A Novel Class of C_{3d} Symmetrical Molecules Synthesized by a Six-Fold Substitution from 1,4,5,8,9,12-Hexabromododecahydrotriphenylene

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1. General Information.

Unless otherwise mentioned, all commercial reagents were used as received without further purification. The reactions were monitored using analytical thin layer chromatography (TLC) with Merck silica gel plate (GF-254). Flash chromatography was performed using Merck silica gel 60 with freshly distilled solvents. ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were recorded on Bruker Avance spectrometers using $CDCl_3$, CD_3COCD_3 or DMSO-d_6 as a solvent. Chemical shifts (δ) are reported in ppm, using TMS as an internal standard. Data are presented as follows: chemical shift (ppm), coupling constant J (Hz) and integration. Elemental analysis was performed on a PE-2400CHN (U.S) analyzer. Melting points were uncorrected. Infrared spectra were recorded using EQUINX55 FT-IR spectrometer (Brucher). The crystal structure was recorded on Bruker APEX II CCD area-detector X-ray diffraction spectrometer.

2. Experimental details and characterization of the compounds

The synthesis of the hexaazide (3a) To a suspension of NaN_3 (0.65 g, 10 mmol) in DMSO (15 mL) in a 25 mL round-bottle flask was added the hexabromide (0.714 g, 1 mmol). The reaction mixture was stirred electromagnetically at room temperature until the hexabromide could not be detected by TLC. The resulting mixture was then poured into 150 mL water. The white participate was collected by vacuum filtration, washed with water, and dried over $CaCl_2$, yielded **3a** as a off-white solid (0.39 g, 81 %). Recrystallization in petroleum ether/chloroform gave the hexaazide as colorless plates.

mp 160.0-161.0 °C.

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 5.06 (s, 6H), 2.28 (s, 12H).

^{13}C NMR (75.45 MHz, $CDCl_3$): δ (ppm) 134.70, 53.60, 23.38.

IR (KBr, cm^{-1}): 2958, 2085, 1636, 1308, 1276, 1308.

Elemental analysis: calcd. for $C_{18}H_{18}N_{18}$: C, 44.44; H, 3.73; N, 51.83; found: C, 43.35; H, 3.31; N, 51.00.

The synthesis of the hexathiocyanide (3b) To a suspension of NaSCN (0.81 g, 10 mmol) in DMF (15 mL) in a 25 mL round-bottle flask was added the hexabromide (0.714 g, 1 mmol). The reaction mixture was stirred electromagnetically at room temperature until the hexabromide could not be detected by TLC. The resultant mixture was then poured into 150 mL water. The white participate was collected by vacuum filtration, washed with water, and dried under vacuum conditions to yield **3b** as a white solid (0.54 g, 92 %). Recrystallization in acetone gave the hexathiocyanide as a white powder.

mp 205.6-206.9 °C.

^{1}H NMR (300 MHz, CD_3COCD_3): δ (ppm) 5.77 (s, 6H), 2.99 (d, J = 9.0Hz, 6H), 2.59 (d, J = 9.3 Hz, 6H).

Elemental analysis: calcd. for $C_{24}H_{18}N_6S_6$: C, 49.46; H, 3.11; N, 14.42; S, 33.01; found: C, 49.40; H, 3.08; N, 14.33; S, 33.00.

The procedure for the synthesis of hexasulfide 3c-j exemplified by 3f: 4-Chlorothiophenol (10 mmol) and powdery KOH (0.56 g, 10 mmol) was added in 10 mL methanol in a 25 mL round-bottle flask and stirred electromagnetically at room temperature until the solid completely

was dissolved. Upon removal of methanol by rotary evaporation, 12 mL DMF was added to dissolve the residue. After the resulting solution was stirred in an ice-water bath for 10 min, the hexabromide 0.714 g (1 mmol) was added and stirred until the hexabromide could not be detected by TLC. The resulted mixture was then poured into 150 mL water. The white participate was collected by vacuum filtration, washed with water and cold ethanol, and dried under vacuum conditions. Column chromatography with petroleum ether/ethyl acetate as eluent gave **3f** as a white solid. Recrystallization in chloroform/etheyl acetate/ethanol gave the product as white block crystals.

3c: yield 57 %; mp 242.0-244.0 °C.

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.24 (m, 30H), 5.45 (s, 6H), 2.72 (d, J = 9.9 Hz, 6H), 1.92 (d, J = 9.6 Hz, 6H).

^{13}C NMR (75.45 MHz, $CDCl_3$): δ (ppm) 136.17, 135.38, 130.45, 129.09, 126.69, 43.62, 22.90.

Elemental analysis: calcd. for $C_{54}H_{48}S_6$: C, 72.93; H, 5.44; S, 21.63; found: C, 72.89; H, 5.43; S, 21.60.

3d: yield 51 %; mp 203.0-205.0 °C.

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.19 (d, J = 6.9 Hz, 12H), 7.06 (d, J = 6.9 Hz ,12H), 5.33 (s, 6H), 2.66 (d, J = 9.6 Hz, 6H); 1.86 (d, J = 9.6 Hz, 6H), 2.35 (s, 18H)

^{13}C NMR (75.45 MHz, $CDCl_3$): δ (ppm) 136.93, 135.20, 131.64, 129.77, 126.23, 124.86 ,

44.34, 22.78 , 21.17.

Elemental analysis: calcd. for $C_{60}H_{60}S_6$: C, 74.03; H, 6.21; S,19.76; found: C, 74.01; H, 6.18; S,19.70.

3e: yield 48 %; mp 211.6-212.9 °C.

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.07 (m, 24H), 5.24 (s, 6H), 2.65 (d, J = 10.2 Hz, 6H), 1.88 (d, J = 9.9 Hz, 6H).

^{13}C NMR (75.45 MHz, $CDCl_3$): δ (ppm) 164.02, 160.73, 135.06, 133.99, 133.89, 116.42, 116.14, 44.69, 22.77.

Elemental analysis: calcd. for $C_{54}H_{42}F_6S_6$: C, 65.03; H, 4.24; S, 19.29; found: C, 65.00; H, 4.10; S, 19.18.

3f: yield 80 %; mp 217.0-219.0 °C.

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.23 (d, J = 8.4 Hz, 12H), 7.14 (d, J = 8.4 Hz, 12H), 5.24 (s, 6H), 2.61 (d, J = 9.9 Hz, 6H), 1.89 (d, J = 9.8 Hz, 6H).

^{13}C NMR (75.45 MHz, $CDCl_3$): δ (ppm) 135.08, 133.96, 133.23, 131.99, 129.34, 43.74, 23.10.

Elemental analysis: calcd. for $C_{54}H_{42}Cl_6S_6$: C, 59.18; H, 3.86; S, 17.55; found: C, 59.17; H, 3.67, S, 17.41.

3g: yield 99 %; mp 208.5-210.0 °C.

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.37 (d, *J* = 8.4 Hz, 12H), 7.07 (d, *J* = 8.4Hz, 12H), 5.22 (s, 6H), 2.60 (d, *J* = 9.9 Hz, 6H), 1.89 (d, *J* = 9.9 Hz, 6H).

^{13}C NMR (75.45 MHz, $CDCl_3$): δ (ppm) 135.08, 134.65, 132.27, 132.08, 121.20, 43.56, 23.18.

Elemental analysis: calcd. for $C_{54}H_{42}Br_6S_6$: C, 47.59; H, 3.11; S, 14.12; found: C, 47.56; H, 3.15; S, 14.10.

3h: yield 61 %; mp 158.0-160.0 °C.

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 5.87 (s, 6H), 2.75 (s, 18H), 2.68 (d, overlaped by $-CH_3$ at δ 2.75, 6H), 2.42 (d, *J* = 9.9 Hz, 6H).

^{13}C NMR (75.45 MHz, $CDCl_3$): δ (ppm) 165.84, 163.55, 136.08, 45.50, 25.11, 15.69

Elemental analysis: calcd. for $C_{36}H_{36}N_{12}S_{12}$: C, 42.33; H, 3.55; N, 16.45; S, 37.67; found: C, 42.30; H, 3.53; N, 16.47; S, 37.7.

3i: yield 85 %; mp 263.0-267.0 °C.

^{1}H NMR (300 MHz, DMSO-d_6): δ (ppm) 5.66 (s, 6H), 4.00 (s, 18H), 2.89 (s, 6H), 2.73 (s, 6H).

Elemental analysis: calcd. for $C_{30}H_{36}N_{24}S_6$: C, 38.95; H, 3.92; N, 36.34; S, 20.80; found: C, 38.94; H, 3.95; N, 36.37; S, 26.74.

3j: yield 98 %; mp 275.0-277.0 °C.

^{1}H NMR (300 MHz, $CDCl_3$): 7.52 (d, *J* = 7.8 Hz, 6H), 7.22 (d, *J* = 8.1 Hz, 6H), 7.13 (t, *J* = 7.2 Hz, *J* = 7.5 Hz, 6H), 7.04 (t, *J* = 7.2Hz, *J* = 7.5 Hz, 6H), 6.03 (s, 6H), 2.82 (d, *J* = 11.1 Hz, 6H), 2.43 (d, *J* = 10.2 Hz, 6H).

Elemental analysis: calcd. for $C_{60}H_{42}N_6S_{12}$: C, 58.50; H, 3.44; N, 6.82; S, 31.24; found: C, 58.43; H, 3.40; N, 6.75; S, 31.82.

3. Copies of IR, ^{1}H NMR, ^{13}C NMR Spectra.

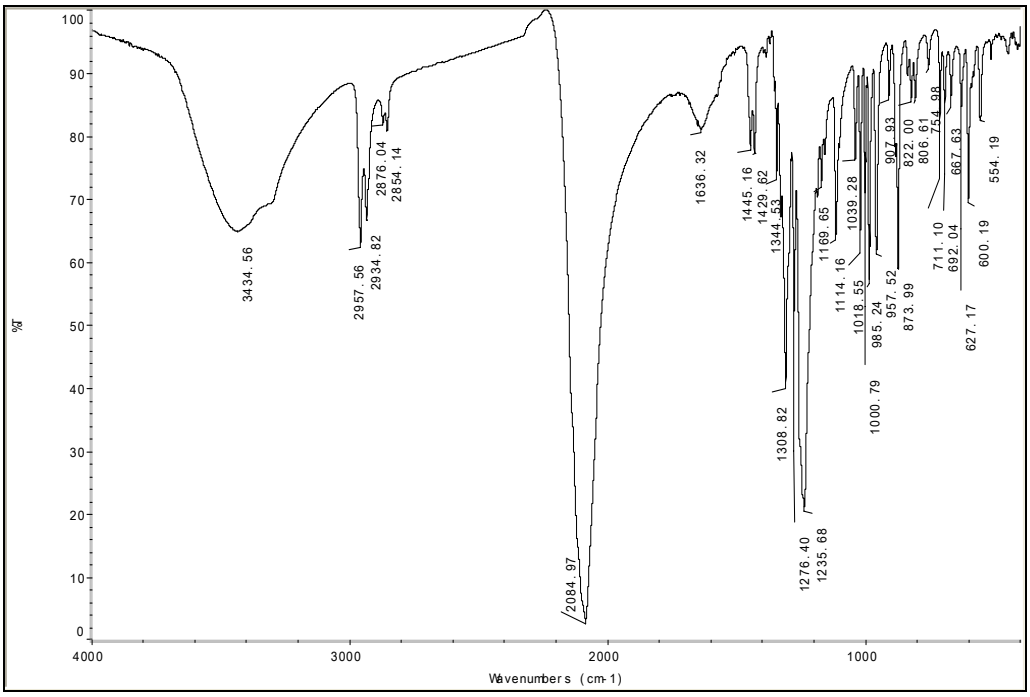

Figure 1S. IR spectrum of 3a.

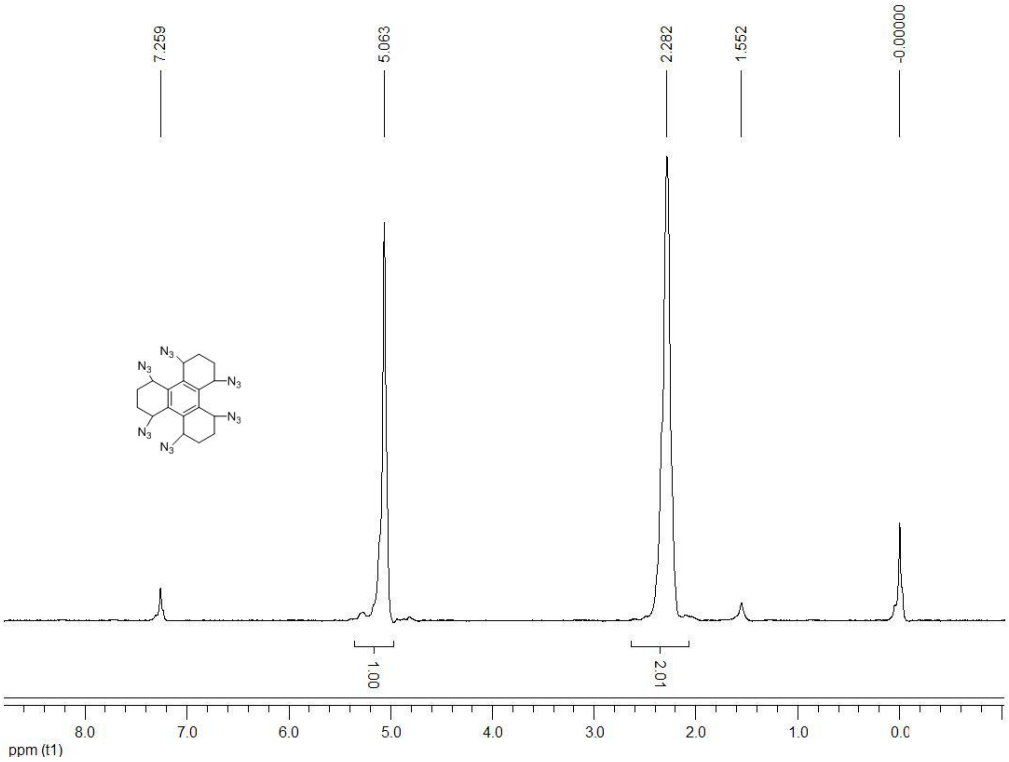

Figure 2S. ^{1}H NMR spectrum of 3a.

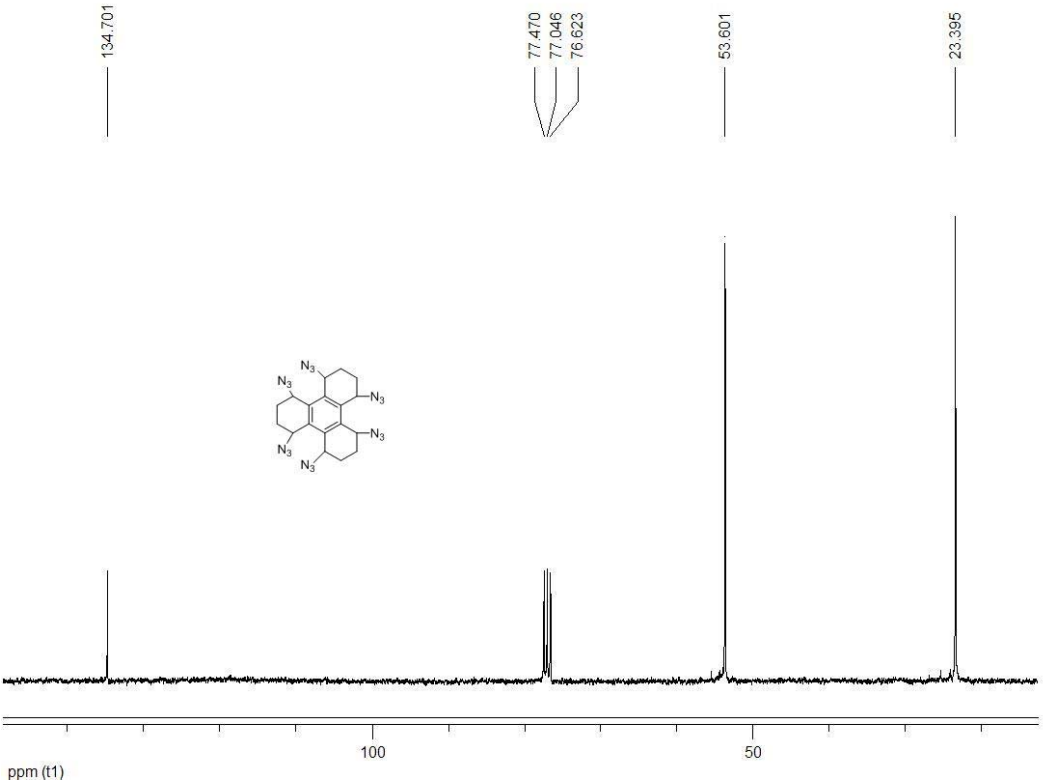

Figure 3S. ^{13}C NMR spectrum of 3a.

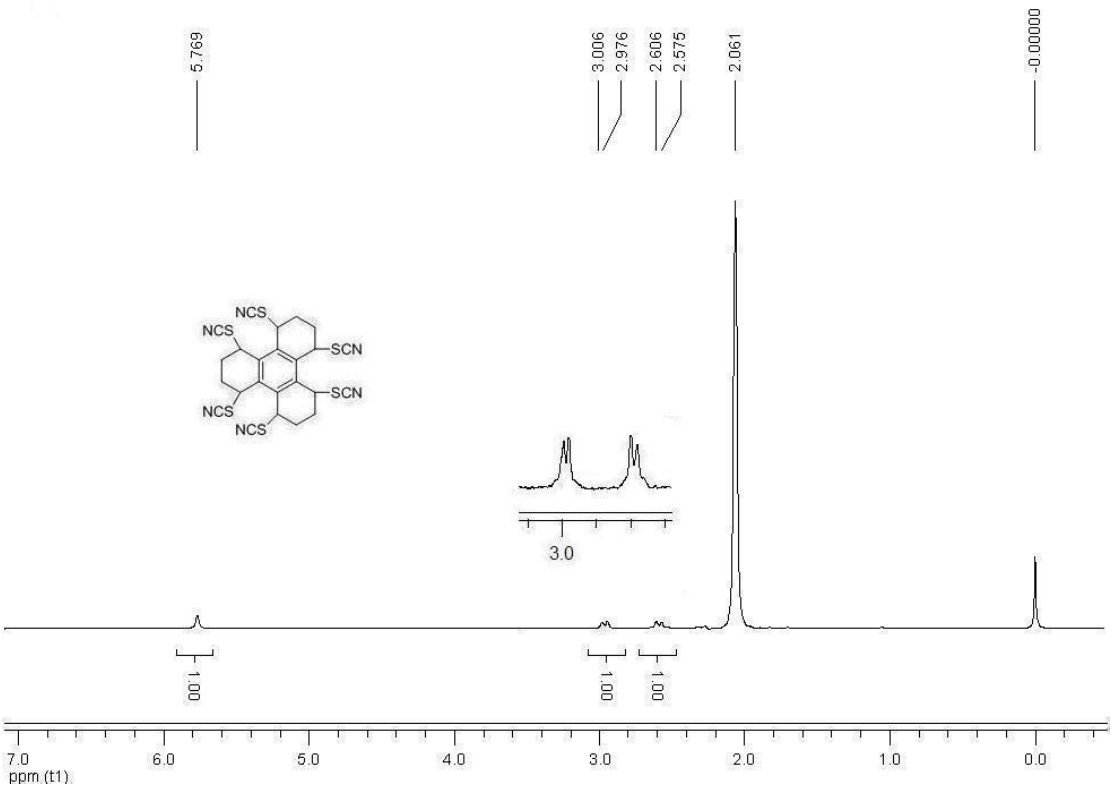

Figure 4S. ^{1}H NMR spectrum of 3b.

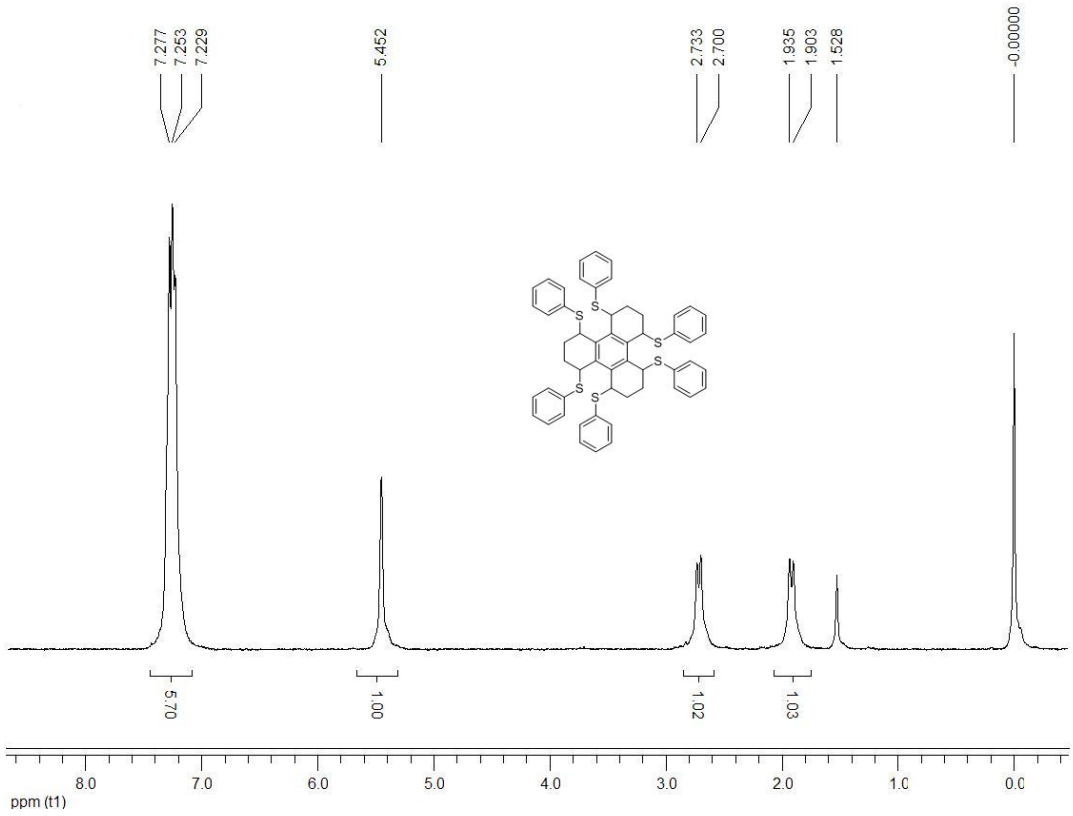

Figure 5S. ^{1}H NMR spectrum of 3c.

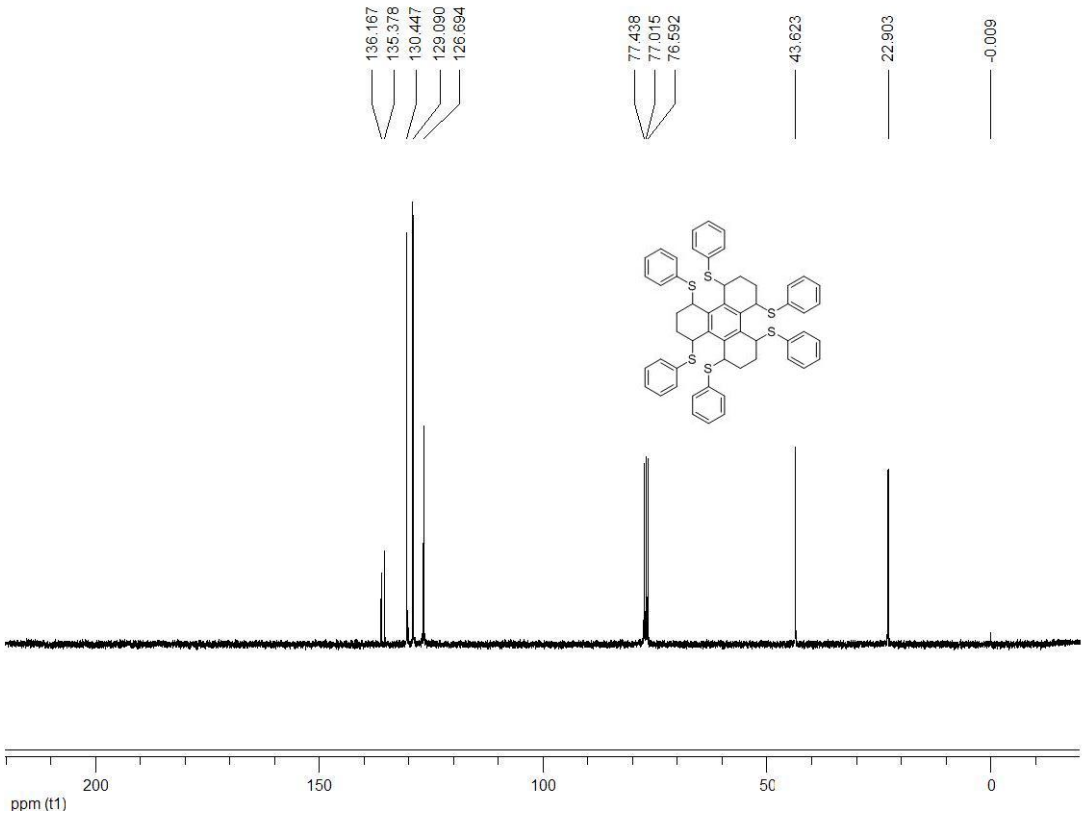

Figure 6S. ^{13}C NMR spectrum of 3c.

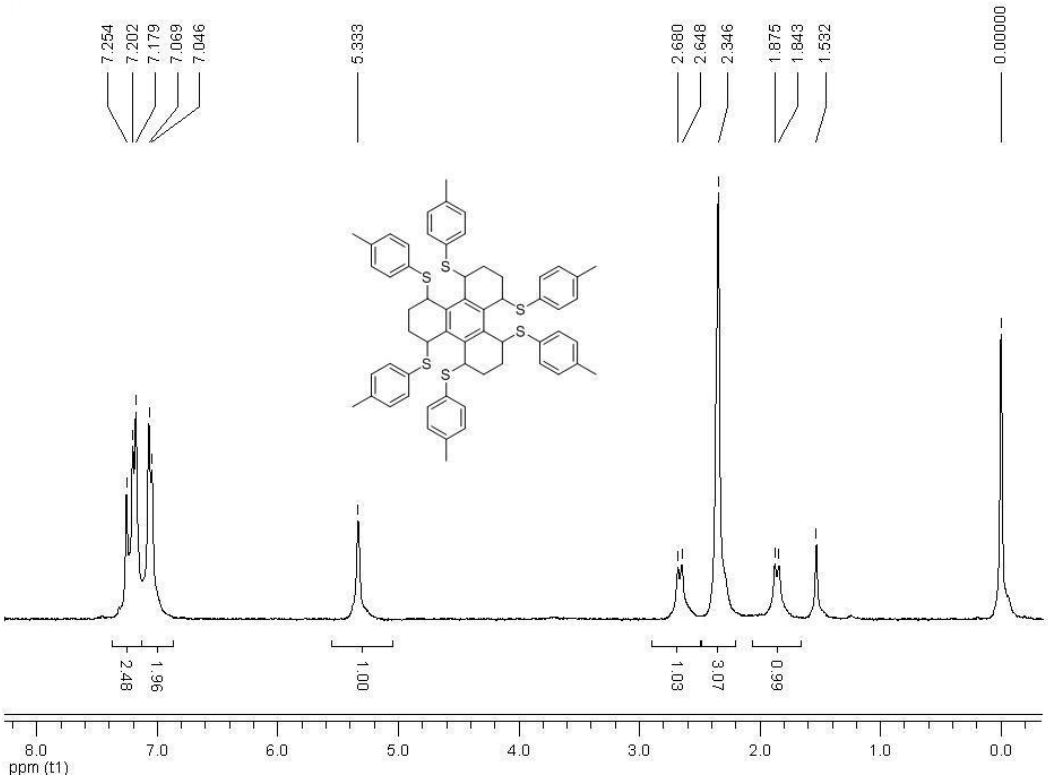

Figure 7S. **^{1}H NMR spectrum of 3d.**

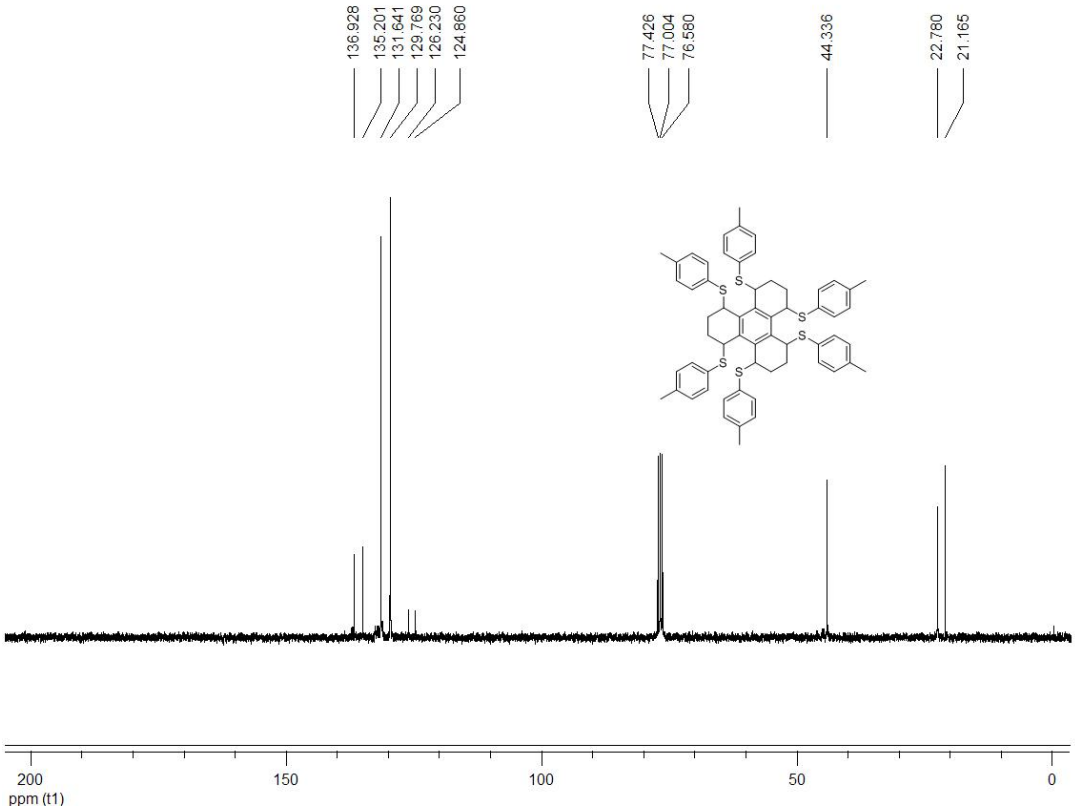

Figure 8S. **^{13}C NMR spectrum of 3d.**

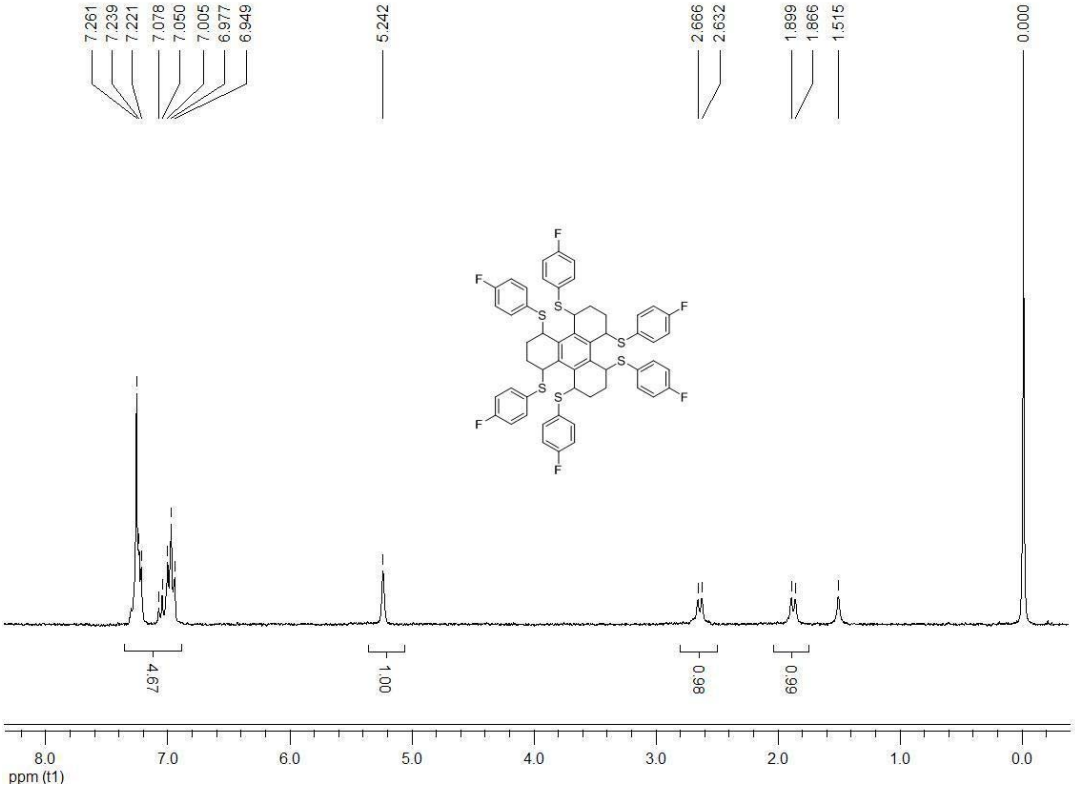

Figure 9S. ^{1}H NMR spectrum of 3e.

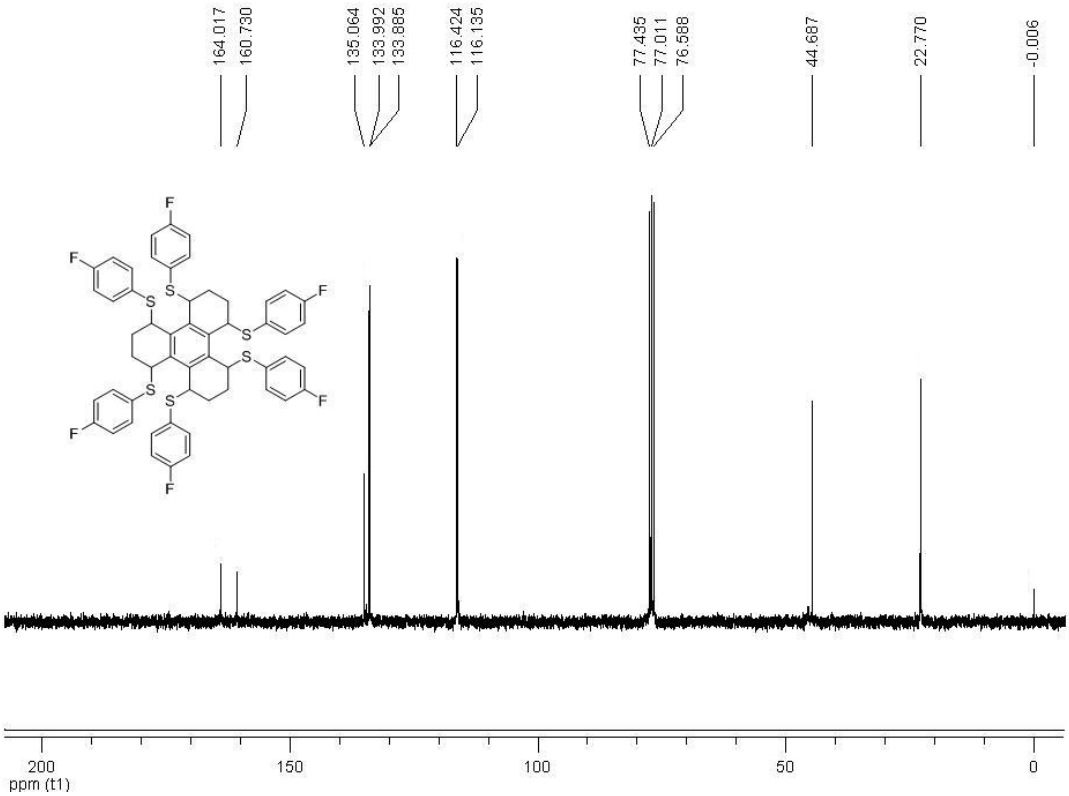

Figure 10S. ^{13}C NMR spectrum of 3e.

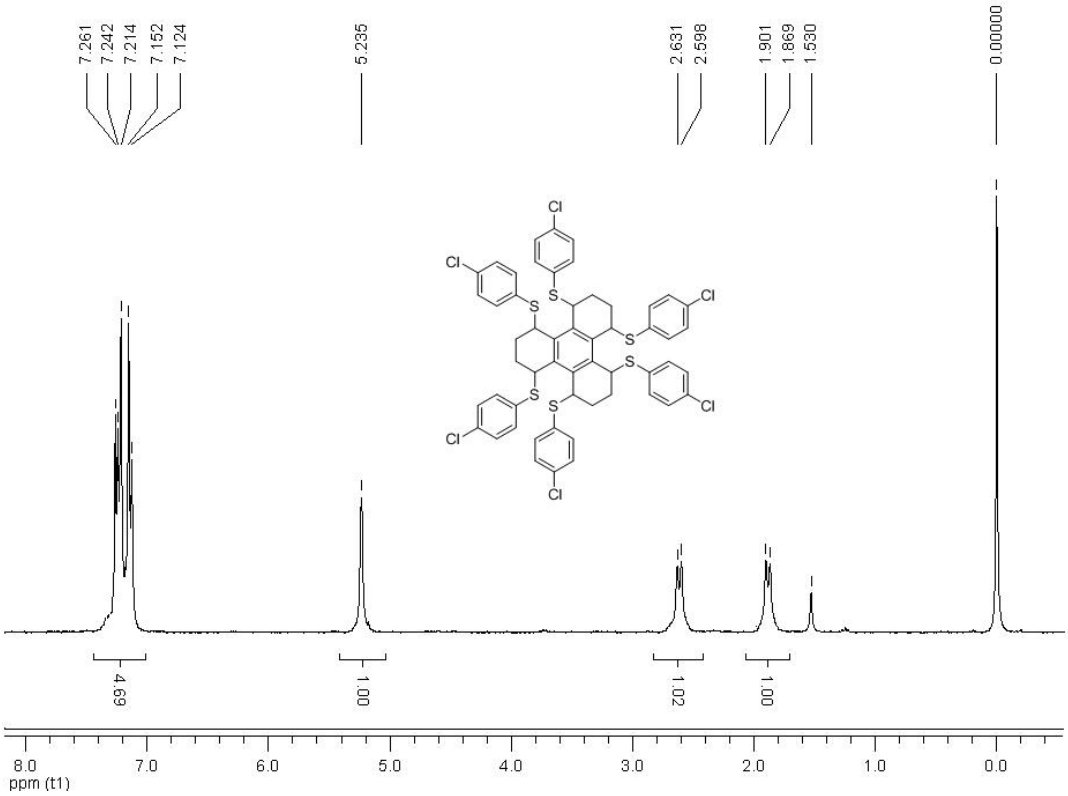

Figure 11S. ^{1}H NMR spectrum of 3f.

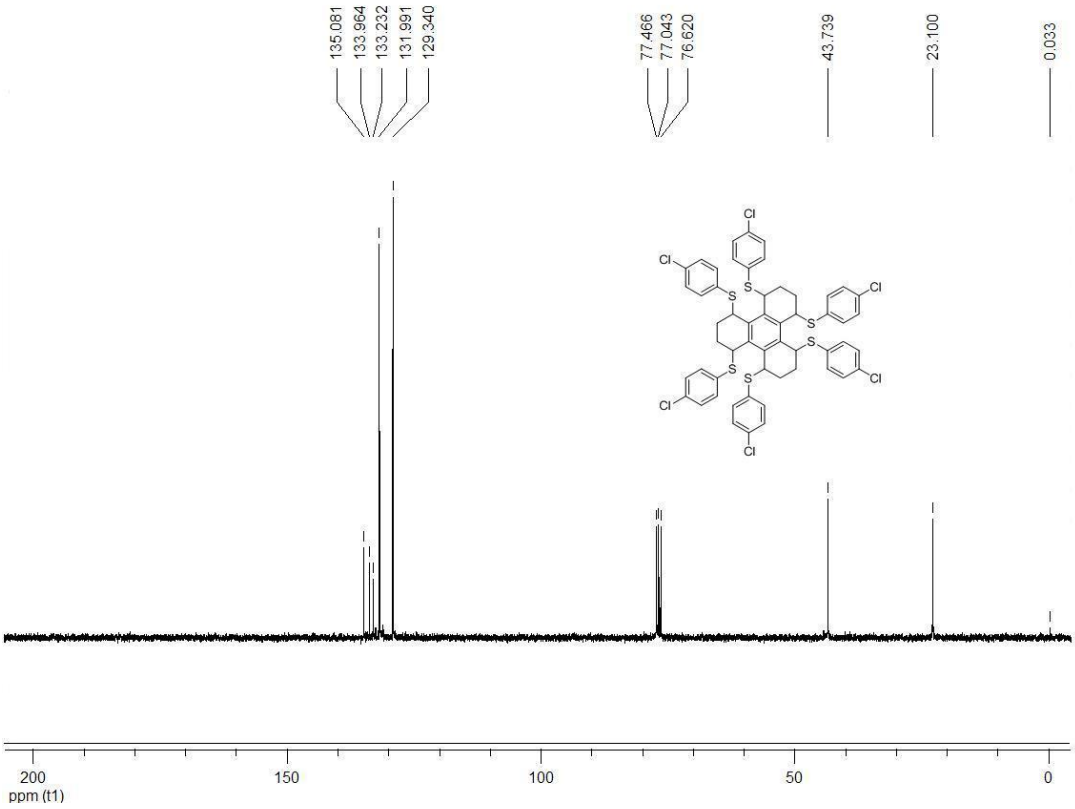

Figure 12S. ^{13}C NMR spectrum of 3f.

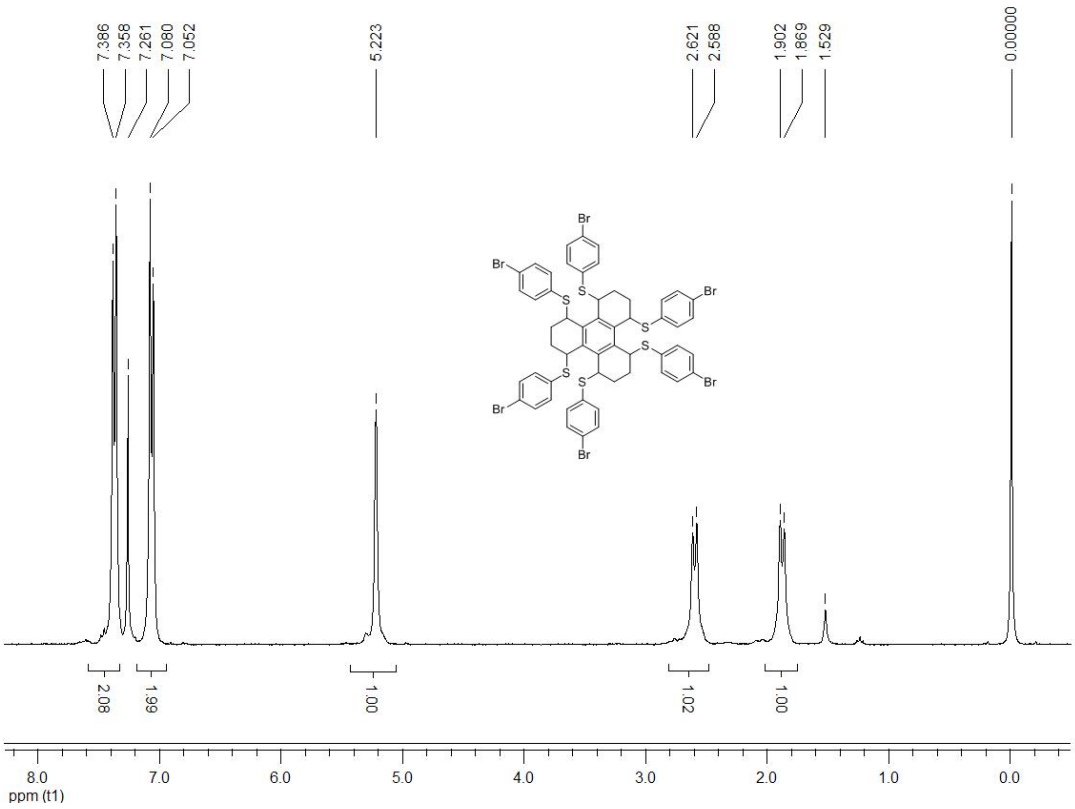

Figure 13S. ^{1}H NMR spectrum of 3g.

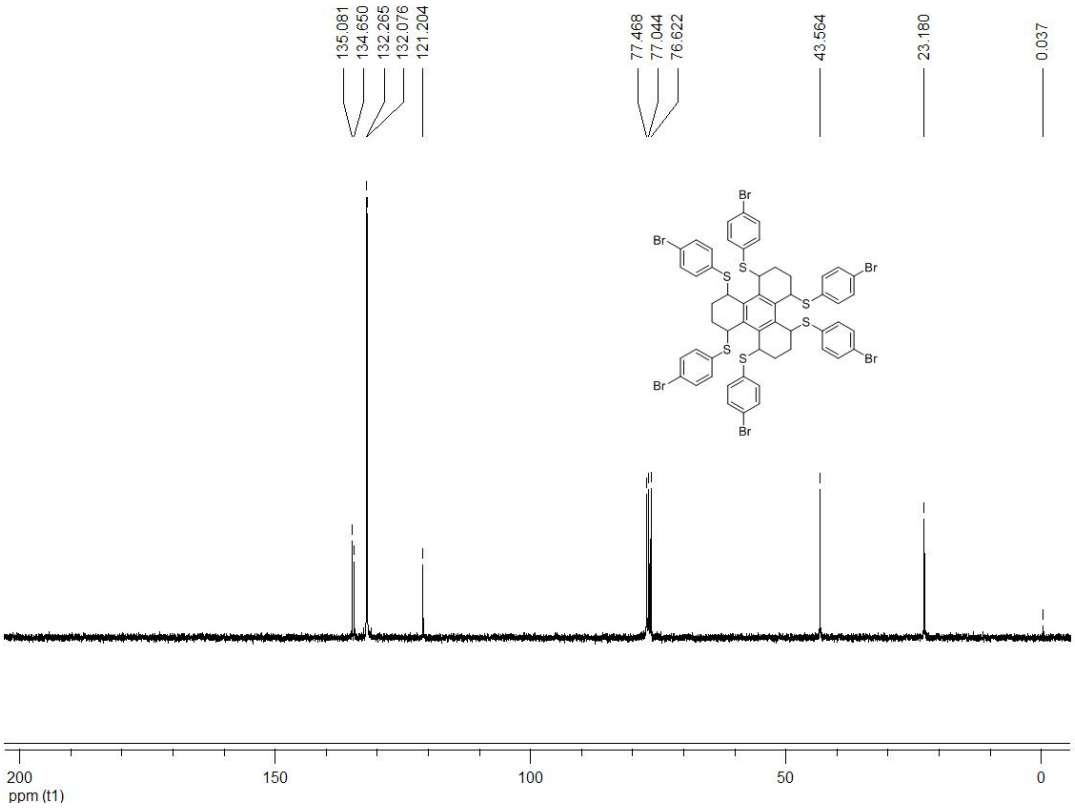

Figure 14S. ^{13}C NMR spectrum of 3g.

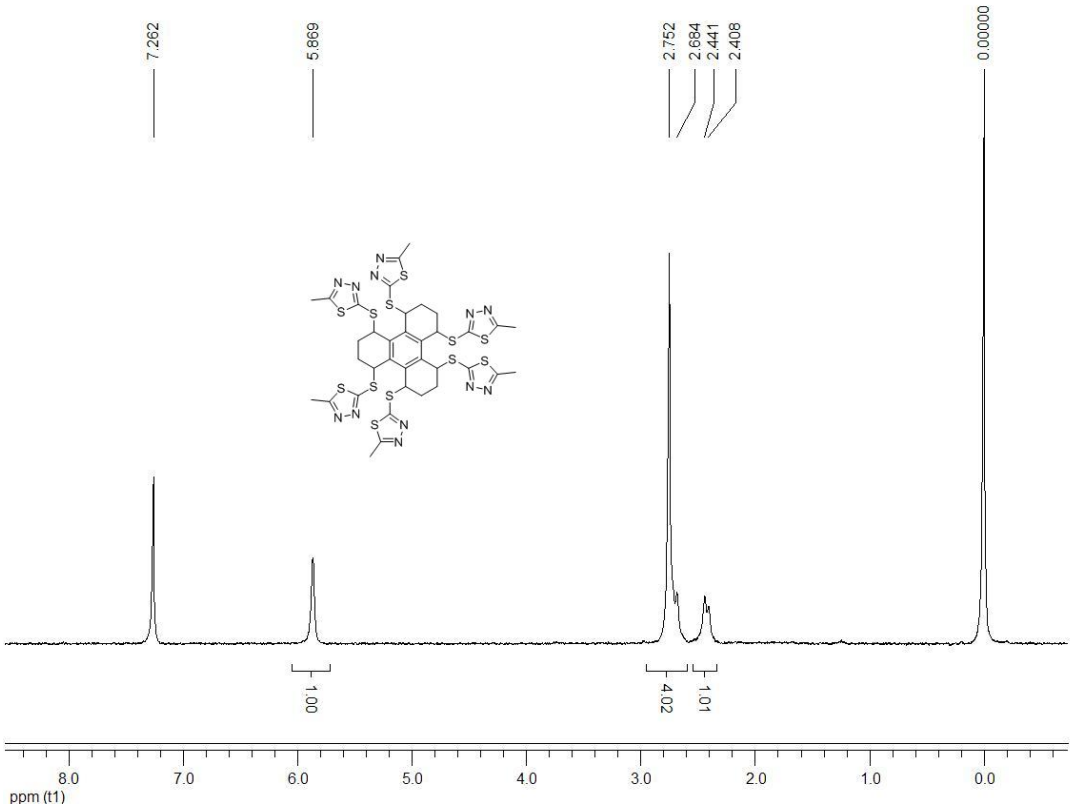

Figure 15. ^{1}H NMR spectrum of 3h.

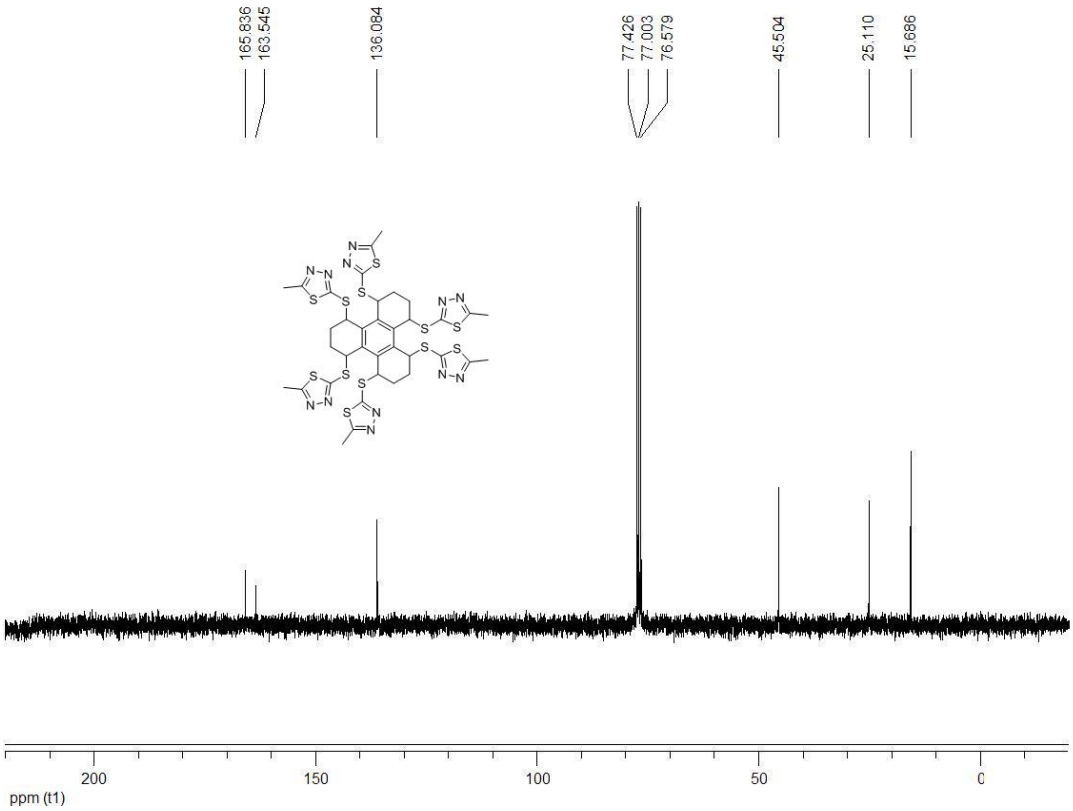

Figure 16S. ^{13}C NMR spectrum of 3h.

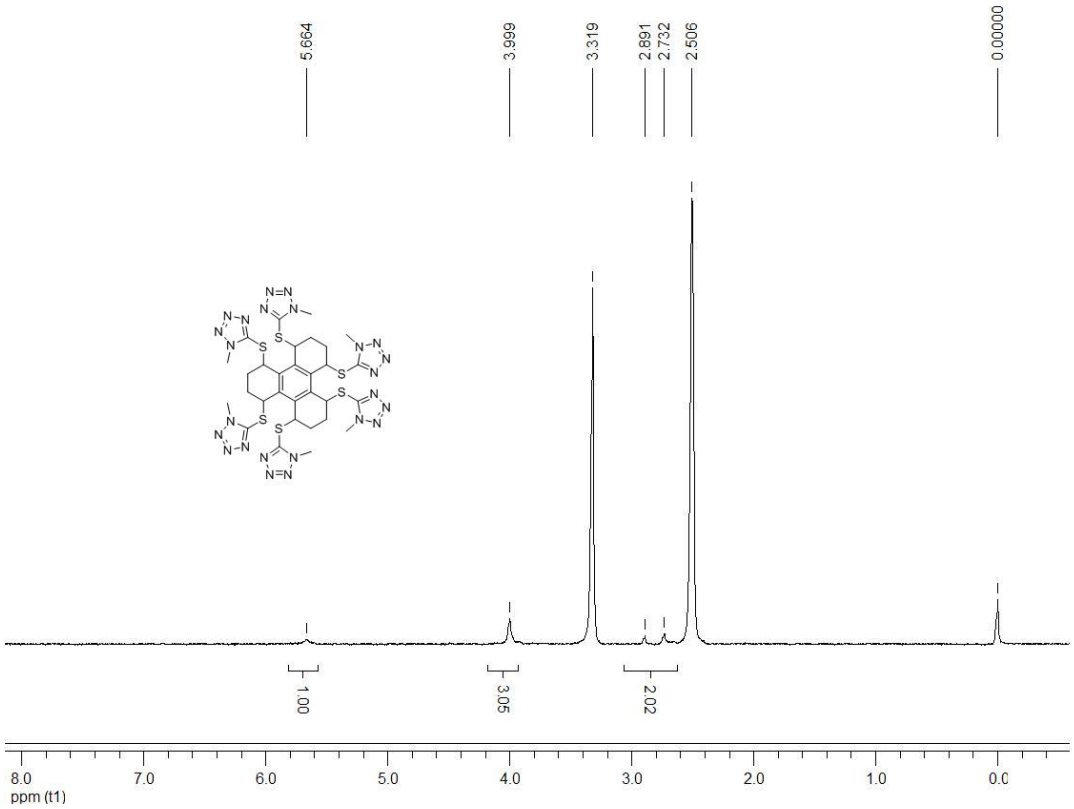

Figure 17. ^{1}H NMR spectrum of 3i.

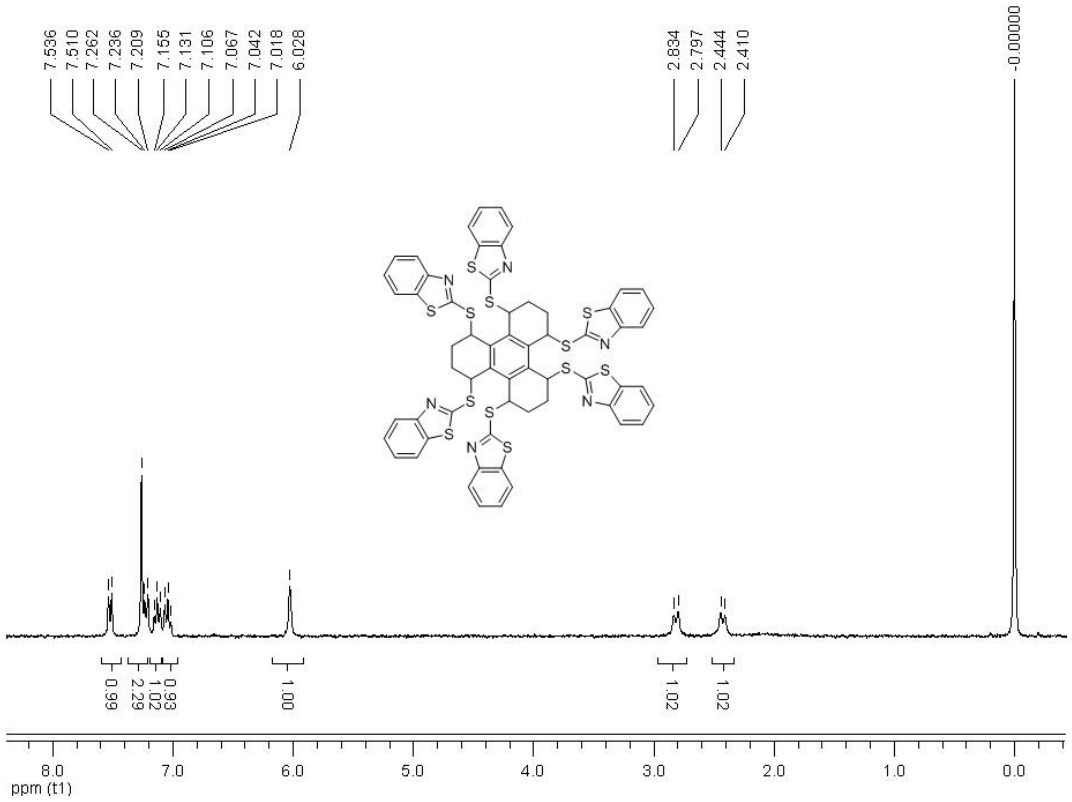

Figure 18. ^{1}H NMR spectrum of 3j.

4. Crystal structure determination of 3a and 3f

Data for both compounds were measured on a Bruker SMART diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71073 Å) using 0.3 ° width steps accumulating area detector frames spanning a hemisphere of reciprocal space for both structures; the reflections were corrected for Lorentz and polarisation effects. Absorption effects were corrected on the basis of multiple equivalent reflections.

The structures were solved by direct methods and refined by full matrix least squares on F2 using the program SHELXTL. All hydrogen atoms were included in calculated positions using a riding model. All non-hydrogen atoms were refined as anisotropic.

Crystal data for compound 3a: $C_{18}H_{18}N_{18}$, M = 486.46, Monoclinic, P2(1)/c, a = 17.280(6) Å, b = 10.589(4) Å, c = 11.979(5) Å, α = 90 °, β = 94.513(8)°, γ = 90 °, V = 2185.1(14) Å^3, T = 296(2) K, Z = 4, μ(Mo-Kα) = 0.71073 Å, colorless square-plate crystal, crystal dimensions 0.31 mm × 0.27 mm × 0.13 mm, crystal density 1.479 Mg m^{-3}. Full matrix least-squares based on F^2 gave R_1 = 0.0508 and wR_2 = 0.0989 for 3894 ($I \geq 2\sigma(I)$), GOF = 1.044 for 325 parameters.

Table 1S Bond Lengths and Bond Angles of 3a

N(1)-N(2)	1.136(4)	C(6)-C(7)	1.529(4)
N(2)-N(3)	1.219(4)	C(7)-C(8)	1.513(4)
N(3)-C(11)	1.508(4)	C(7)-H(7)	0.9800
N(4)-N(5)	1.223(4)	C(8)-C(9)	1.483(5)
N(4)-C(14)	1.501(4)	C(8)-H(8A)	0.9700
N(5)-N(6)	1.133(4)	C(8)-H(8B)	0.9700
N(7)-N(8)	1.122(4)	C(9)-C(10)	1.516(4)
N(8)-N(9)	1.239(4)	C(9)-H(9A)	0.9700
N(9)-C(15)	1.493(4)	C(9)-H(9B)	0.9700
N(10)-N(11)	1.131(4)	C(10)-H(10)	0.9800
N(11)-N(12)	1.219(4)	C(11)-C(12)	1.512(4)
N(12)-C(18)	1.499(4)	C(11)-H(11)	0.9800
N(13)-N(14)	1.141(5)	C(12)-C(13)	1.510(4)
N(14)-N(15)	1.210(4)	C(12)-H(12A)	0.9700
N(15)-C(7)	1.492(4)	C(12)-H(12B)	0.9700
N(16)-N(17)	1.239(5)	C(13)-C(14)	1.515(5)
N(16)-C(10)	1.517(5)	C(13)-H(13A)	0.9700
N(17)-N(18)	1.132(5)	C(13)-H(13B)	0.9700
C(1)-C(6)	1.398(4)	C(14)-H(14)	0.9800
C(1)-C(2)	1.407(4)	C(15)-C(16)	1.519(5)
C(1)-C(10)	1.510(4)	C(15)-H(15)	0.9800
C(2)-C(3)	1.394(4)	C(16)-C(17)	1.510(4)
C(2)-C(11)	1.524(4)	C(16)-H(16A)	0.9700
C(3)-C(4)	1.413(4)	C(16)-H(16B)	0.9700
C(3)-C(14)	1.504(4)	C(17)-C(18)	1.520(4)
C(4)-C(5)	1.387(4)	C(17)-H(17A)	0.9700
C(4)-C(15)	1.520(4)	C(17)-H(17B)	0.9700
C(5)-C(6)	1.410(4)	C(18)-H(18)	0.9800

C(5)-C(18)	1.522(4)	N(1)-N(2)-N(3)	172.6(4)
N(2)-N(3)-C(11)	113.1(3)	C(1)-C(10)-H(10)	107.9
N(5)-N(4)-C(14)	115.3(3)	C(9)-C(10)-H(10)	107.9
N(6)-N(5)-N(4)	174.6(4)	N(16)-C(10)-H(10)	107.9
N(7)-N(8)-N(9)	173.3(5)	N(3)-C(11)-C(12)	111.1(3)
N(8)-N(9)-C(15)	116.2(3)	N(3)-C(11)-C(2)	105.3(3)
N(10)-N(11)-N(12)	173.3(5)	C(12)-C(11)-C(2)	112.3(3)

Crystal data for compound 3f: $C_{54}H_{42}Cl_6S_6$, M = 1095.94, Triclinic, space group: P-1, a = 11.5162(16) Å, b = 14.2283(19) Å, c = 17.692(2) Å, α = 100.364(2)°, β = 108.708(2)°, γ = 102.865(2) °,V = 2575.8(6) Å^3, T = 296(2) K, Z = 2, μ(Mo-Kα) = 0.71073 Å, block colorless crystal, crystal dimensions: 0.12 mm × 0.10 mm × 0.08 mm, crystal density: 1.413 Mg m^{-3}. Full matrix least-squares based on F^2 gave R_1 = 0.0428 and wR_2 = 0.1437 for 9021 ($I \geq 2\sigma(I)$), GOF = 1.001 for 595 parameters.

Table 2S. Bond Lengths and Bond Angles of 3f.

C(1)-C(2)	1.352(6)	C(30)-H(30)	0.9300
C(1)-C(6)	1.362(6)	C(31)-C(32)	1.368(5)
C(1)-Cl(6)	1.755(3)	C(31)-C(36)	1.372(5)
C(2)-C(3)	1.380(5)	C(31)-Cl(1)	1.731(3)
C(2)-H(2)	0.9300	C(32)-C(33)	1.389(4)
C(3)-C(4)	1.366(4)	C(32)-H(32)	0.9300
C(3)-H(3)	0.9300	C(33)-C(34)	1.381(4)
C(4)-C(5)	1.382(4)	C(33)-H(33)	0.9300
C(4)-S(1)	1.770(3)	C(34)-C(35)	1.396(4)
C(5)-C(6)	1.377(5)	C(34)-S(6)	1.774(3)
C(5)-H(5)	0.9300	C(35)-C(36)	1.386(4)
C(6)-H(6)	0.9300	C(35)-H(35)	0.9300
C(7)-C(12)	1.368(4)	C(36)-H(36)	0.9300
C(7)-C(8)	1.367(4)	C(37)-C(38)	1.521(4)
C(7)-Cl(2)	1.741(3)	C(37)-C(42)	1.524(3)
C(8)-C(9)	1.387(4)	C(37)-S(2)	1.848(3)
C(8)-H(8)	0.9300	C(37)-H(37)	0.9800
C(9)-C(10)	1.388(4)	C(38)-C(39)	1.513(4)
C(9)-H(9)	0.9300	C(38)-H(38A)	0.9700
C(10)-C(11)	1.379(4)	C(38)-H(38B)	0.9700
C(10)-S(2)	1.778(3)	C(39)-C(40)	1.514(3)
C(11)-C(12)	1.388(4)	C(39)-H(39A)	0.9700
C(11)-H(11)	0.9300	C(39)-H(39B)	0.9700
C(12)-H(12)	0.9300	C(40)-C(41)	1.523(3)
C(13)-C(18)	1.357(5)	C(40)-S(1)	1.860(3)
C(13)-C(14)	1.365(5)	C(40)-H(40)	0.9800
C(13)-Cl(3)	1.749(3)	C(41)-C(42)	1.394(3)
C(14)-C(15)	1.387(4)	C(41)-C(50)	1.425(3)

C(14)-H(14)	0.9300	C(42)-C(43)	1.411(3)
C(15)-C(16)	1.386(4)	C(43)-C(48)	1.397(3)
C(15)-H(15)	0.9300	C(43)-C(44)	1.531(3)
C(16)-C(17)	1.385(4)	C(44)-C(45)	1.523(4)
C(16)-S(3)	1.779(3)	C(44)-S(3)	1.857(3)
C(17)-C(18)	1.392(5)	C(44)-H(44)	0.9800
C(17)-H(17)	0.9300	C(45)-C(46)	1.514(4)
C(18)-H(18)	0.9300	C(45)-H(45A)	0.9700
C(19)-C(24)	1.378(6)	C(45)-H(45B)	0.9700
C(19)-C(20)	1.360(5)	C(46)-C(47)	1.525(4)
C(19)-Cl(4)	1.744(4)	C(46)-H(46A)	0.9700
C(20)-C(21)	1.388(5)	C(46)-H(46B)	0.9700
C(20)-H(20)	0.9300	C(47)-C(48)	1.528(3)
C(21)-C(22)	1.384(5)	C(47)-S(4)	1.859(3)
C(21)-H(21)	0.9300	C(47)-H(47)	0.9800
C(22)-C(23)	1.383(4)	C(48)-C(49)	1.418(3)
C(22)-S(4)	1.773(3)	C(49)-C(50)	1.402(3)
C(23)-C(24)	1.375(5)	C(49)-C(52)	1.530(3)
C(23)-H(23)	0.9300	C(50)-C(51)	1.510(3)
C(24)-H(24)	0.9300	C(51)-C(53)	1.524(3)
C(25)-C(26)	1.373(4)	C(51)-S(6)	1.880(3)
C(25)-C(30)	1.370(4)	C(51)-H(51)	0.9800
C(25)-Cl(5)	1.746(3)	C(52)-C(54)	1.530(3)
C(26)-C(27)	1.384(4)	C(52)-S(5)	1.852(2)
C(26)-H(26)	0.9300	C(52)-H(52)	0.9800
C(27)-C(28)	1.389(4)	C(53)-C(54)	1.517(4)
C(27)-H(27)	0.9300	C(53)-H(53A)	0.9700
C(28)-C(29)	1.384(4)	C(53)-H(53B)	0.9700
C(28)-S(5)	1.779(2)	C(54)-H(54A)	0.9700
C(29)-C(30)	1.387(4)	C(54)-H(54B)	0.9700
C(29)-H(29)	0.9300	C(2)-C(1)-C(6)	121.1(3)
C(2)-C(1)-Cl(6)	119.0(3)	C(18)-C(13)-C(14)	121.5(3)
C(6)-C(1)-Cl(6)	119.8(3)	C(18)-C(13)-Cl(3)	119.6(3)
C(1)-C(2)-C(3)	119.1(3)	C(14)-C(13)-Cl(3)	118.9(3)
C(1)-C(2)-H(2)	120.5	C(15)-C(14)-C(13)	118.8(3)
C(3)-C(2)-H(2)	120.5	C(15)-C(14)-H(14)	120.6
C(2)-C(3)-C(4)	121.5(3)	C(13)-C(14)-H(14)	120.6
C(2)-C(3)-H(3)	119.2	C(14)-C(15)-C(16)	121.4(3)
C(4)-C(3)-H(3)	119.2	C(14)-C(15)-H(15)	119.3
C(5)-C(4)-C(3)	118.0(3)	C(16)-C(15)-H(15)	119.3
C(5)-C(4)-S(1)	122.8(2)	C(17)-C(16)-C(15)	118.1(3)
C(3)-C(4)-S(1)	119.0(2)	C(17)-C(16)-S(3)	120.2(2)
C(4)-C(5)-C(6)	120.7(3)	C(15)-C(16)-S(3)	121.6(2)
C(4)-C(5)-H(5)	119.7	C(16)-C(17)-C(18)	120.4(3)

C(6)-C(5)-H(5)	119.7	C(16)-C(17)-H(17)	119.8
C(5)-C(6)-C(1)	119.4(4)	C(18)-C(17)-H(17)	119.8
C(5)-C(6)-H(6)	120.3	C(13)-C(18)-C(17)	119.8(3)
C(1)-C(6)-H(6)	120.3	C(13)-C(18)-H(18)	120.1
C(12)-C(7)-C(8)	120.9(3)	C(17)-C(18)-H(18)	120.1
C(12)-C(7)-Cl(2)	120.0(2)	C(24)-C(19)-C(20)	120.3(3)
C(8)-C(7)-Cl(2)	119.0(2)	C(24)-C(19)-Cl(4)	120.2(3)
C(7)-C(8)-C(9)	119.3(3)	C(20)-C(19)-Cl(4)	119.4(4)
C(7)-C(8)-H(8)	120.4	C(19)-C(20)-C(21)	119.6(4)
C(9)-C(8)-H(8)	120.4	C(19)-C(20)-H(20)	120.2
C(8)-C(9)-C(10)	120.7(3)	C(21)-C(20)-H(20)	120.2
C(8)-C(9)-H(9)	119.6	C(22)-C(21)-C(20)	121.2(3)
C(10)-C(9)-H(9)	119.6	C(22)-C(21)-H(21)	119.4
C(11)-C(10)-C(9)	118.8(3)	C(20)-C(21)-H(21)	119.4
C(11)-C(10)-S(2)	119.2(2)	C(21)-C(22)-C(23)	117.9(3)
C(9)-C(10)-S(2)	121.6(2)	C(21)-C(22)-S(4)	123.8(2)
C(10)-C(11)-C(12)	120.3(3)	C(23)-C(22)-S(4)	118.3(3)
C(10)-C(11)-H(11)	119.8	C(22)-C(23)-C(24)	121.1(4)
C(12)-C(11)-H(11)	119.8	C(22)-C(23)-H(23)	119.5
C(7)-C(12)-C(11)	119.8(3)	C(24)-C(23)-H(23)	119.5
C(7)-C(12)-H(12)	120.1	C(19)-C(24)-C(23)	119.9(3)
C(11)-C(12)-H(12)	120.1	C(19)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1	C(39)-C(38)-H(38A)	109.5
C(26)-C(25)-C(30)	120.5(3)	C(37)-C(38)-H(38A)	109.5
C(26)-C(25)-Cl(5)	119.8(2)	C(39)-C(38)-H(38B)	109.5
C(30)-C(25)-Cl(5)	119.7(2)	C(37)-C(38)-H(38B)	109.5
C(25)-C(26)-C(27)	119.9(3)	H(38A)-C(38)-H(38B)	108.0
C(25)-C(26)-H(26)	120.1	C(38)-C(39)-C(40)	110.9(2)
C(27)-C(26)-H(26)	120.0	C(38)-C(39)-H(39A)	109.5
C(26)-C(27)-C(28)	120.5(3)	C(40)-C(39)-H(39A)	109.5
C(26)-C(27)-H(27)	119.8	C(38)-C(39)-H(39B)	109.5
C(28)-C(27)-H(27)	119.8	C(40)-C(39)-H(39B)	109.5
C(29)-C(28)-C(27)	118.7(2)	H(39A)-C(39)-H(39B)	108.0
C(29)-C(28)-S(5)	116.42(19)	C(39)-C(40)-C(41)	114.9(2)
C(27)-C(28)-S(5)	124.9(2)	C(39)-C(40)-S(1)	110.91(18)
C(28)-C(29)-C(30)	120.6(3)	C(41)-C(40)-S(1)	104.35(16)
C(28)-C(29)-H(29)	119.7	C(39)-C(40)-H(40)	108.8
C(30)-C(29)-H(29)	119.7	C(41)-C(40)-H(40)	108.8
C(25)-C(30)-C(29)	119.8(3)	S(1)-C(40)-H(40)	108.8
C(25)-C(30)-H(30)	120.1	C(42)-C(41)-C(50)	119.7(2)
C(29)-C(30)-H(30)	120.1	C(42)-C(41)-C(40)	120.4(2)
C(32)-C(31)-C(36)	121.1(3)	C(50)-C(41)-C(40)	119.7(2)
C(32)-C(31)-Cl(1)	118.9(3)	C(41)-C(42)-C(43)	120.6(2)
C(36)-C(31)-Cl(1)	120.0(3)	C(41)-C(42)-C(37)	120.0(2)

C(31)-C(32)-C(33)	119.5(3)	C(43)-C(42)-C(37)	119.1(2)
C(31)-C(32)-H(32)	120.3	C(48)-C(43)-C(42)	119.9(2)
C(33)-C(32)-H(32)	120.3	C(48)-C(43)-C(44)	120.9(2)
C(34)-C(33)-C(32)	120.6(3)	C(42)-C(43)-C(44)	119.1(2)
C(34)-C(33)-H(33)	119.7	C(45)-C(44)-C(43)	113.7(2)
C(32)-C(33)-H(33)	119.7	C(45)-C(44)-S(3)	112.22(19)
C(33)-C(34)-C(35)	119.2(3)	C(43)-C(44)-S(3)	105.12(17)
C(33)-C(34)-S(6)	118.6(2)	C(45)-C(44)-H(44)	108.6
C(35)-C(34)-S(6)	121.9(2)	C(43)-C(44)-H(44)	108.6
C(36)-C(35)-C(34)	119.9(3)	S(3)-C(44)-H(44)	108.6
C(36)-C(35)-H(35)	120.0	C(46)-C(45)-C(44)	110.3(2)
C(34)-C(35)-H(35)	120.1	C(46)-C(45)-H(45A)	109.6
C(35)-C(36)-C(31)	119.8(3)	C(44)-C(45)-H(45A)	109.6
C(35)-C(36)-H(36)	120.1	C(46)-C(45)-H(45B)	109.6
C(31)-C(36)-H(36)	120.1	C(44)-C(45)-H(45B)	109.6
C(38)-C(37)-C(42)	114.5(2)	H(45A)-C(45)-H(45B)	108.1
C(38)-C(37)-S(2)	112.03(18)	C(45)-C(46)-C(47)	110.5(2)
C(42)-C(37)-S(2)	102.82(16)	C(45)-C(46)-H(46A)	109.5
C(38)-C(37)-H(37)	109.1	C(47)-C(46)-H(46A)	109.6
C(42)-C(37)-H(37)	109.1	C(45)-C(46)-H(46B)	109.6
S(2)-C(37)-H(37)	109.1	C(47)-C(46)-H(46B)	109.6
C(39)-C(38)-C(37)	110.9(2)	H(46A)-C(46)-H(46B)	108.1
C(46)-C(47)-C(48)	113.8(2)	C(49)-C(52)-S(5)	106.44(16)
C(46)-C(47)-S(4)	110.07(18)	C(54)-C(52)-H(52)	108.7
C(48)-C(47)-S(4)	107.92(16)	C(49)-C(52)-H(52)	108.7
C(46)-C(47)-H(47)	108.3	S(5)-C(52)-H(52)	108.7
C(48)-C(47)-H(47)	108.3	C(54)-C(53)-C(51)	109.7(2)
S(4)-C(47)-H(47)	108.3	C(54)-C(53)-H(53A)	109.7
C(43)-C(48)-C(49)	120.0(2)	C(51)-C(53)-H(53A)	109.7
C(43)-C(48)-C(47)	120.7(2)	C(54)-C(53)-H(53B)	109.7
C(49)-C(48)-C(47)	119.2(2)	C(51)-C(53)-H(53B)	109.7
C(50)-C(49)-C(48)	120.1(2)	H(53A)-C(53)-H(53B)	108.2
C(50)-C(49)-C(52)	120.3(2)	C(52)-C(54)-C(53)	110.2(2)
C(48)-C(49)-C(52)	119.6(2)	C(52)-C(54)-H(54A)	109.6
C(49)-C(50)-C(41)	119.6(2)	C(53)-C(54)-H(54A)	109.6
C(49)-C(50)-C(51)	121.6(2)	C(52)-C(54)-H(54B)	109.6
C(41)-C(50)-C(51)	118.8(2)	C(53)-C(54)-H(54B)	109.6
C(53)-C(51)-C(50)	114.4(2)	H(54A)-C(54)-H(54B)	108.1
C(53)-C(51)-S(6)	105.39(18)	C(4)-S(1)-C(40)	102.07(12)
C(50)-C(51)-S(6)	114.48(17)	C(10)-S(2)-C(37)	103.65(12)
C(53)-C(51)-H(51)	107.4	C(16)-S(3)-C(44)	101.38(12)
C(50)-C(51)-H(51)	107.4	C(22)-S(4)-C(47)	101.26(13)
S(6)-C(51)-H(51)	107.4	C(28)-S(5)-C(52)	103.79(11)
C(54)-C(52)-C(49)	113.5(2)	C(34)-S(6)-C(51)	108.67(12)

C(54)-C(52)-S(5)	110.68(17)