.0796	A(14,11,29)	122.776	A(22,24,40)	120.4404
R(7,16)	1.4814	R(30,32)	1.3934	A(4,12,9)	113.2556	A(23,24,40)	119.8222
R(8,23)	1.4055	R(30,46)	1.084	A(4,12,13)	113.2556	A(15,25,26)	122.5356
R(9,10)	1.4593	R(31,32)	1.3852	A(9,12,13)	130.6381	A(15,25,41)	119.2336
R(9,12)	1.4814	R(31,47)	1.0796	A(11,13,12)	119.4655	A(26,25,41)	118.2014
R(9,17)	1.4055	R(32,48)	1.084	A(11,13,31)	117.7322	A(25,26,28)	119.7319
R(10,19)	1.4055	A(2,1,4)	90.0	A(12,13,31)	122.776	A(25,26,42)	119.8222
R(11,13)	1.4593	A(2,1,14)	122.6148	A(1,14,11)	113.2556	A(28,26,42)	120.4404
R(11,14)	1.4814	A(4,1,14)	122.6148	A(1,14,15)	113.2556	A(16,27,28)	122.5356
R(11,29)	1.4055	A(1,2,3)	90.0	A(11,14,15)	130.6381	A(16,27,43)	119.2336
R(12,13)	1.4814	A(1,2,7)	122.6148	A(14,15,16)	119.4655	A(28,27,43)	118.2014
R(13,31)	1.4055	A(3,2,7)	122.6148	A(14,15,25)	122.776	A(26,28,27)	119.7319

R(14,15)	1.4814	A(2,3,4)	90.0	A(16,15,25)	117.7322	A(26,28,44)	120.4404
R(15,16)	1.4593	A(2,3,5)	122.6148	A(7,16,15)	119.4655	A(27,28,44)	119.8222
R(15,25)	1.4055	A(4,3,5)	122.6148	A(7,16,27)	122.776	A(11,29,30)	122.5356
R(16,27)	1.4055	A(1,4,3)	90.0	A(15,16,27)	117.7322	A(11,29,45)	119.2336
R(17,18)	1.3852	A(1,4,12)	122.6148	A(9,17,18)	122.5356	A(30,29,45)	118.2014
R(17,33)	1.0796	A(3,4,12)	122.6148	A(9,17,33)	119.2336	A(29,30,32)	119.7319
R(18,20)	1.3934	A(3,5,6)	113.2556	A(18,17,33)	118.2014	A(29,30,46)	119.8222
R(18,34)	1.084	A(3,5,10)	113.2556	A(17,18,20)	119.7319	A(32,30,46)	120.4404
R(19,20)	1.3852	A(6,5,10)	130.6381	A(17,18,34)	119.8222	A(13,31,32)	122.5356
R(19,35)	1.0796	A(5,6,8)	119.4655	A(20,18,34)	120.4404	A(13,31,47)	119.2336
R(20,36)	1.084	A(5,6,21)	122.776	A(10,19,20)	122.5356	A(32,31,47)	118.2014
R(21,22)	1.3852	A(8,6,21)	117.7322	A(10,19,35)	119.2336	A(30,32,31)	119.7319
R(21,37)	1.0796	A(2,7,8)	113.2556	A(20,19,35)	118.2014	A(30,32,48)	120.4404
R(22,24)	1.3934	A(2,7,16)	113.2556	A(18,20,19)	119.7319	A(31,32,48)	119.8222



**1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene**

Level of theory: B3LYP/6-311G\*\*

Point group:  $C_s$

Total Energy [Hartree]: -2864.1324373

C1	0.807382	-2.387357	0.727077
C2	-0.645442	-2.434245	0.728011
C3	-0.645442	-2.434245	-0.728011
C4	0.807382	-2.387357	-0.727077
C5	-1.406926	-1.578036	-1.455604
C6	-2.614233	-1.117040	-0.729118
C7	-1.406926	-1.578036	1.455604
C8	-2.614233	-1.117040	0.729118
C9	0.757117	-0.968740	-2.622805
C10	-0.689944	-0.998596	-2.613340
C11	2.669054	-0.917737	0.729632
C12	1.510975	-1.486069	-1.458011



C13	2.669054	-0.917737	-0.729632
C14	1.510975	-1.486069	1.458011
C15	0.757117	-0.968740	2.622805
C16	-0.689944	-0.998596	2.613340
C17	1.376870	-0.396392	-3.745996
C18	0.712810	0.162227	-4.842649
C19	-1.345211	-0.411602	-3.709015
C20	-0.716471	0.171385	-4.813759
C21	-3.771239	-0.663526	-1.384349
C22	-4.887815	-0.214945	-0.696588
C23	-3.771239	-0.663526	1.384349
C24	-4.887815	-0.214945	0.696588
C25	1.376870	-0.396392	3.745996
C26	0.712810	0.162227	4.842649
C27	-1.345211	-0.411602	3.709015
C28	-0.716471	0.171385	4.813759
C29	3.765431	-0.330410	1.384069
C30	4.824717	0.239240	0.696779
C31	3.765431	-0.330410	-1.384069
C32	4.824717	0.239240	-0.696779
H33	2.454958	-0.421837	-3.766320
H34	-2.422963	-0.436069	-3.697084
H35	-3.816236	-0.704101	-2.462709
H36	-5.763017	0.113353	-1.245610
H37	-3.816236	-0.704101	2.462709
H38	-5.763017	0.113353	1.245610
H39	2.454958	-0.421837	3.766320
H40	-2.422963	-0.436069	3.697084
H41	3.806268	-0.345971	2.462784
H42	5.653954	0.670061	1.246242
H43	3.806268	-0.345971	-2.462784
H44	5.653954	0.670061	-1.246242

Si45	-1.931135	0.957775	6.069857
Si46	1.890175	0.710866	6.252166
Si47	-1.931135	0.957775	-6.069857
Si48	1.890175	0.710866	-6.252166
C49	-1.612607	0.472381	7.870660
H50	-1.633056	-0.615273	7.986713
H51	-0.670312	0.835655	8.279741
H52	-2.416663	0.882449	8.490811
C53	-1.949785	2.838071	5.863986
H54	-2.662823	3.290866	6.560799
H55	-0.976443	3.299937	6.033859
H56	-2.266062	3.098826	4.849488
C57	-3.689932	0.357126	5.698190
H58	-4.064385	0.713379	4.734666
H59	-3.773222	-0.733349	5.717261
H60	-4.363102	0.749327	6.467316
C61	-1.612607	0.472381	-7.870660
H62	-0.670312	0.835655	-8.279741
H63	-1.633056	-0.615273	-7.986713
H64	-2.416663	0.882449	-8.490811
C65	-1.949785	2.838071	-5.863986
H66	-0.976443	3.299937	-6.033859
H67	-2.662823	3.290866	-6.560799
H68	-2.266062	3.098826	-4.849488
C69	-3.689932	0.357126	-5.698190
H70	-3.773222	-0.733349	-5.717261
H71	-4.064385	0.713379	-4.734666
H72	-4.363102	0.749327	-6.467316
C73	1.928251	-0.610560	7.605191
H74	0.951101	-0.790286	8.056106
H75	2.279106	-1.560596	7.191010
H76	2.619243	-0.320769	8.403545

C77	1.514241	2.414156	6.986712
H78	0.577802	2.476162	7.540876
H79	2.320184	2.674439	7.681049
H80	1.496657	3.180325	6.206199
C81	3.654077	0.847971	5.570936
H82	4.072814	-0.116752	5.271662
H83	3.718942	1.529596	4.718030
H84	4.302774	1.245832	6.357991
C85	1.928251	-0.610560	-7.605191
H86	2.279106	-1.560596	-7.191010
H87	0.951101	-0.790286	-8.056106
H88	2.619243	-0.320769	-8.403545
C89	1.514241	2.414156	-6.986712
H90	2.320184	2.674439	-7.681049
H91	0.577802	2.476162	-7.540876
H92	1.496657	3.180325	-6.206199
C93	3.654077	0.847971	-5.570936
H94	3.718942	1.529596	-4.718030
H95	4.072814	-0.116752	-5.271662
H96	4.302774	1.245832	-6.357991

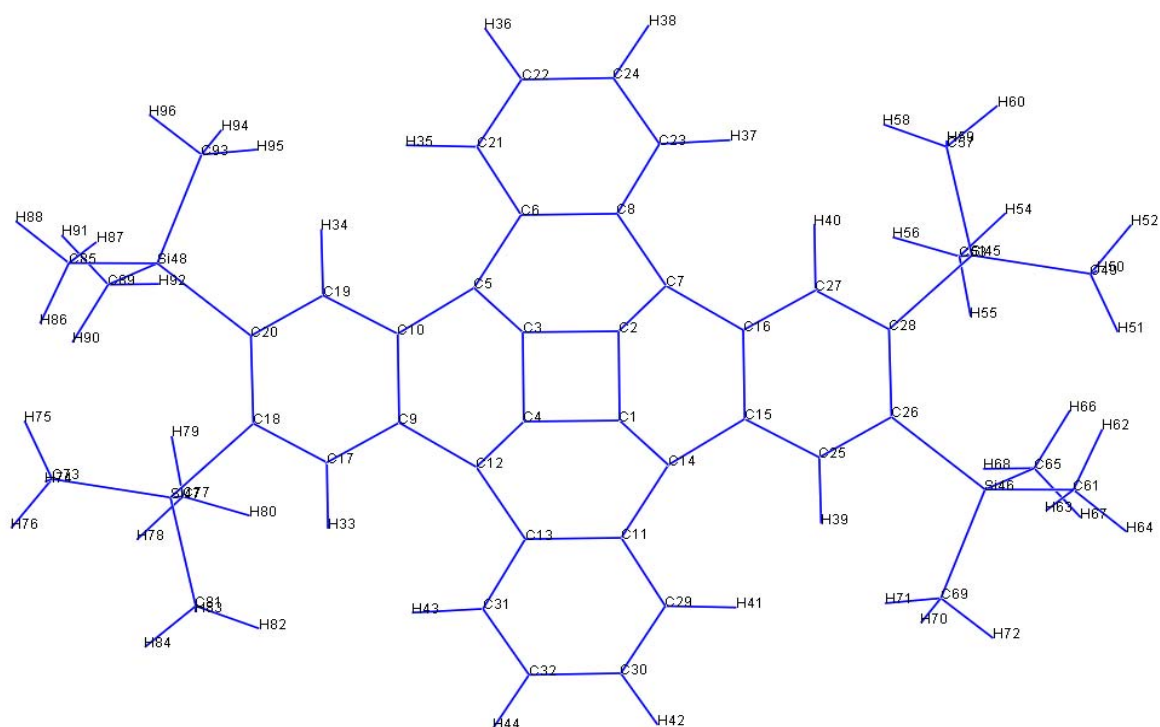
Bond lengths [Å] and bonds angles [deg]

Parameter	Value	Parameter	Value	Parameter	Value	Parameter	Value
R(1,2)	1.4536	R(57,58)	1.0934	A(16,15,25)	117.0472	A(85,48,93)	106.7865
R(1,4)	1.4542	R(57,59)	1.0938	A(7,16,15)	119.8382	A(89,48,93)	105.0214
R(1,14)	1.3571	R(57,60)	1.0948	A(7,16,27)	123.2051	A(45,49,50)	110.6626
R(2,3)	1.456	R(61,62)	1.0896	A(15,16,27)	116.9047	A(45,49,51)	114.6697
R(2,7)	1.3573	R(61,63)	1.094	A(9,17,18)	125.4702	A(45,49,52)	108.6211
R(3,4)	1.4536	R(61,64)	1.0951	A(9,17,33)	116.516	A(50,49,51)	107.9266
R(3,5)	1.3573	R(65,66)	1.0907	A(18,17,33)	117.9877	A(50,49,52)	107.3664
R(4,12)	1.3571	R(65,67)	1.095	A(17,18,20)	117.4812	A(51,49,52)	107.3082

R(5,6)	1.4825	R(65,68)	1.0942	A(17,18,48)	113.5361	A(45,53,54)	110.3775
R(5,10)	1.4799	R(69,70)	1.0938	A(20,18,48)	128.8394	A(45,53,55)	113.2774
R(6,8)	1.4582	R(69,71)	1.0934	A(10,19,20)	125.4844	A(45,53,56)	109.9159
R(6,21)	1.4049	R(69,72)	1.0948	A(10,19,34)	116.6202	A(54,53,55)	107.8728
R(7,8)	1.4825	R(73,74)	1.0911	A(20,19,34)	117.8825	A(54,53,56)	107.653
R(7,16)	1.4799	R(73,75)	1.0942	A(18,20,19)	117.5675	A(55,53,56)	107.5446
R(8,23)	1.4049	R(73,76)	1.0949	A(18,20,47)	128.5466	A(45,57,58)	112.7895
R(9,10)	1.4474	R(77,78)	1.0899	A(19,20,47)	113.8249	A(45,57,59)	112.5309
R(9,12)	1.4808	R(77,79)	1.0952	A(6,21,22)	122.447	A(45,57,60)	108.6206
R(9,17)	1.4047	R(77,80)	1.0939	A(6,21,35)	119.1992	A(58,57,59)	108.3074
R(10,19)	1.4051	R(81,82)	1.0934	A(22,21,35)	118.2966	A(58,57,60)	106.9652
R(11,13)	1.4593	R(81,83)	1.0937	A(21,22,24)	119.7504	A(59,57,60)	107.3425
R(11,14)	1.4814	R(81,84)	1.0948	A(21,22,36)	119.8087	A(47,61,62)	114.6697
R(11,29)	1.4054	R(85,86)	1.0942	A(24,22,36)	120.4277	A(47,61,63)	110.6626
R(12,13)	1.4814	R(85,87)	1.0911	A(8,23,24)	122.447	A(47,61,64)	108.6211
R(13,31)	1.4054	R(85,88)	1.0949	A(8,23,37)	119.1992	A(62,61,63)	107.9266
R(14,15)	1.4808	R(89,90)	1.0952	A(24,23,37)	118.2966	A(62,61,64)	107.3082
R(15,16)	1.4474	R(89,91)	1.0899	A(22,24,23)	119.7504	A(63,61,64)	107.3664
R(15,25)	1.4047	R(89,92)	1.0939	A(22,24,38)	120.4277	A(47,65,66)	113.2774
R(16,27)	1.4051	R(93,94)	1.0937	A(23,24,38)	119.8087	A(47,65,67)	110.3775
R(17,18)	1.3985	R(93,95)	1.0934	A(15,25,26)	125.4702	A(47,65,68)	109.9159
R(17,33)	1.0786	R(93,96)	1.0948	A(15,25,39)	116.516	A(66,65,67)	107.8728
R(18,20)	1.4296	A(2,1,4)	90.0368	A(26,25,39)	117.9877	A(66,65,68)	107.5446
R(18,48)	1.9167	A(2,1,14)	122.6342	A(25,26,28)	117.4812	A(67,65,68)	107.653
R(19,20)	1.3984	A(4,1,14)	122.5893	A(25,26,46)	113.5361	A(47,69,70)	112.5309
R(19,34)	1.0781	A(1,2,3)	89.9632	A(28,26,46)	128.8394	A(47,69,71)	112.7895
R(20,47)	1.9161	A(1,2,7)	122.7327	A(16,27,28)	125.4844	A(47,69,72)	108.6206
R(21,22)	1.386	A(3,2,7)	122.415	A(16,27,40)	116.6202	A(70,69,71)	108.3074
R(21,35)	1.0801	A(2,3,4)	89.9632	A(28,27,40)	117.8825	A(70,69,72)	107.3425
R(22,24)	1.3932	A(2,3,5)	122.415	A(26,28,27)	117.5675	A(71,69,72)	106.9652
R(22,36)	1.0841	A(4,3,5)	122.7327	A(26,28,45)	128.5466	A(46,73,74)	113.1192

R(23,24)	1.386	A(1,4,3)	90.0368	A(27,28,45)	113.8249	A(46,73,75)	110.0135
R(23,37)	1.0801	A(1,4,12)	122.5893	A(11,29,30)	122.5029	A(46,73,76)	110.4477
R(24,38)	1.0841	A(3,4,12)	122.6342	A(11,29,41)	119.2582	A(74,73,75)	107.4931
R(25,26)	1.3985	A(3,5,6)	112.9755	A(30,29,41)	118.2122	A(74,73,76)	107.9061
R(25,39)	1.0786	A(3,5,10)	113.2368	A(29,30,32)	119.7452	A(75,73,76)	107.6649
R(26,28)	1.4296	A(6,5,10)	131.0058	A(29,30,42)	119.7946	A(46,77,78)	114.7841
R(26,46)	1.9167	A(5,6,8)	119.3427	A(32,30,42)	120.4552	A(46,77,79)	108.2869
R(27,28)	1.3984	A(5,6,21)	122.8545	A(13,31,32)	122.5029	A(46,77,80)	110.8925
R(27,40)	1.0781	A(8,6,21)	117.8008	A(13,31,43)	119.2582	A(78,77,79)	107.2422
R(28,45)	1.9161	A(2,7,8)	112.9755	A(32,31,43)	118.2122	A(78,77,80)	108.0077
R(29,30)	1.3853	A(2,7,16)	113.2368	A(30,32,31)	119.7452	A(79,77,80)	107.3224
R(29,41)	1.0796	A(8,7,16)	131.0058	A(30,32,44)	120.4552	A(46,81,82)	113.0072
R(30,32)	1.3936	A(6,8,7)	119.3427	A(31,32,44)	119.7946	A(46,81,83)	112.3618
R(30,42)	1.084	A(6,8,23)	117.8008	A(28,45,49)	114.3248	A(46,81,84)	108.6177
R(31,32)	1.3853	A(7,8,23)	122.8545	A(28,45,53)	110.0507	A(82,81,83)	108.2825
R(31,43)	1.0796	A(10,9,12)	119.7772	A(28,45,57)	109.2468	A(82,81,84)	106.8872
R(32,44)	1.084	A(10,9,17)	117.0472	A(49,45,53)	111.1153	A(83,81,84)	107.397
R(45,49)	1.8921	A(12,9,17)	123.141	A(49,45,57)	105.1625	A(48,85,86)	110.0135
R(45,53)	1.8916	A(5,10,9)	119.8382	A(53,45,57)	106.5302	A(48,85,87)	113.1192
R(45,57)	1.8953	A(5,10,19)	123.2051	A(26,46,73)	109.7792	A(48,85,88)	110.4477
R(46,73)	1.8916	A(9,10,19)	116.9047	A(26,46,77)	114.8972	A(86,85,87)	107.4931
R(46,77)	1.8926	A(13,11,14)	119.4502	A(26,46,81)	109.1452	A(86,85,88)	107.6649
R(46,81)	1.8958	A(13,11,29)	117.7518	A(73,46,77)	110.7979	A(87,85,88)	107.9061
R(47,61)	1.8921	A(14,11,29)	122.7647	A(73,46,81)	106.7865	A(48,89,90)	108.2869
R(47,65)	1.8916	A(4,12,9)	113.064	A(77,46,81)	105.0214	A(48,89,91)	114.7841
R(47,69)	1.8953	A(4,12,13)	113.2825	A(20,47,61)	114.3248	A(48,89,92)	110.8925
R(48,85)	1.8916	A(9,12,13)	130.5943	A(20,47,65)	110.0507	A(90,89,91)	107.2422
R(48,89)	1.8926	A(11,13,12)	119.4502	A(20,47,69)	109.2468	A(90,89,92)	107.3224
R(48,93)	1.8958	A(11,13,31)	117.7518	A(61,47,65)	111.1153	A(91,89,92)	108.0077
R(49,50)	1.094	A(12,13,31)	122.7647	A(61,47,69)	105.1625	A(48,93,94)	112.3618
R(49,51)	1.0896	A(1,14,11)	113.2825	A(65,47,69)	106.5302	A(48,93,95)	113.0072

R(49,52)	1.0951	A(1,14,15)	113.064	A(18,48,85)	109.7792	A(48,93,96)	108.6177
R(53,54)	1.095	A(11,14,15)	130.5943	A(18,48,89)	114.8972	A(94,93,95)	108.2825
R(53,55)	1.0907	A(14,15,16)	119.7772	A(18,48,93)	109.1452	A(94,93,96)	107.397
R(53,56)	1.0942	A(14,15,25)	123.141	A(85,48,89)	110.7979	A(95,93,96)	106.8872



**1,8,9,16-tetrakis(trimethylsilyl)5,6:11,12-di[2,3]naphthalenodibenz[b,h]biphenylene**

Level of theory: B3LYP/6-311G\*\*

Point group:  $C_2$

Total Energy [Hartree]: -2864.1324388

C1	-0.719044	0.735207	-2.393134
C2	0.734873	0.719353	-2.392403
C3	0.719044	-0.735207	-2.393134
C4	-0.734873	-0.719353	-2.392403
C5	1.442457	-1.474815	-1.514859
C6	2.629104	-0.761172	-0.988150
C7	1.475876	1.439873	-1.512594
C8	2.649383	0.697628	-0.995108
C9	-0.753731	-2.611417	-0.966097
C10	0.693383	-2.633946	-0.978383
C11	-2.629104	0.761172	-0.988150
C12	-1.475876	-1.439873	-1.512594
C13	-2.649383	-0.697628	-0.995108

C14	-1.442457	1.474815	-1.514859
C15	-0.693383	2.633946	-0.978383
C16	0.753731	2.611417	-0.966097
C17	-1.402029	-3.709526	-0.376520
C18	-0.766916	-4.824932	0.179113
C19	1.319199	-3.766179	-0.431042
C20	0.661394	-4.862287	0.136149
C21	3.739813	-1.428221	-0.443797
C22	4.834925	-0.753128	0.070551
C23	3.785914	1.339394	-0.474382
C24	4.860316	0.639937	0.050989
C25	-1.319199	3.766179	-0.431042
C26	-0.661394	4.862287	0.136149
C27	1.402029	3.709526	-0.376520
C28	0.766916	4.824932	0.179113
C29	-3.739813	1.428221	-0.443797
C30	-4.834925	0.753128	0.070551
C31	-3.785914	-1.339394	-0.474382
C32	-4.860316	-0.639937	0.050989
H33	-2.480009	-3.692160	-0.378506
H34	2.396069	-3.794863	-0.485049
H35	3.763466	-2.507541	-0.451873
H36	5.673694	-1.312304	0.469185
H37	3.848028	2.416650	-0.516830
H38	5.720882	1.178973	0.430522
H39	-2.396069	3.794863	-0.485049
H40	2.480009	3.692160	-0.378506
H41	-3.763466	2.507541	-0.451873
H42	-5.673694	1.312304	0.469185
H43	-3.848028	-2.416650	-0.516830
H44	-5.720882	-1.178973	0.430522
Si45	1.971846	6.083267	0.976935



Si46	-1.841763	6.282689	0.648624
Si47	-1.971846	-6.083267	0.976935
Si48	1.841763	-6.282689	0.648624
C49	1.671462	7.881045	0.469029
H50	1.716567	7.987169	-0.618944
H51	0.723490	8.298496	0.807073
H52	2.469350	8.501192	0.891000
C53	1.954968	5.893634	2.858950
H54	2.658940	6.594774	3.319142
H55	0.973123	6.065820	3.301607
H56	2.267309	4.881598	3.133733
C57	3.739813	5.699133	0.412272
H58	4.104997	4.739363	0.787689
H59	3.842102	5.703549	-0.676691
H60	4.408470	6.471309	0.806161
C61	-1.846192	7.624590	-0.684660
H62	-0.861416	8.062342	-0.854774
H63	-2.188710	7.206222	-1.635925
H64	-2.531591	8.433510	-0.411437
C65	-1.495302	7.028979	2.352938
H66	-0.553728	7.572109	2.431362
H67	-2.298378	7.735349	2.588538
H68	-1.504612	6.255508	3.126393
C69	-3.611803	5.612228	0.756790
H70	-4.013888	5.308540	-0.213629
H71	-3.694566	4.764310	1.442686
H72	-4.263610	6.405491	1.136826
C73	-1.671462	-7.881045	0.469029
H74	-1.716567	-7.987169	-0.618944
H75	-0.723490	-8.298496	0.807073
H76	-2.469350	-8.501192	0.891000
C77	-1.954968	-5.893634	2.858950

H78	-2.658940	-6.594774	3.319142
H79	-0.973123	-6.065820	3.301607
H80	-2.267309	-4.881598	3.133733
C81	-3.739813	-5.699133	0.412272
H82	-4.104997	-4.739363	0.787689
H83	-3.842102	-5.703549	-0.676691
H84	-4.408470	-6.471309	0.806161
C85	1.846192	-7.624590	-0.684660
H86	0.861416	-8.062342	-0.854774
H87	2.188710	-7.206222	-1.635925
H88	2.531591	-8.433510	-0.411437
C89	1.495302	-7.028979	2.352938
H90	0.553728	-7.572109	2.431362
H91	2.298378	-7.735349	2.588538
H92	1.504612	-6.255508	3.126393
C93	3.611803	-5.612228	0.756790
H94	4.013888	-5.308540	-0.213629
H95	3.694566	-4.764310	1.442686
H96	4.263610	-6.405491	1.136826

Bond lengths [ $\text{\AA}$ ] and bonds angles [deg]

Parameter	Value	Parameter	Value	Parameter	Value	Parameter	Value
R(1,2)	1.454	R(57,58)	1.0934	A(16,15,25)	117.0446	A(85,48,93)	106.7919
R(1,4)	1.4546	R(57,59)	1.0938	A(7,16,15)	119.7878	A(89,48,93)	105.0103
R(1,14)	1.3571	R(57,60)	1.0948	A(7,16,27)	123.2464	A(45,49,50)	110.6434
R(2,3)	1.4546	R(61,62)	1.091	A(15,16,27)	116.9222	A(45,49,51)	114.7628
R(2,7)	1.3573	R(61,63)	1.0942	A(9,17,18)	125.4865	A(45,49,52)	108.5992
R(3,4)	1.454	R(61,64)	1.0949	A(9,17,33)	116.6175	A(50,49,51)	107.8923
R(3,5)	1.3571	R(65,66)	1.0898	A(18,17,33)	117.8791	A(50,49,52)	107.3501
R(4,12)	1.3573	R(65,67)	1.0952	A(17,18,20)	117.5569	A(51,49,52)	107.3009
R(5,6)	1.4815	R(65,68)	1.0939	A(17,18,47)	113.8011	A(45,53,54)	110.3783

R(5,10)	1.4807	R(69,70)	1.0934	A(20,18,47)	128.5846	A(45,53,55)	113.3279
R(6,8)	1.459	R(69,71)	1.0937	A(10,19,20)	125.4656	A(45,53,56)	109.8784
R(6,21)	1.4053	R(69,72)	1.0948	A(10,19,34)	116.5337	A(54,53,55)	107.8844
R(7,8)	1.4818	R(73,74)	1.0941	A(20,19,34)	117.9736	A(54,53,56)	107.6488
R(7,16)	1.4808	R(73,75)	1.0896	A(18,20,19)	117.4963	A(55,53,56)	107.5211
R(8,23)	1.4052	R(73,76)	1.0951	A(18,20,48)	128.8071	A(45,57,58)	112.7791
R(9,10)	1.4473	R(77,78)	1.095	A(19,20,48)	113.5539	A(45,57,59)	112.5222
R(9,12)	1.4808	R(77,79)	1.0907	A(6,21,22)	122.4951	A(45,57,60)	108.6386
R(9,17)	1.4049	R(77,80)	1.0942	A(6,21,35)	119.2715	A(58,57,59)	108.31
R(10,19)	1.4047	R(81,82)	1.0934	A(22,21,35)	118.2025	A(58,57,60)	106.9545
R(11,13)	1.459	R(81,83)	1.0938	A(21,22,24)	119.757	A(59,57,60)	107.3523
R(11,14)	1.4815	R(81,84)	1.0948	A(21,22,36)	119.7858	A(46,61,62)	113.1043
R(11,29)	1.4053	R(85,86)	1.091	A(24,22,36)	120.4481	A(46,61,63)	110.0145
R(12,13)	1.4818	R(85,87)	1.0942	A(8,23,24)	122.4887	A(46,61,64)	110.4679
R(13,31)	1.4052	R(85,88)	1.0949	A(8,23,37)	119.1788	A(62,61,63)	107.4818
R(14,15)	1.4807	R(89,90)	1.0898	A(24,23,37)	118.2889	A(62,61,64)	107.9092
R(15,16)	1.4473	R(89,91)	1.0952	A(22,24,23)	119.7293	A(63,61,64)	107.6666
R(15,25)	1.4047	R(89,92)	1.0939	A(22,24,38)	120.4415	A(46,65,66)	114.8026
R(16,27)	1.4049	R(93,94)	1.0934	A(23,24,38)	119.823	A(46,65,67)	108.2903
R(17,18)	1.3987	R(93,95)	1.0937	A(15,25,26)	125.4656	A(46,65,68)	110.8772
R(17,33)	1.0781	R(93,96)	1.0948	A(15,25,39)	116.5337	A(66,65,67)	107.2548
R(18,20)	1.4294	A(2,1,4)	89.9987	A(26,25,39)	117.9736	A(66,65,68)	107.9906
R(18,47)	1.9162	A(2,1,14)	122.5914	A(25,26,28)	117.4963	A(67,65,68)	107.3202
R(19,20)	1.3985	A(4,1,14)	122.6043	A(25,26,46)	113.5539	A(46,69,70)	113.0109
R(19,34)	1.0786	A(1,2,3)	90.0012	A(28,26,46)	128.8071	A(46,69,71)	112.3703
R(20,48)	1.9166	A(1,2,7)	122.7136	A(16,27,28)	125.4865	A(46,69,72)	108.6281
R(21,22)	1.3855	A(3,2,7)	122.4849	A(16,27,40)	116.6175	A(70,69,71)	108.2652
R(21,35)	1.0796	A(2,3,4)	89.9987	A(28,27,40)	117.8791	A(70,69,72)	106.8811
R(22,24)	1.3934	A(2,3,5)	122.6043	A(26,28,27)	117.5569	A(71,69,72)	107.3969
R(22,36)	1.084	A(4,3,5)	122.5914	A(26,28,45)	128.5846	A(47,73,74)	110.6434
R(23,24)	1.3855	A(1,4,3)	90.0012	A(27,28,45)	113.8011	A(47,73,75)	114.7628

R(23,37)	1.0799	A(1,4,12)	122.4849	A(11,29,30)	122.4951	A(47,73,76)	108.5992
R(24,38)	1.0841	A(3,4,12)	122.7136	A(11,29,41)	119.2715	A(74,73,75)	107.8923
R(25,26)	1.3985	A(3,5,6)	113.2366	A(30,29,41)	118.2025	A(74,73,76)	107.3501
R(25,39)	1.0786	A(3,5,10)	113.0441	A(29,30,32)	119.757	A(75,73,76)	107.3009
R(26,28)	1.4294	A(6,5,10)	130.8047	A(29,30,42)	119.7858	A(47,77,78)	110.3783
R(26,46)	1.9166	A(5,6,8)	119.4122	A(32,30,42)	120.4481	A(47,77,79)	113.3279
R(27,28)	1.3987	A(5,6,21)	122.8284	A(13,31,32)	122.4887	A(47,77,80)	109.8784
R(27,40)	1.0781	A(8,6,21)	117.7405	A(13,31,43)	119.1788	A(78,77,79)	107.8844
R(28,45)	1.9162	A(2,7,8)	113.1293	A(32,31,43)	118.2889	A(78,77,80)	107.6488
R(29,30)	1.3855	A(2,7,16)	113.1396	A(30,32,31)	119.7293	A(79,77,80)	107.5211
R(29,41)	1.0796	A(8,7,16)	130.8152	A(30,32,44)	120.4415	A(47,81,82)	112.7791
R(30,32)	1.3934	A(6,8,7)	119.4392	A(31,32,44)	119.823	A(47,81,83)	112.5222
R(30,42)	1.084	A(6,8,23)	117.7825	A(28,45,49)	114.3523	A(47,81,84)	108.6386
R(31,32)	1.3855	A(7,8,23)	122.7615	A(28,45,53)	110.0477	A(82,81,83)	108.31
R(31,43)	1.0799	A(10,9,12)	119.7878	A(28,45,57)	109.2343	A(82,81,84)	106.9545
R(32,44)	1.0841	A(10,9,17)	116.9222	A(49,45,53)	111.1554	A(83,81,84)	107.3523
R(45,49)	1.8921	A(12,9,17)	123.2464	A(49,45,57)	105.1108	A(48,85,86)	113.1043
R(45,53)	1.8916	A(5,10,9)	119.7819	A(53,45,57)	106.5243	A(48,85,87)	110.0145
R(45,57)	1.8953	A(5,10,19)	123.1458	A(26,46,61)	109.7978	A(48,85,88)	110.4679
R(46,61)	1.8917	A(9,10,19)	117.0446	A(26,46,65)	114.8528	A(86,85,87)	107.4818
R(46,65)	1.8925	A(13,11,14)	119.4122	A(26,46,69)	109.157	A(86,85,88)	107.9092
R(46,69)	1.8959	A(13,11,29)	117.7405	A(61,46,65)	110.8194	A(87,85,88)	107.6666
R(47,73)	1.8921	A(14,11,29)	122.8284	A(61,46,69)	106.7919	A(48,89,90)	114.8026
R(47,77)	1.8916	A(4,12,9)	113.1396	A(65,46,69)	105.0103	A(48,89,91)	108.2903
R(47,81)	1.8953	A(4,12,13)	113.1293	A(18,47,73)	114.3523	A(48,89,92)	110.8772
R(48,85)	1.8917	A(9,12,13)	130.8152	A(18,47,77)	110.0477	A(90,89,91)	107.2548
R(48,89)	1.8925	A(11,13,12)	119.4392	A(18,47,81)	109.2343	A(90,89,92)	107.9906
R(48,93)	1.8959	A(11,13,31)	117.7825	A(73,47,77)	111.1554	A(91,89,92)	107.3202
R(49,50)	1.0941	A(12,13,31)	122.7615	A(73,47,81)	105.1108	A(48,93,94)	113.0109
R(49,51)	1.0896	A(1,14,11)	113.2366	A(77,47,81)	106.5243	A(48,93,95)	112.3703
R(49,52)	1.0951	A(1,14,15)	113.0441	A(20,48,85)	109.7978	A(48,93,96)	108.6281

R(53,54)	1.095	A(11,14,15)	130.8047	A(20,48,89)	114.8528	A(94,93,95)	108.2652
R(53,55)	1.0907	A(14,15,16)	119.7819	A(20,48,93)	109.157	A(94,93,96)	106.8811
R(53,56)	1.0942	A(14,15,25)	123.1458	A(85,48,89)	110.8194	A(95,93,96)	107.3969

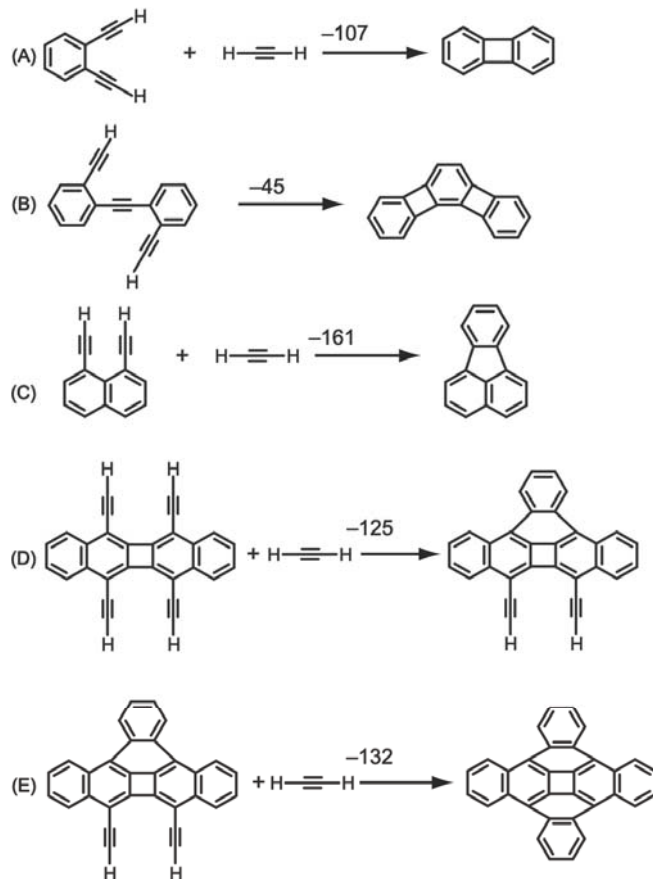
## References

- (1) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, T. Vreven, Jr., K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J.A. Pople, Gaussian, Inc., Wallingford CT, 2004.
- (2) See *e.g.* M. A. Dobrowolski, M. K. Cyrański, B. L. Merner, G. J. Bodwell, J. I. Wu, P. v. Ragué Schleyer, *J. Org. Chem.* 73, 8001 (2008).

## Cyclotrimerization Thermochemistry

$\Delta E$ , M05-2X/6-311+G(d,p)

M. D. Wodrich, C. Corminboeuf, P. R. Schreiner, A. A. Fokin, P. V. R. Schleyer, *Org. Lett.* **9**, 1851-1854 (2007). Energy in kcal/mol.



## NMR Chemical Shift Calculations

GIAO/WP04/6-31G(d,p)//M05-2X/6-311+G(d,p)

according the methods of R. Jain, T. Bally, P. R. Rablen, *J. Org. Chem.* **74**, 4017-4023 (2009) and M. D. Wodrich, C. Corminboeuf, P. R. Schreiner, A. A. Fokin, P. V. R. Schleyer, *Organic Letters* **9**, 1851-1854 (2007).

Referenced to benzene (measured for benzene (CD<sub>2</sub>Cl<sub>2</sub>) <sup>1</sup>H δ, 7.42, <sup>13</sup>C δ, 129.9)

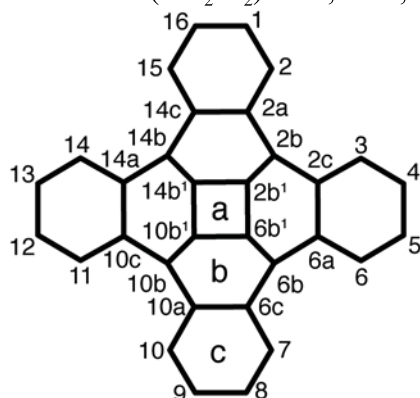


Table. Calculated and measured chemical shifts for TMS<sub>4</sub>-TBQ.

Position	<sup>1</sup> H δ calcd.	<sup>1</sup> H δ exp.	<sup>13</sup> C δ calcd.	<sup>13</sup> C δ exp.
1	–	–	146.2	145.5
2	8.64	8.93	136.7	133.9
2a	–	–	143.5	140.6
2b	–	–	134.1	128.8
2b1	–	–	148.9	145.3
2c	–	–	146.3	141.9
3	8.50	8.63	129.7	127.6
4	7.80	7.57	128.9	127.7
CH <sub>3</sub>	0.65	0.5	12.6	2.2



## NICS Calculations

GIAO/WP04/6-31G(d,p)//M05-2X/6-311+G(d,p)

Chemical shifts calculated according the methods of R. Jain, T. Bally, P. R. Rablen, *J. Org. Chem.* 74, 4017-4023 (2009) at the geometry calculated according to M. D. Wodrich, C. Corminboeuf, P. R. Schreiner, A. A. Fokin, P. V. R. Schleyer, *Org. Lett.* 9, 1851-1854 (2007).

	NICS(0)	NICS(1) convex	NICS(1) concave
[4]radialene	5.3	-2.3	
benzene	-9.7	-10.9	
cyclobutadiene	23.7	16.5	
corannulene - five membered	8.9	2.7	-2.7
corannulene - six membered	-7.0	-6.0	-12.3
C <sub>60</sub> - five membered	11.0	5.9	2.1
C <sub>60</sub> - six membered	-2.7	-0.6	-5.7
TBQ - four membered A	4.5	4.0	-5.8
TBQ - medial B	-3.7	-2.2	-9.0
TBQ - distal C	-9.7	-10.8	-10.6

## Excited State Calculations

TD-DFT B3LYP/6-31G(d)//B3LYP/6-31G(d)

tetrakis(TMS)[4]circulene, B3LYP/6-31G\* geometry (C2v):

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.697867	4.911190	-0.137394
2	6	-1.387086	3.806029	-0.619646
3	6	-0.730690	2.660949	-1.107057
4	6	0.730690	2.660949	-1.107057
5	6	1.387086	3.806029	-0.619646
6	6	0.697867	4.911190	-0.137394
7	6	-1.457350	1.463830	-1.598194
8	6	-0.728384	0.726429	-2.479285
9	6	0.728384	0.726429	-2.479285
10	6	1.457350	1.463830	-1.598194
11	6	-2.607364	0.724220	-1.030671
12	6	-2.607364	-0.724220	-1.030671
13	6	-1.457350	-1.463830	-1.598194
14	6	-0.728384	-0.726429	-2.479285
15	6	-3.701241	-1.359993	-0.413930
16	6	-4.789212	-0.717757	0.193233
17	6	-4.789212	0.717757	0.193233
18	6	-3.701241	1.359993	-0.413930
19	6	0.728384	-0.726429	-2.479285
20	6	1.457350	-1.463830	-1.598194
21	6	0.730690	-2.660949	-1.107057
22	6	-0.730690	-2.660949	-1.107057
23	6	2.607364	0.724220	-1.030671
24	6	2.607364	-0.724220	-1.030671
25	6	-1.387086	-3.806029	-0.619646
26	6	-0.697867	-4.911190	-0.137394
27	6	0.697867	-4.911190	-0.137394
28	6	1.387086	-3.806029	-0.619646
29	6	3.701241	-1.359993	-0.413930
30	6	4.789212	-0.717757	0.193233
31	6	4.789212	0.717757	0.193233
32	6	3.701241	1.359993	-0.413930
33	1	-3.696653	-2.438857	-0.430918
34	14	-6.079719	-1.950605	0.904846
35	14	-6.079719	1.950605	0.904846
36	1	-3.696653	2.438857	-0.430918
37	1	3.696653	-2.438857	-0.430918
38	14	6.079719	1.950605	0.904846
39	14	6.079719	-1.950605	0.904846
40	1	3.696653	2.438857	-0.430918
41	1	2.468071	-3.852213	-0.657479
42	1	1.248653	-5.777412	0.218918

43	1	-1.248653	-5.777412	0.218918
44	1	-2.468071	-3.852213	-0.657479
45	1	2.468071	3.852213	-0.657479
46	1	1.248653	5.777412	0.218918
47	1	-1.248653	5.777412	0.218918
48	1	-2.468071	3.852213	-0.657479
49	6	-5.465661	-3.725731	0.607955
50	6	-6.306277	-1.809070	2.783811
51	6	-7.764418	-1.854792	0.037773
52	6	-5.465661	3.725731	0.607955
53	6	-7.764418	1.854792	0.037773
54	6	-6.306277	1.809070	2.783811
55	6	5.465661	-3.725731	0.607955
56	6	7.764418	-1.854792	0.037773
57	6	6.306277	-1.809070	2.783811
58	6	5.465661	3.725731	0.607955
59	6	6.306277	1.809070	2.783811
60	6	7.764418	1.854792	0.037773
61	1	-6.204429	-4.417812	1.031615
62	1	-5.366389	-3.973480	-0.455436
63	1	-4.508297	-3.935834	1.098891
64	1	-8.338396	-2.761092	0.269387
65	1	-8.369664	0.999751	0.348833
66	1	-7.651341	-1.805357	-1.051382
67	1	-6.728955	-2.748272	3.162395
68	1	-5.350539	-1.647566	3.295277
69	1	-6.984145	1.005709	3.082474
70	1	-8.338396	2.761092	0.269387
71	1	-7.651341	1.805357	-1.051382
72	1	-8.369664	-0.999751	0.348833
73	1	-6.204429	4.417812	1.031615
74	1	-4.508297	3.935834	1.098891
75	1	-5.366389	3.973480	-0.455436
76	1	-6.728955	2.748272	3.162395
77	1	-6.984145	-1.005709	3.082474
78	1	-5.350539	1.647566	3.295277
79	1	6.204429	-4.417812	1.031615
80	1	4.508297	-3.935834	1.098891
81	1	5.366389	-3.973480	-0.455436
82	1	8.338396	-2.761092	0.269387
83	1	7.651341	-1.805357	-1.051382
84	1	8.369664	0.999751	0.348833
85	1	6.728955	-2.748272	3.162395
86	1	6.984145	1.005709	3.082474
87	1	5.350539	-1.647566	3.295277
88	1	8.338396	2.761092	0.269387
89	1	8.369664	-0.999751	0.348833
90	1	7.651341	1.805357	-1.051382
91	1	6.204429	4.417812	1.031615
92	1	5.366389	3.973480	-0.455436
93	1	4.508297	3.935834	1.098891

94	1	6.728955	2.748272	3.162395
95	1	5.350539	1.647566	3.295277
96	1	6.984145	-1.005709	3.082474

---

total Energy: -2863.61743421

zero-point correction: 0.430519

Low frequencies --- -81.1259 -81.1091 -0.0027 -0.0016

Low frequencies --- 0.0017 3.1618 4.7503 7.4040

(the negative frequencies are associated with TMS torsions)

## Ion Thermochemistry

The electron affinity and ionization potential were calculated at the B3LYP/6-31G\* level.