10.1071/CH11375_AC

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~~Supplementary Material~~

First synthesis of diindeno[1,2-*g*:1',2'-*s*]rubicene derivatives and their evaluation as semiconductors

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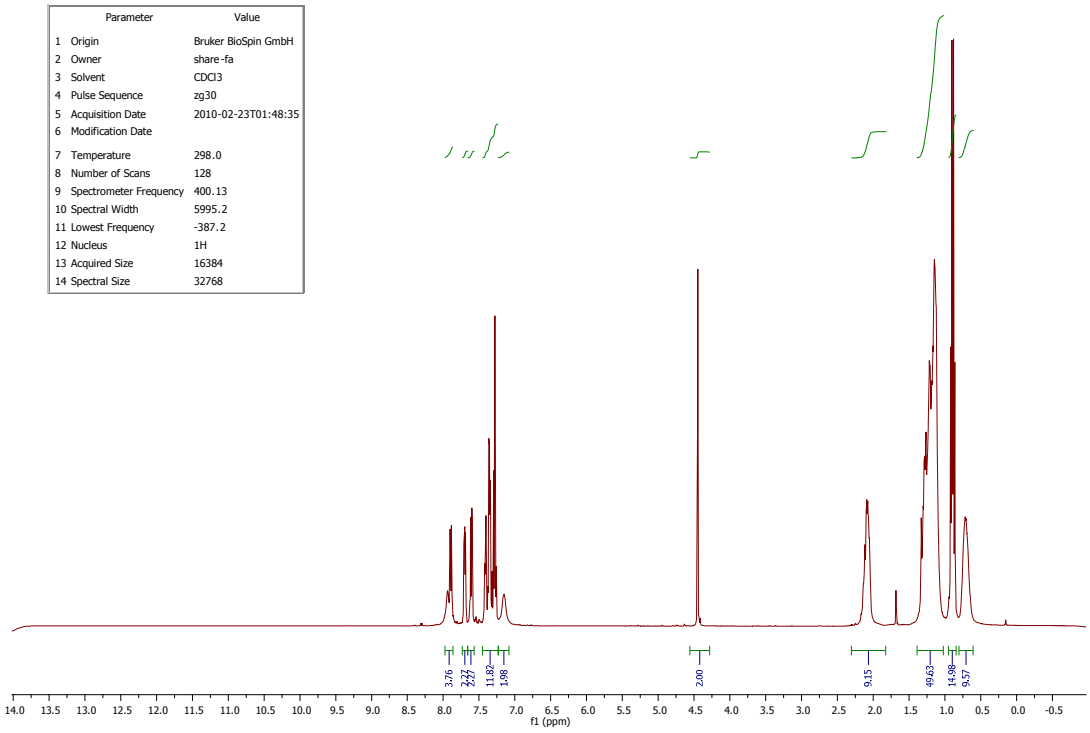
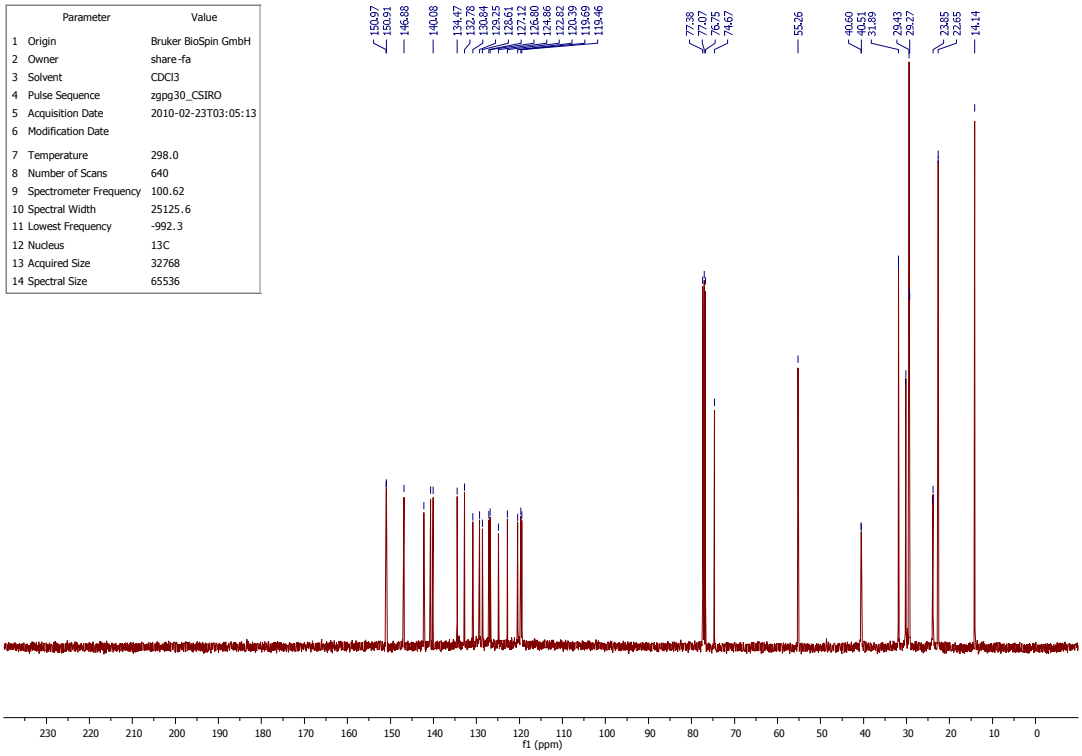
*^{1}H and ^{13}C NMR data for compounds **7a-d**, **8a-d**, **4a**.*

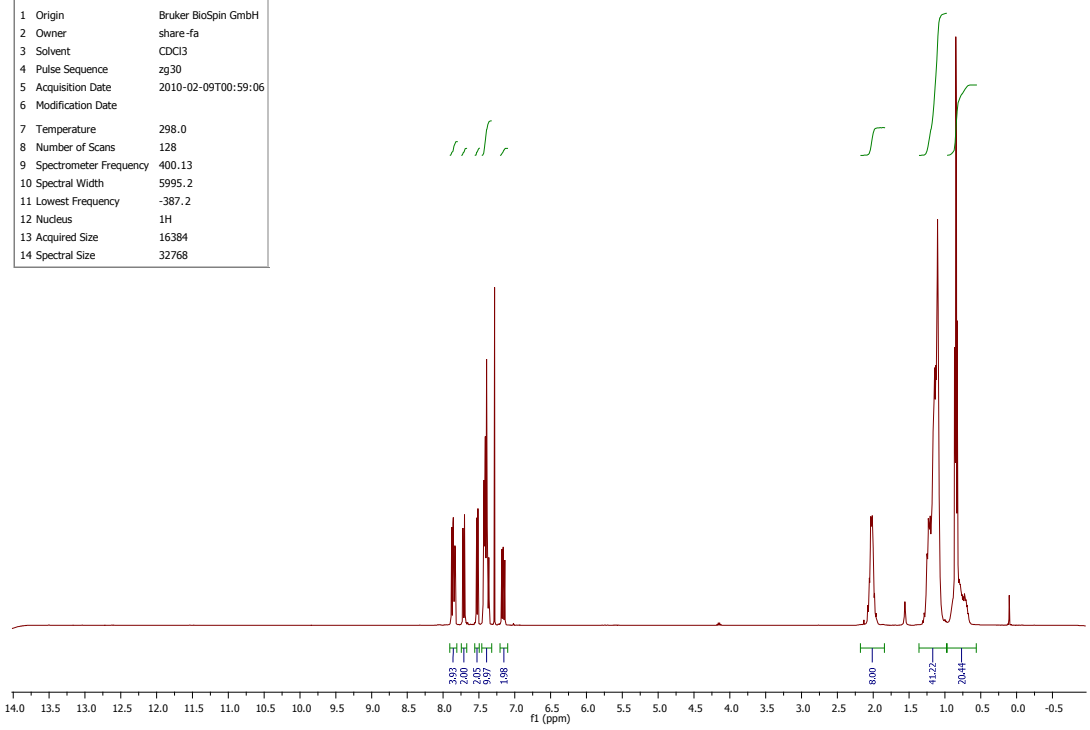
*1,5-dichloro-9,10-bis(9,9-dioctylfluoren-2-yl)-9,10-dihydroanthracene-9,10-diol **7a***





1,5-dichloro-9,10-bis(9,9-dioctylfluoren-2-yl)anthracene ***8a***

	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zg30
5	Acquisition Date	2010-02-09T00:59:06
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	128
9	Spectrometer Frequency	400.13
10	Spectral Width	5995.2
11	Lowest Frequency	-387.2
12	Nucleus	1H
13	Acquired Size	16384
14	Spectral Size	32768



	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zgpg30_CSIRO
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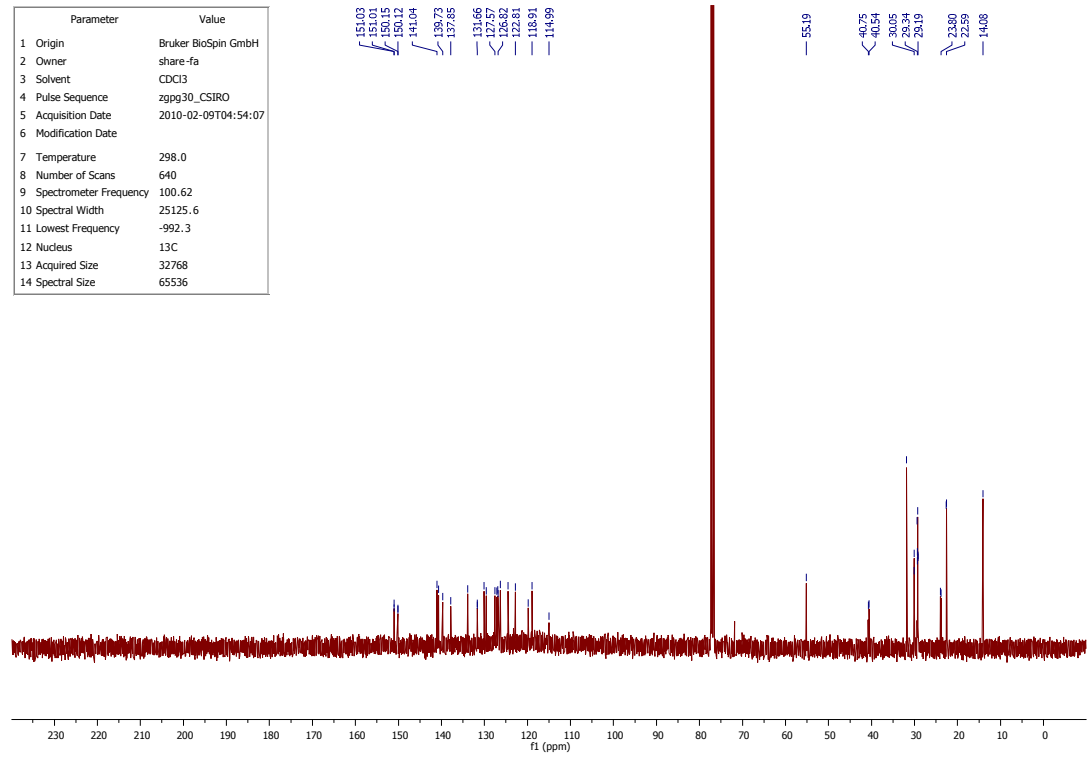
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	640
9	Spectrometer Frequency	100.62
10	Spectral Width	25125.6
11	Lowest Frequency	-992.3
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536



9,9,19,19-tetraoctyl-9,19-dihydrodiindeno[1,2-g:1',2'-s]rubicene **4a**

	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zg30
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9	Spectrometer Frequency	400.13
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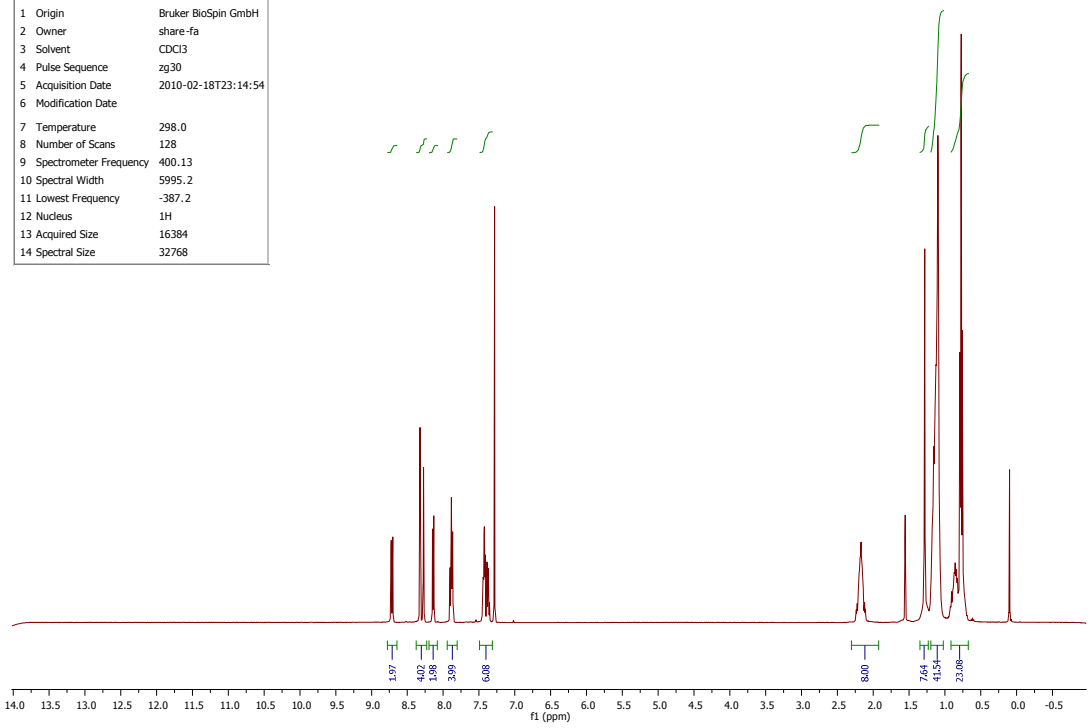
11	Lowest Frequency	-387.2
12	Nucleus	1H
13	Acquired Size	16384
14	Spectral Size	32768



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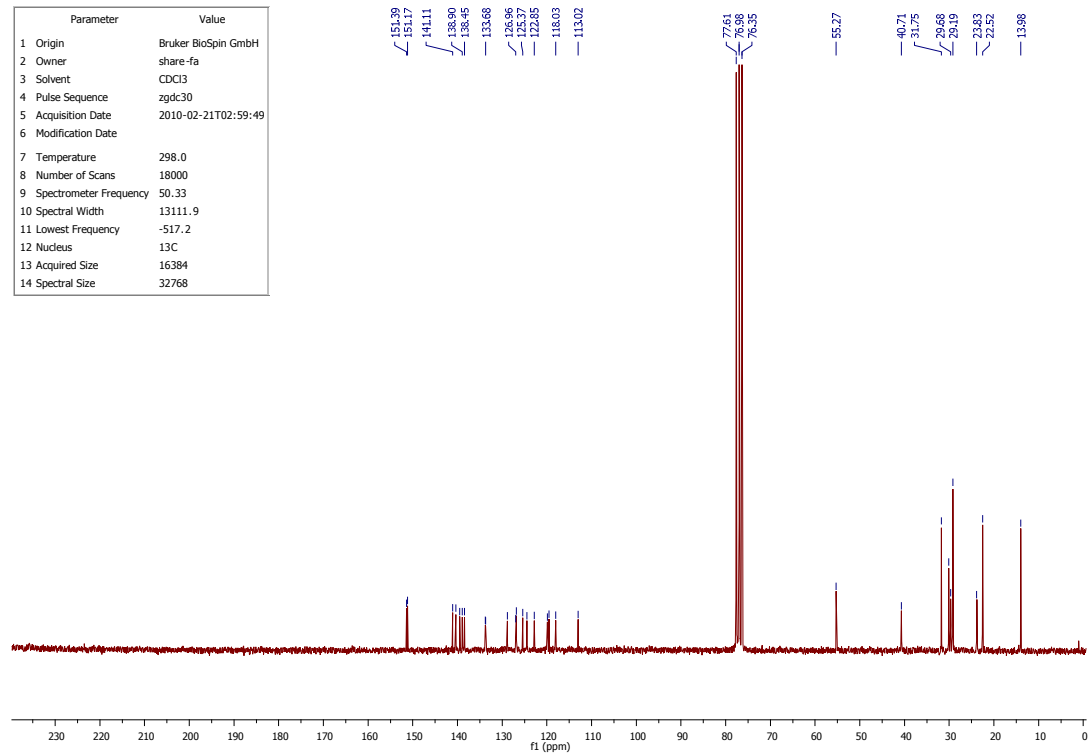
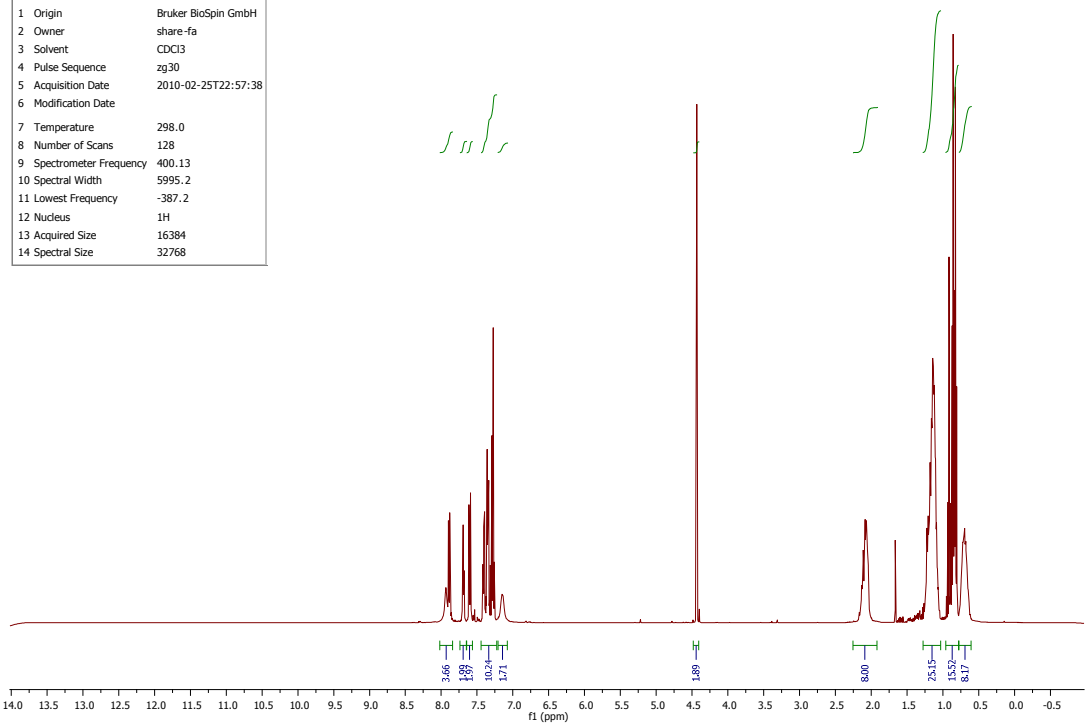
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zgdc30
5	Acquisition Date	2010-02-21T02:59:49
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	18000
9	Spectrometer Frequency	50.33
10	Spectral Width	13111.9
11	Lowest Frequency	-517.2
12	Nucleus	13C
13	Acquired Size	16384
14	Spectral Size	32768



1,5-dichloro-9,10-bis(9,9-dihexylfluoren-2-yl)-9,10-dihydroanthracene-9,10-diol ***7b***

	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zg30
5	Acquisition Date	2010-02-25T22:57:38
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	128
9	Spectrometer Frequency	400.13
10	Spectral Width	5995.2
11	Lowest Frequency	-387.2
12	Nucleus	1H
13	Acquired Size	16384
14	Spectral Size	32768



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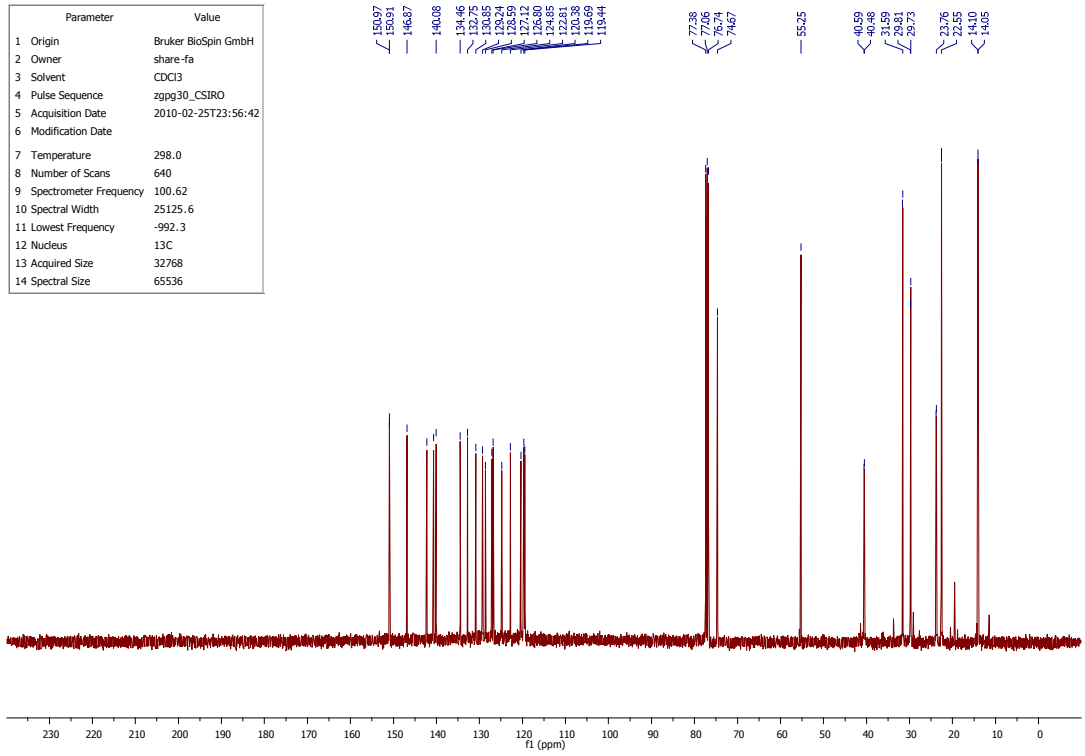
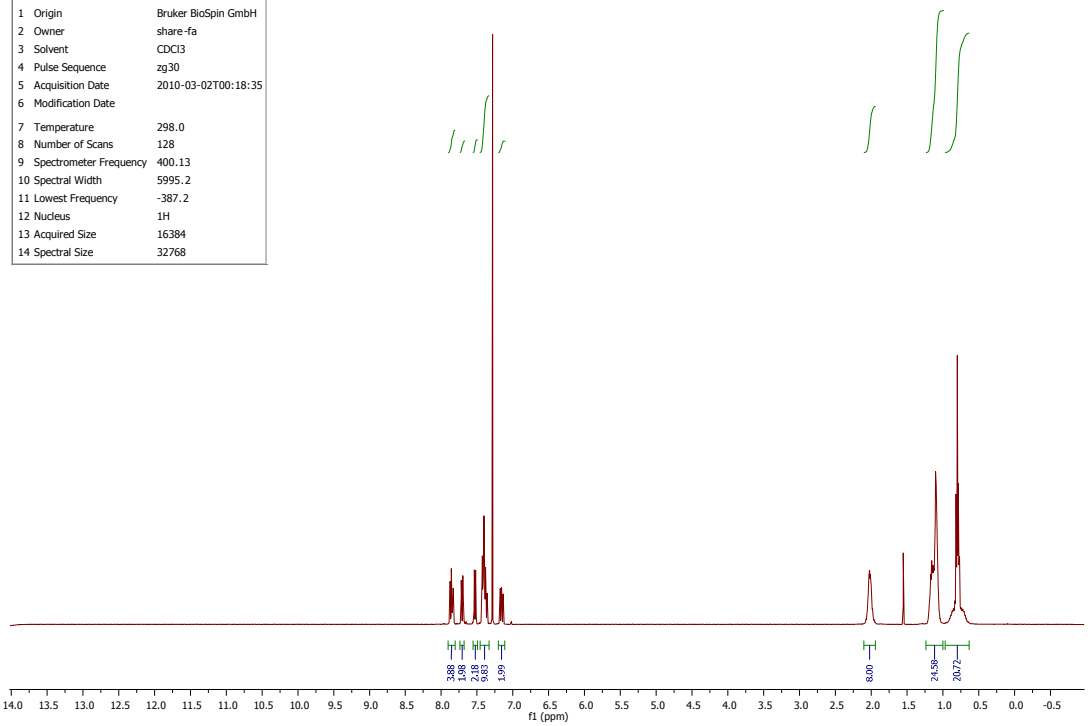
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zgpg30_CSIRO
5	Acquisition Date	2010-02-25T23:56:42
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	640
9	Spectrometer Frequency	100.62
10	Spectral Width	25125.6
11	Lowest Frequency	-992.3
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

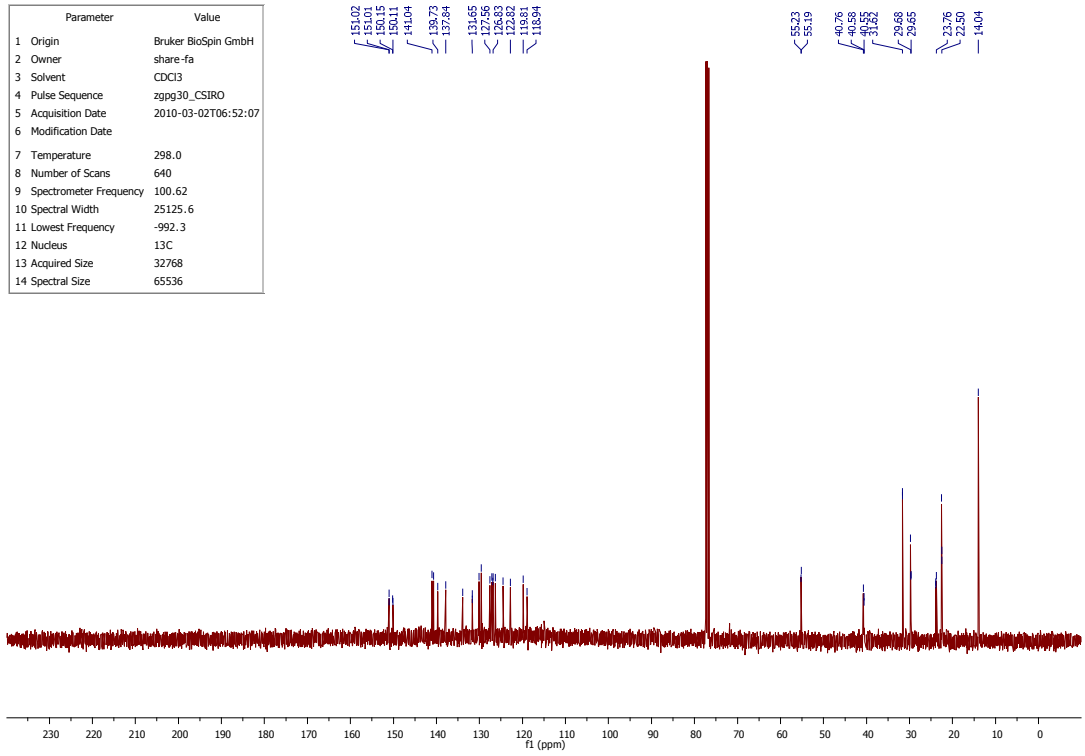


1,5-dichloro-9,10-bis(9,9-dihexylfluoren-2-yl)anthracene **8b**

	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zg30
5	Acquisition Date	2010-03-02T00:18:35
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	128
9	Spectrometer Frequency	400.13
10	Spectral Width	5995.2
11	Lowest Frequency	-387.2
12	Nucleus	1H
13	Acquired Size	16384
14	Spectral Size	32768

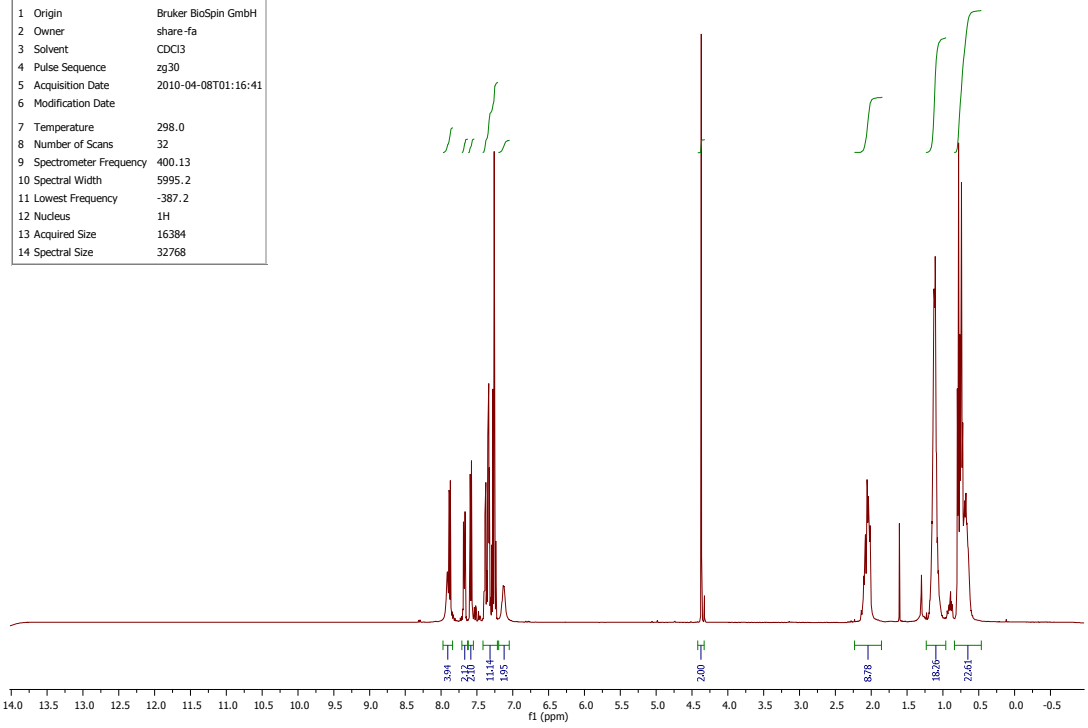


	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zgpg30_CSIRO
5	Acquisition Date	2010-03-02T06:52:07
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	640
9	Spectrometer Frequency	100.62
10	Spectral Width	25125.6
11	Lowest Frequency	-992.3
12	Nucleus	13C
13	Acquired Size	32768
14	Spectral Size	65536

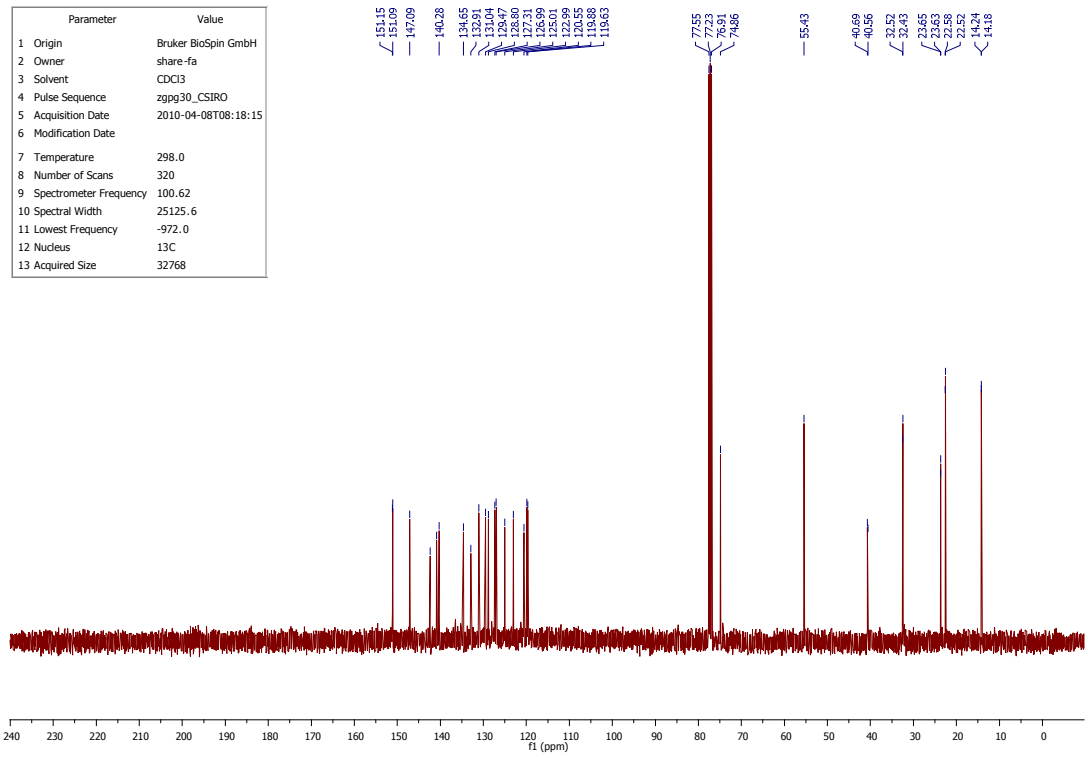


1,5-dichloro-9,10-bis(9,9-dipentylfluoren-2-yl)-9,10-dihydroanthracene-9,10-diol **7c**

	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zg30
5	Acquisition Date	2010-04-08T01:16:41
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	32
9	Spectrometer Frequency	400.13
10	Spectral Width	5995.2
11	Lowest Frequency	-387.2
12	Nucleus	1H
13	Acquired Size	16384
14	Spectral Size	32768

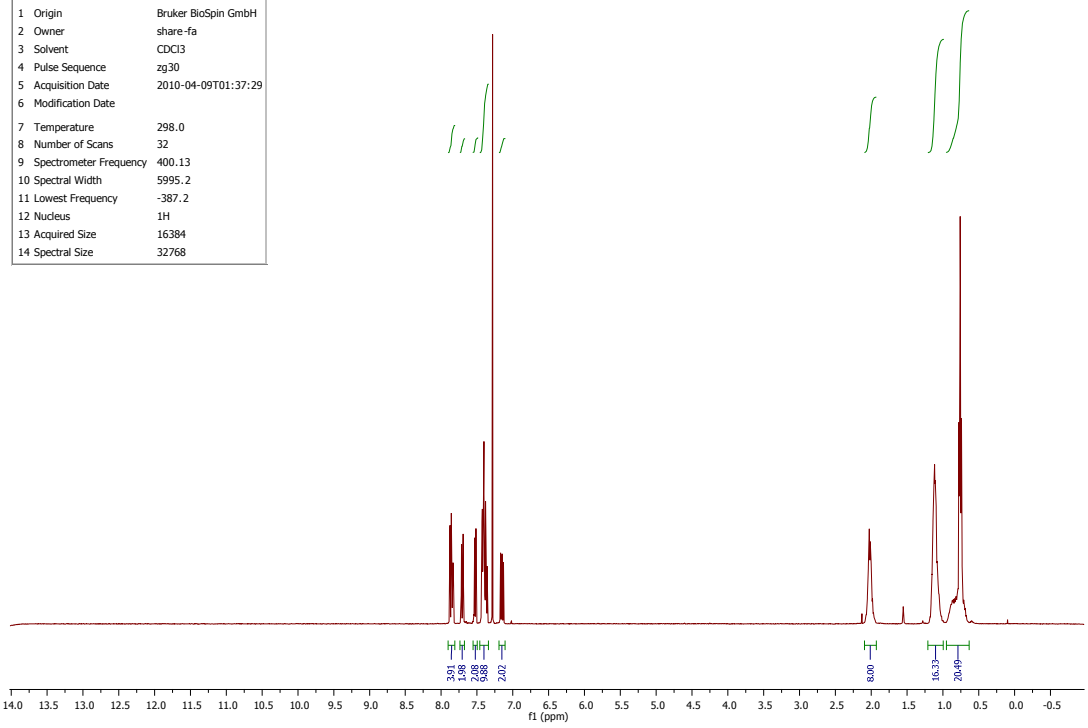


	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zgpg30_CSIRO
5	Acquisition Date	2010-04-08T08:18:15
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	320
9	Spectrometer Frequency	100.62
10	Spectral Width	25125.6
11	Lowest Frequency	-972.0
12	Nucleus	13C
13	Acquired Size	32768

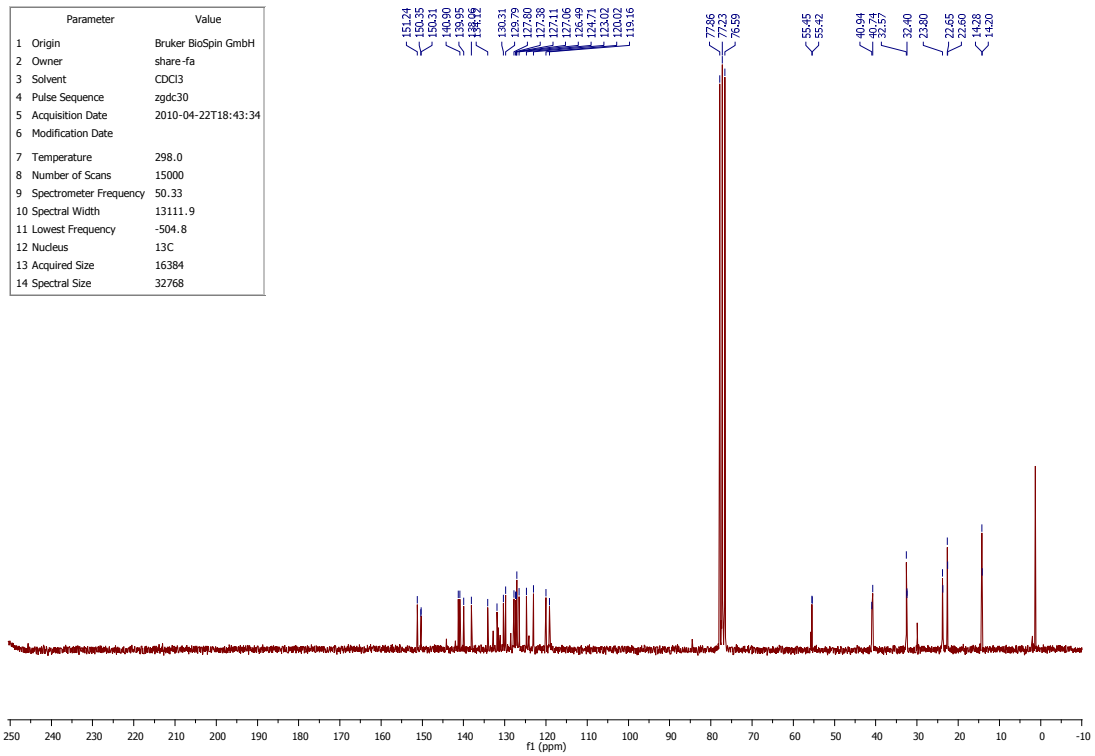


1,5-dichloro-9,10-bis(9,9-dipentylfluoren-2-yl)anthracene **8c**

	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zg30
5	Acquisition Date	2010-04-09T01:37:29
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	32
9	Spectrometer Frequency	400.13
10	Spectral Width	5995.2
11	Lowest Frequency	-387.2
12	Nucleus	1H
13	Acquired Size	16384
14	Spectral Size	32768

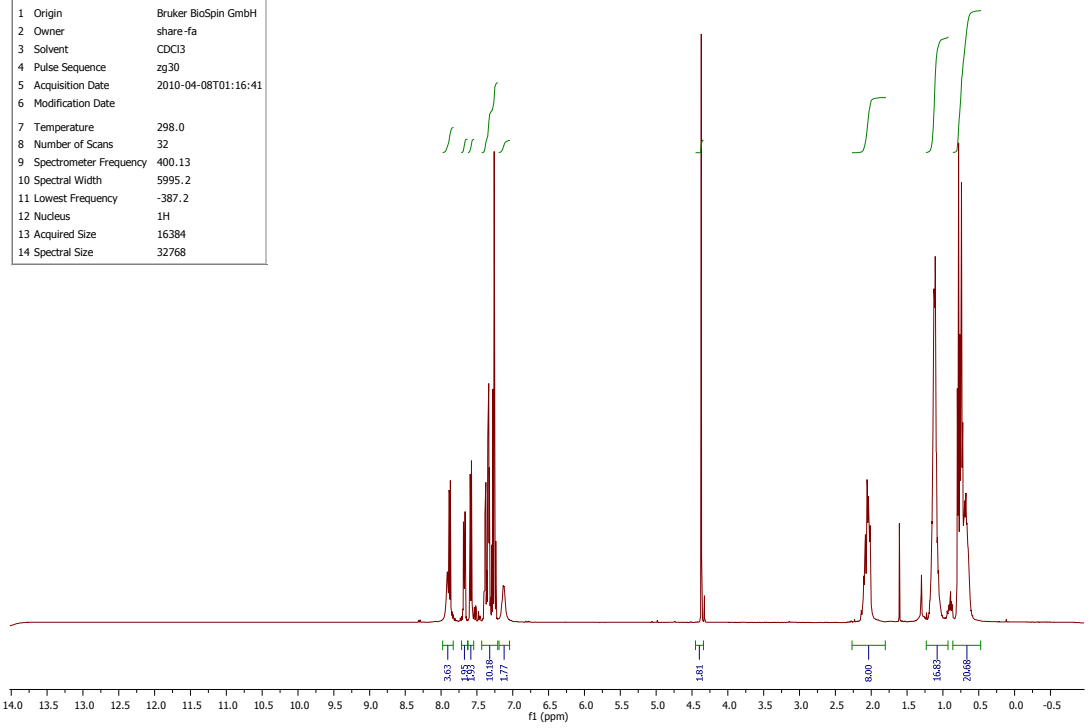


	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zgdc30
5	Acquisition Date	2010-04-22T18:43:34
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	15000
9	Spectrometer Frequency	50.33
10	Spectral Width	13111.9
11	Lowest Frequency	-504.8
12	Nucleus	13C
13	Acquired Size	16384
14	Spectral Size	32768

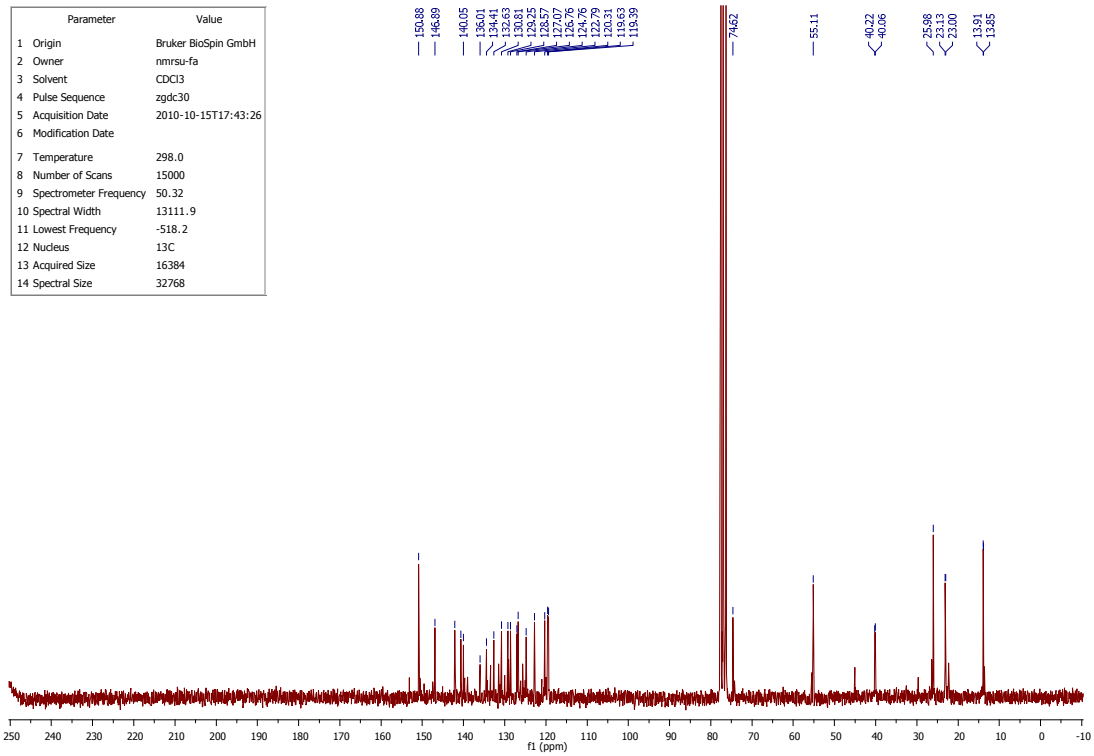


1,5-dichloro-9,10-bis(9,9-dibutylfluoren-2-yl)-9,10-dihydroanthracene-9,10-diol **7d**

	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zg30
5	Acquisition Date	2010-04-08T01:16:41
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	32
9	Spectrometer Frequency	400.13
10	Spectral Width	5995.2
11	Lowest Frequency	-387.2
12	Nucleus	1H
13	Acquired Size	16384
14	Spectral Size	32768

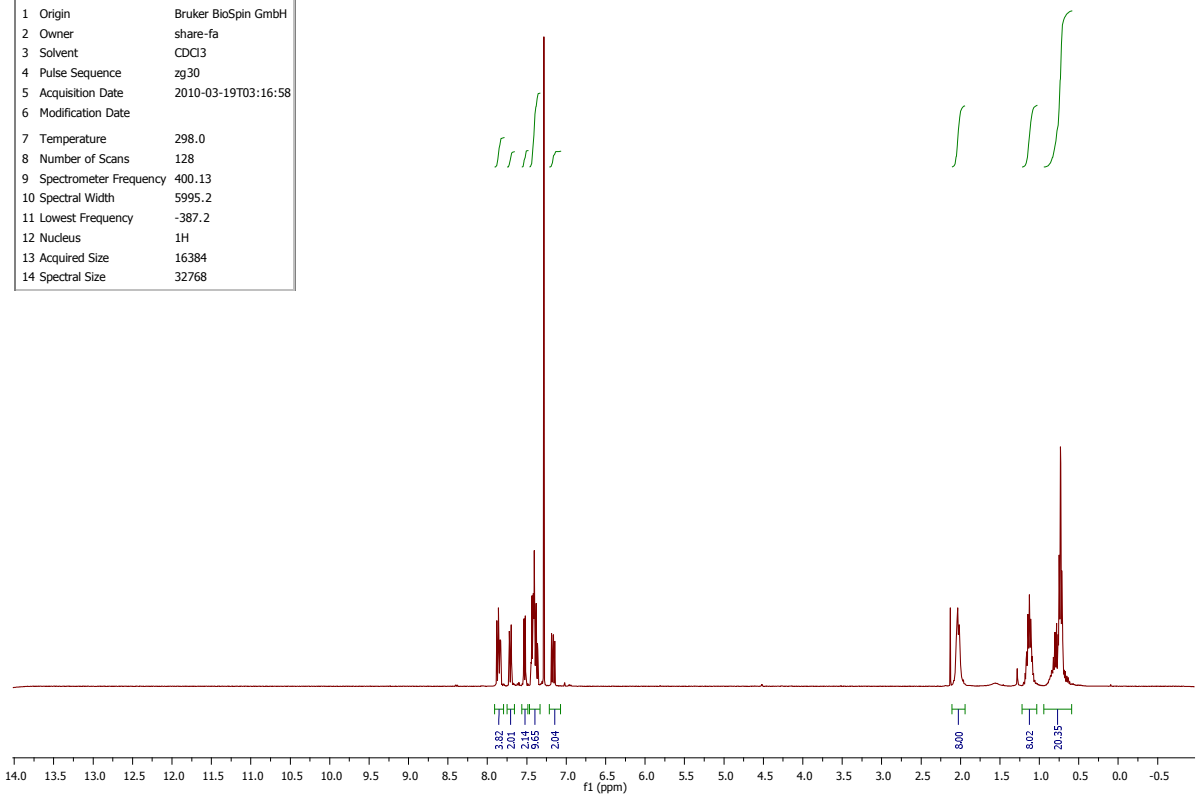


	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	nmrsu-fa
3	Solvent	CDCl3
4	Pulse Sequence	zgdc30
5	Acquisition Date	2010-10-15T17:43:26
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	15000
9	Spectrometer Frequency	50.32
10	Spectral Width	13111.9
11	Lowest Frequency	-518.2
12	Nucleus	13C
13	Acquired Size	16384
14	Spectral Size	32768



1,5-dichloro-9,10-bis(9,9-dibutylfluoren-2-yl)anthracene **8d**

	Parameter	Value
1	Origin	Bruker BioSpin GmbH
2	Owner	share-fa
3	Solvent	CDCl3
4	Pulse Sequence	zg30
5	Acquisition Date	2010-03-19T03:16:58
6	Modification Date	
7	Temperature	298.0
8	Number of Scans	128
9	Spectrometer Frequency	400.13
10	Spectral Width	5995.2
11	Lowest Frequency	-387.2
12	Nucleus	1H
13	Acquired Size	16384
14	Spectral Size	32768



Crystallographic data

4b C64 H70

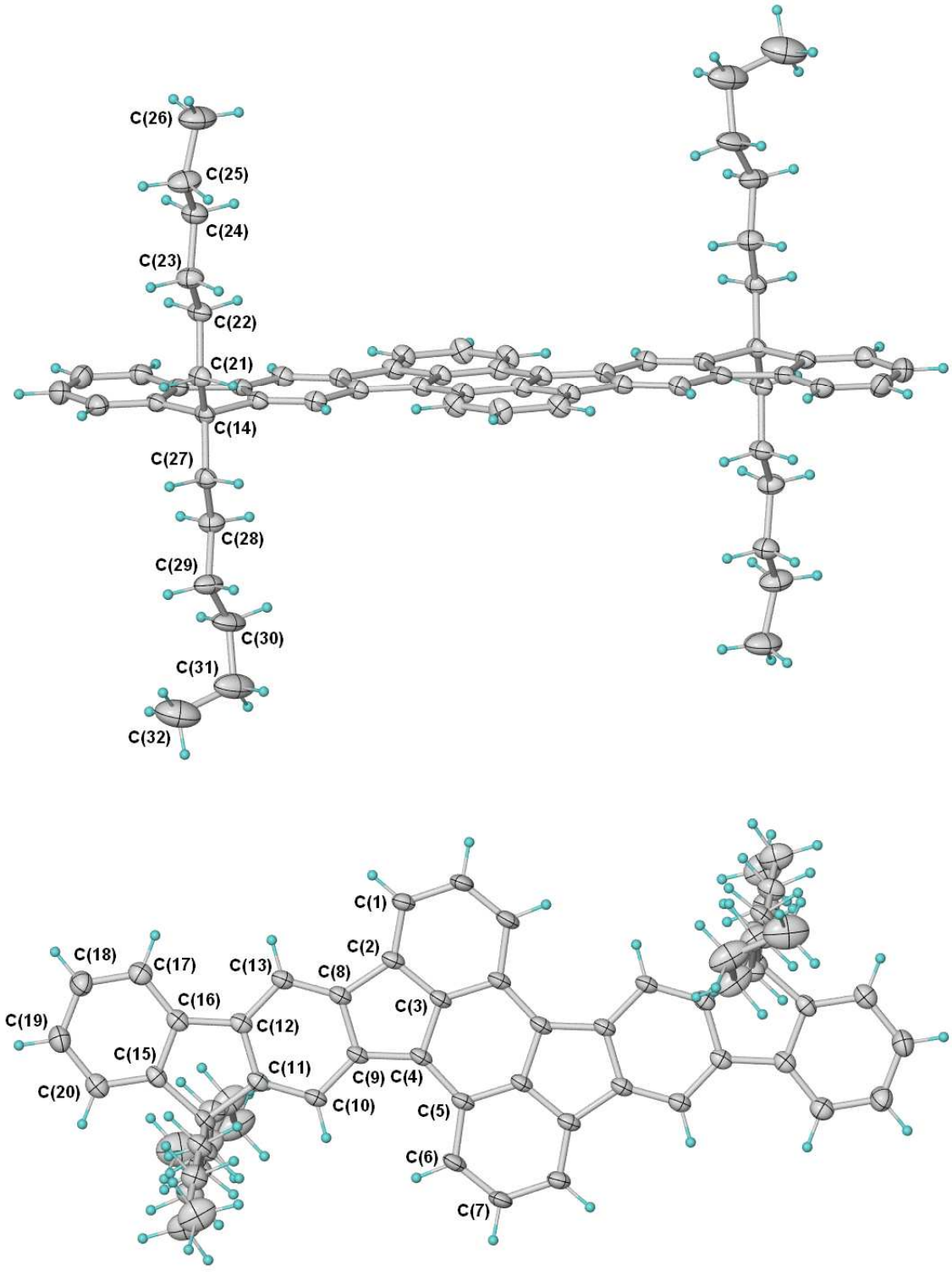


Figure 1. Molecular diagram of molecule 1 as shown with 30% thermal ellipsoids and hydrogen atoms as spheres of arbitrary size (a) side view (b) top view. Only one component

of the disordered hexyl chains is shown. The C-C bond lengths and C-C-C bond angles within the disordered hexyl chains have been restrained to reasonable values.

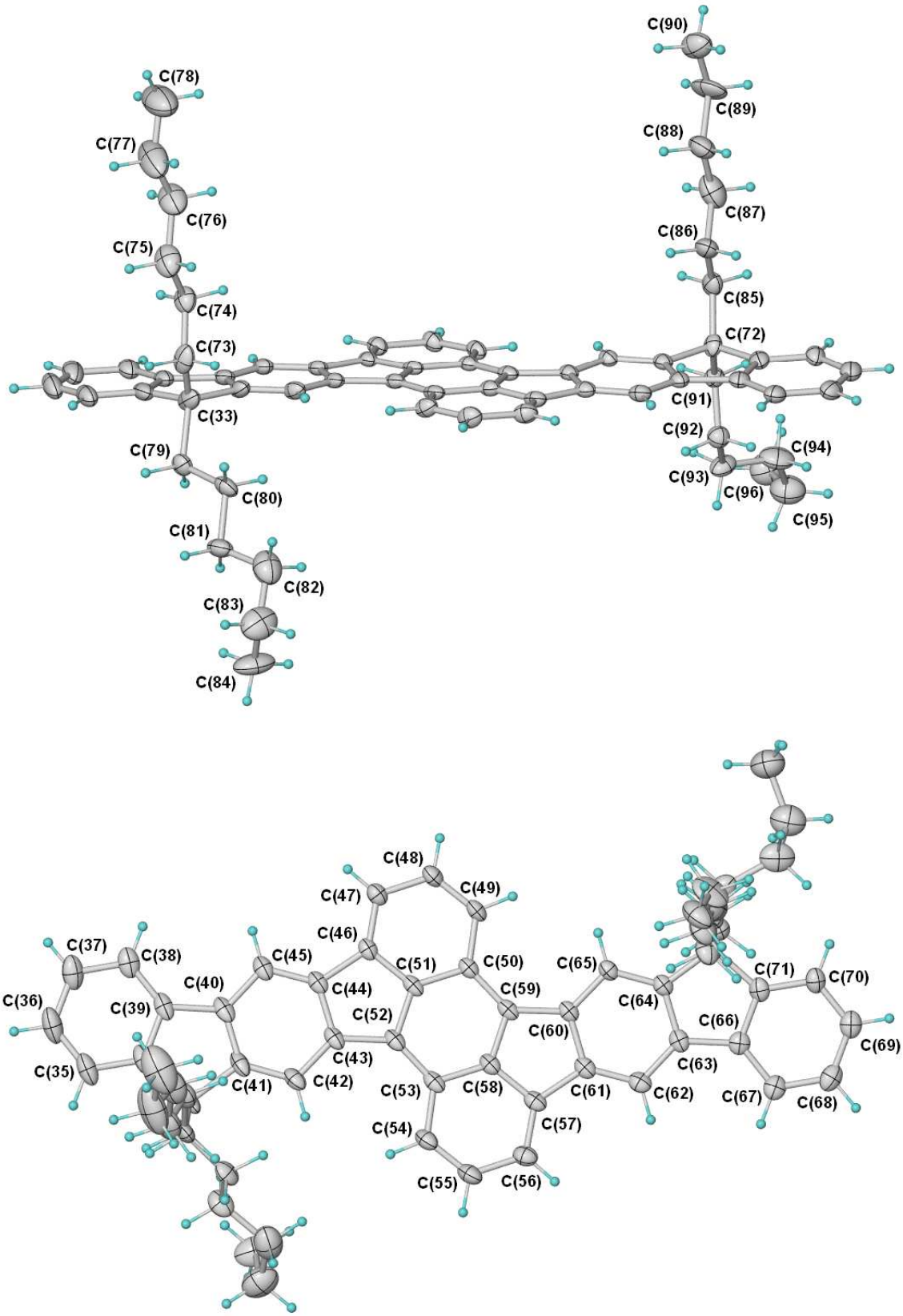


Figure 2. Molecular diagram of molecule 2 as shown with 30% thermal ellipsoids and hydrogen atoms as spheres of arbitrary size (a) side view (b) top view. Only one component of the disordered hexyl chains is shown. The C-C bond lengths and C-C-C bond angles within the disordered hexyl chains have been restrained to reasonable values.

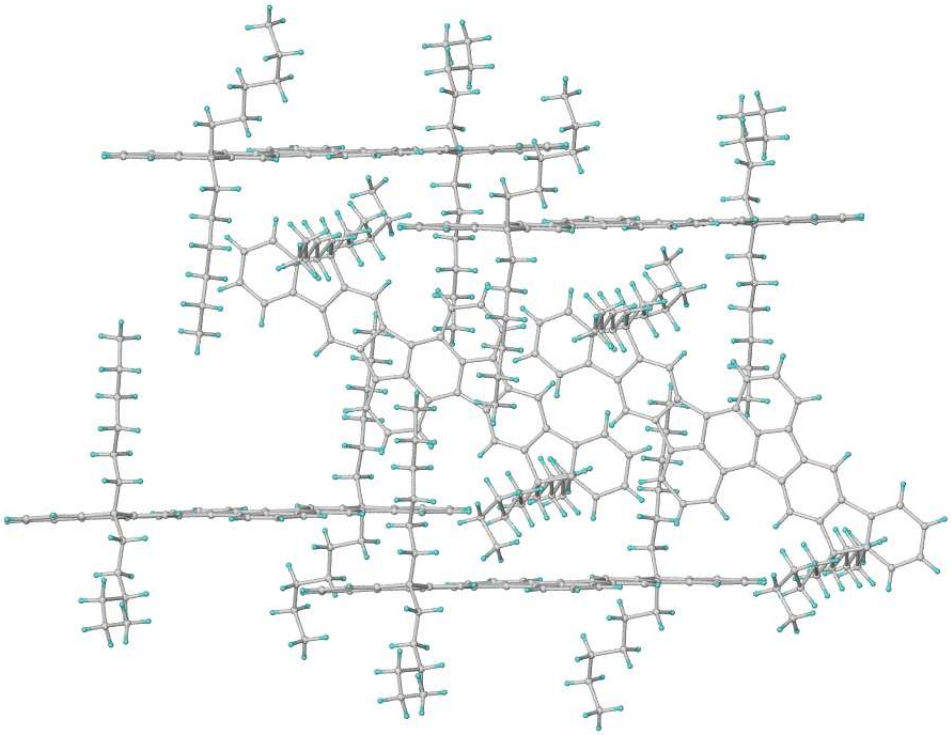


Figure 3 Ball and stick representation showing packing of adjacent molecules. Interplanar separation between parallel polycyclic aromatic ring planes is ca 3.4-3.6Å

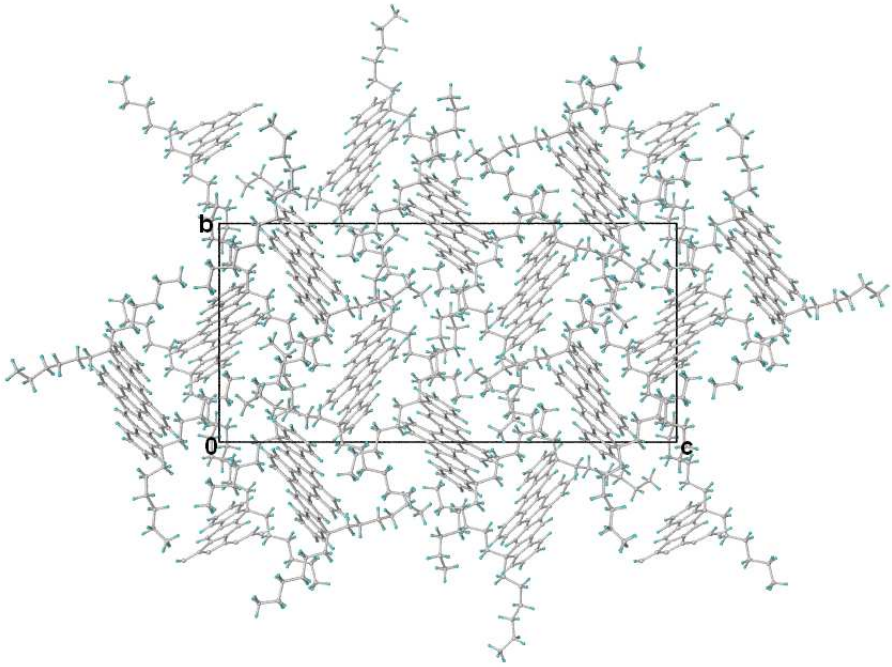


Figure 4. Cell contents as viewed down the ‘a’ axis direction.

Table 1. Crystal data and structure refinement for A3_10a.

Identification code	a3_10a
Empirical formula	C64 H70
Formula weight	839.20
Temperature	173(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 13.070(4) A alpha = 90 deg. b = 16.387(6) A beta = 99.187(10) deg. c = 34.727(13) A gamma = 90 deg.
Volume	7342(4) A^3
Z, Calculated density	6, 1.139 Mg/m^3
Absorption coefficient	0.064 mm^-1
F(000)	2724
Crystal size	0.20 x 0.13 x 0.10 mm
Theta range for data collection	3.31 to 25.00 deg.
Limiting indices	-14<=h<=7, -19<=k<=19, -41<=l<=41
Reflections collected / unique	32784 / 12435 [R(int) = 0.0513]
Completeness to theta = 25.00	96.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0 and 0.48
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12435 / 262 / 1038
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0887, wR2 = 0.2179
R indices (all data)	R1 = 0.1449, wR2 = 0.2607
Largest diff. peak and hole	0.540 and -0.537 e.A^-3

Table 2. Bond lengths [A] and angles [deg] for A3_10a.

C(1)-C(2)	1.360(5)
C(1)-C(7)#1	1.415(6)
C(2)-C(3)	1.413(5)
C(2)-C(8)	1.471(5)
C(3)-C(4)	1.407(5)
C(3)-C(5)#1	1.419(5)
C(4)-C(5)	1.408(5)
C(4)-C(9)	1.464(5)
C(5)-C(6)	1.419(5)
C(5)-C(3)#1	1.419(5)
C(6)-C(7)	1.358(6)
C(7)-C(1)#1	1.415(6)
C(8)-C(13)	1.373(5)
C(8)-C(9)	1.423(5)
C(9)-C(10)	1.395(5)
C(10)-C(11)	1.377(5)
C(11)-C(12)	1.400(5)
C(11)-C(14)	1.521(5)
C(12)-C(13)	1.388(5)
C(12)-C(16)	1.465(6)
C(14)-C(15)	1.502(5)
C(14)-C(21)	1.535(5)
C(14)-C(27)	1.545(5)
C(15)-C(20)	1.383(6)
C(15)-C(16)	1.394(5)
C(16)-C(17)	1.385(6)
C(17)-C(18)	1.383(6)
C(18)-C(19)	1.382(6)
C(19)-C(20)	1.386(6)
C(21)-C(22)	1.514(5)
C(22)-C(23)	1.499(5)
C(23)-C(24)	1.495(6)
C(24)-C(25)	1.495(6)
C(25)-C(26)	1.487(7)
C(27)-C(28)	1.499(5)
C(28)-C(29)	1.506(5)
C(29)-C(30)	1.515(7)
C(30)-C(31)	1.514(7)
C(30')-C(31')	1.518(9)
C(31)-C(32)	1.511(7)
C(31')-C(32')	1.512(9)
C(33)-C(34)	1.505(7)
C(33)-C(41)	1.532(5)
C(33)-C(73)	1.538(7)
C(33)-C(79')	1.560(12)
C(33)-C(79)	1.602(10)
C(34)-C(39)	1.392(6)
C(34)-C(35)	1.393(6)
C(35)-C(36)	1.369(8)
C(36)-C(37)	1.383(8)
C(37)-C(38)	1.387(7)

C(38)-C(39)	1.372(7)
C(39)-C(40)	1.476(6)
C(40)-C(45)	1.389(5)
C(40)-C(41)	1.391(6)
C(41)-C(42)	1.388(6)
C(42)-C(43)	1.394(5)
C(43)-C(44)	1.420(6)
C(43)-C(52)	1.476(6)
C(44)-C(45)	1.379(6)
C(44)-C(46)	1.469(5)
C(46)-C(47)	1.360(5)
C(46)-C(51)	1.415(5)
C(47)-C(48)	1.427(5)
C(48)-C(49)	1.356(6)
C(49)-C(50)	1.416(5)
C(50)-C(59)	1.404(5)
C(50)-C(51)	1.418(5)
C(51)-C(52)	1.407(5)
C(52)-C(53)	1.397(6)
C(53)-C(58)	1.424(5)
C(53)-C(54)	1.427(5)
C(54)-C(55)	1.347(6)
C(55)-C(56)	1.424(6)
C(56)-C(57)	1.362(5)
C(57)-C(58)	1.419(6)
C(57)-C(61)	1.462(5)
C(58)-C(59)	1.402(5)
C(59)-C(60)	1.476(5)
C(60)-C(65)	1.391(5)
C(60)-C(61)	1.431(5)
C(61)-C(62)	1.383(6)
C(62)-C(63)	1.391(5)
C(63)-C(64)	1.406(5)
C(63)-C(66)	1.467(6)
C(64)-C(65)	1.379(5)
C(64)-C(72)	1.515(5)
C(66)-C(67)	1.382(6)
C(66)-C(71)	1.390(6)
C(67)-C(68)	1.389(6)
C(68)-C(69)	1.385(6)
C(69)-C(70)	1.373(6)
C(70)-C(71)	1.388(6)
C(71)-C(72)	1.504(6)
C(72)-C(85)	1.520(6)
C(72)-C(91')	1.5492(12)
C(72)-C(91)	1.561(8)
C(73)-C(74)	1.508(7)
C(74)-C(75)	1.492(7)
C(75)-C(76)	1.564(9)
C(76)-C(77)	1.441(8)
C(77)-C(78)	1.517(12)
C(79)-C(80)	1.504(8)
C(79')-C(80')	1.504(9)
C(80)-C(81)	1.519(8)
C(80')-C(81')	1.505(8)

C(81')-C(82')	1.471(9)
C(81)-C(82)	1.503(9)
C(82)-C(83)	1.469(9)
C(83)-C(84)	1.524(9)
C(83')-C(84')	1.525(10)
C(83')-C(82')	1.536(9)
C(85)-C(86)	1.478(7)
C(86)-C(87)	1.529(12)
C(87)-C(88)	1.466(8)
C(88)-C(89)	1.494(8)
C(89)-C(90)	1.469(9)
C(91)-C(92)	1.448(8)
C(91')-C(92')	1.492(9)
C(92)-C(93)	1.519(7)
C(92')-C(93')	1.500(9)
C(93)-C(94)	1.511(8)
C(93')-C(94')	1.491(9)
C(94)-C(95)	1.490(8)
C(94')-C(95')	1.521(8)
C(95)-C(96)	1.460(9)
C(95')-C(96')	1.513(10)
C(89')-C(90')	1.468(10)
C(89')-C(88')	1.518(9)
C(88')-C(87')	1.485(10)

C(2)-C(1)-C(7)#1	118.5(4)
C(1)-C(2)-C(3)	119.3(4)
C(1)-C(2)-C(8)	133.8(4)
C(3)-C(2)-C(8)	106.9(3)
C(4)-C(3)-C(2)	110.8(3)
C(4)-C(3)-C(5)#1	126.0(4)
C(2)-C(3)-C(5)#1	123.2(3)
C(3)-C(4)-C(5)	118.2(3)
C(3)-C(4)-C(9)	106.7(3)
C(5)-C(4)-C(9)	135.1(3)
C(4)-C(5)-C(6)	129.0(4)
C(4)-C(5)-C(3)#1	115.9(3)
C(6)-C(5)-C(3)#1	115.1(4)
C(7)-C(6)-C(5)	121.1(4)
C(6)-C(7)-C(1)#1	122.7(3)
C(13)-C(8)-C(9)	121.9(3)
C(13)-C(8)-C(2)	130.9(3)
C(9)-C(8)-C(2)	107.2(3)
C(10)-C(9)-C(8)	119.1(4)
C(10)-C(9)-C(4)	132.5(3)
C(8)-C(9)-C(4)	108.4(3)
C(11)-C(10)-C(9)	118.6(3)
C(10)-C(11)-C(12)	121.8(3)
C(10)-C(11)-C(14)	128.2(3)
C(12)-C(11)-C(14)	110.0(3)
C(13)-C(12)-C(11)	120.3(4)
C(13)-C(12)-C(16)	131.0(4)
C(11)-C(12)-C(16)	108.7(3)
C(8)-C(13)-C(12)	118.3(4)
C(15)-C(14)-C(11)	101.8(3)

C(15)-C(14)-C(21)	112.1(3)
C(11)-C(14)-C(21)	113.1(3)
C(15)-C(14)-C(27)	111.6(3)
C(11)-C(14)-C(27)	110.4(3)
C(21)-C(14)-C(27)	107.8(3)
C(20)-C(15)-C(16)	119.4(4)
C(20)-C(15)-C(14)	129.3(4)
C(16)-C(15)-C(14)	111.3(3)
C(17)-C(16)-C(15)	121.0(4)
C(17)-C(16)-C(12)	131.0(4)
C(15)-C(16)-C(12)	108.0(4)
C(18)-C(17)-C(16)	118.9(4)
C(19)-C(18)-C(17)	120.7(5)
C(18)-C(19)-C(20)	120.3(4)
C(15)-C(20)-C(19)	119.8(4)
C(22)-C(21)-C(14)	115.6(3)
C(23)-C(22)-C(21)	112.4(3)
C(24)-C(23)-C(22)	116.0(4)
C(25)-C(24)-C(23)	114.1(4)
C(26)-C(25)-C(24)	116.0(5)
C(28)-C(27)-C(14)	115.8(3)
C(27)-C(28)-C(29)	113.0(3)
C(28)-C(29)-C(30)	105.5(5)
C(31)-C(30)-C(29)	115.0(6)
C(32)-C(31)-C(30)	113.4(7)
C(32')-C(31')-C(30')	114.1(8)
C(34)-C(33)-C(41)	101.6(4)
C(34)-C(33)-C(73)	111.2(4)
C(41)-C(33)-C(73)	112.1(4)
C(34)-C(33)-C(79')	126.7(7)
C(41)-C(33)-C(79')	113.1(5)
C(73)-C(33)-C(79')	92.2(5)
C(34)-C(33)-C(79)	97.7(5)
C(41)-C(33)-C(79)	108.7(5)
C(73)-C(33)-C(79)	122.8(5)
C(79')-C(33)-C(79)	34.2(4)
C(39)-C(34)-C(35)	119.8(5)
C(39)-C(34)-C(33)	111.9(4)
C(35)-C(34)-C(33)	128.3(5)
C(36)-C(35)-C(34)	119.0(5)
C(35)-C(36)-C(37)	120.9(5)
C(36)-C(37)-C(38)	120.6(6)
C(39)-C(38)-C(37)	118.6(5)
C(38)-C(39)-C(34)	121.1(4)
C(38)-C(39)-C(40)	131.7(4)
C(34)-C(39)-C(40)	107.2(5)
C(45)-C(40)-C(41)	120.7(4)
C(45)-C(40)-C(39)	129.8(5)
C(41)-C(40)-C(39)	109.5(4)
C(42)-C(41)-C(40)	122.1(4)
C(42)-C(41)-C(33)	128.2(5)
C(40)-C(41)-C(33)	109.7(4)
C(41)-C(42)-C(43)	117.7(4)
C(42)-C(43)-C(44)	119.8(4)
C(42)-C(43)-C(52)	131.6(4)

C(44)-C(43)-C(52)	108.6(3)
C(45)-C(44)-C(43)	121.7(4)
C(45)-C(44)-C(46)	131.4(4)
C(43)-C(44)-C(46)	106.9(4)
C(44)-C(45)-C(40)	118.0(4)
C(47)-C(46)-C(51)	119.5(3)
C(47)-C(46)-C(44)	133.0(4)
C(51)-C(46)-C(44)	107.5(3)
C(46)-C(47)-C(48)	117.7(4)
C(49)-C(48)-C(47)	123.3(4)
C(48)-C(49)-C(50)	120.8(4)
C(59)-C(50)-C(49)	129.0(4)
C(59)-C(50)-C(51)	115.6(3)
C(49)-C(50)-C(51)	115.4(4)
C(52)-C(51)-C(46)	110.6(3)
C(52)-C(51)-C(50)	126.1(4)
C(46)-C(51)-C(50)	123.4(3)
C(53)-C(52)-C(51)	118.3(4)
C(53)-C(52)-C(43)	135.4(4)
C(51)-C(52)-C(43)	106.3(4)
C(52)-C(53)-C(58)	115.8(3)
C(52)-C(53)-C(54)	129.0(4)
C(58)-C(53)-C(54)	115.2(4)
C(55)-C(54)-C(53)	120.8(4)
C(54)-C(55)-C(56)	123.3(4)
C(57)-C(56)-C(55)	118.4(4)
C(56)-C(57)-C(58)	119.0(4)
C(56)-C(57)-C(61)	133.9(4)
C(58)-C(57)-C(61)	107.1(3)
C(59)-C(58)-C(57)	110.9(3)
C(59)-C(58)-C(53)	125.9(4)
C(57)-C(58)-C(53)	123.3(4)
C(58)-C(59)-C(50)	118.4(4)
C(58)-C(59)-C(60)	106.7(4)
C(50)-C(59)-C(60)	135.0(3)
C(65)-C(60)-C(61)	119.6(4)
C(65)-C(60)-C(59)	132.5(4)
C(61)-C(60)-C(59)	107.8(3)
C(62)-C(61)-C(60)	121.0(4)
C(62)-C(61)-C(57)	131.5(4)
C(60)-C(61)-C(57)	107.5(4)
C(61)-C(62)-C(63)	118.6(4)
C(62)-C(63)-C(64)	120.4(4)
C(62)-C(63)-C(66)	131.0(4)
C(64)-C(63)-C(66)	108.6(4)
C(65)-C(64)-C(63)	121.5(4)
C(65)-C(64)-C(72)	128.7(4)
C(63)-C(64)-C(72)	109.7(4)
C(64)-C(65)-C(60)	118.9(4)
C(67)-C(66)-C(71)	120.8(4)
C(67)-C(66)-C(63)	131.0(4)
C(71)-C(66)-C(63)	108.2(4)
C(66)-C(67)-C(68)	118.8(4)
C(69)-C(68)-C(67)	120.2(4)
C(70)-C(69)-C(68)	121.0(5)

C(69)-C(70)-C(71)	119.2(4)
C(70)-C(71)-C(66)	120.0(4)
C(70)-C(71)-C(72)	128.9(4)
C(66)-C(71)-C(72)	111.1(4)
C(71)-C(72)-C(64)	102.2(3)
C(71)-C(72)-C(85)	111.2(4)
C(64)-C(72)-C(85)	111.0(3)
C(71)-C(72)-C(91')	118.1(6)
C(64)-C(72)-C(91')	122.0(7)
C(85)-C(72)-C(91')	92.1(5)
C(71)-C(72)-C(91)	111.9(4)
C(64)-C(72)-C(91)	109.7(4)
C(85)-C(72)-C(91)	110.6(4)
C(91')-C(72)-C(91)	18.8(5)
C(74)-C(73)-C(33)	114.5(4)
C(75)-C(74)-C(73)	113.8(5)
C(74)-C(75)-C(76)	112.3(5)
C(77)-C(76)-C(75)	115.6(7)
C(76)-C(77)-C(78)	112.0(8)
C(80)-C(79)-C(33)	110.3(7)
C(80')-C(79')-C(33)	108.0(9)
C(79)-C(80)-C(81)	112.0(7)
C(79')-C(80')-C(81')	116.6(9)
C(82')-C(81')-C(80')	123.4(9)
C(82)-C(81)-C(80)	109.1(7)
C(83)-C(82)-C(81)	113.0(8)
C(82)-C(83)-C(84)	109.5(8)
C(84')-C(83')-C(82')	115.3(9)
C(86)-C(85)-C(72)	115.4(4)
C(85)-C(86)-C(87)	101.8(6)
C(88)-C(87)-C(86)	112.3(9)
C(87)-C(88)-C(89)	117.8(8)
C(90)-C(89)-C(88)	117.3(8)
C(92)-C(91)-C(72)	121.2(6)
C(92')-C(91')-C(72)	109.3(6)
C(91)-C(92)-C(93)	117.3(6)
C(91')-C(92')-C(93')	111.6(7)
C(94)-C(93)-C(92)	115.7(6)
C(94')-C(93')-C(92')	118.5(8)
C(95)-C(94)-C(93)	119.5(8)
C(93')-C(94')-C(95')	111.2(8)
C(96)-C(95)-C(94)	119.4(9)
C(96')-C(95')-C(94')	114.5(8)
C(81')-C(82')-C(83')	117.2(8)
C(90')-C(89')-C(88')	116.5(9)
C(87')-C(88')-C(89')	115.8(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z

C60H62 **4c**

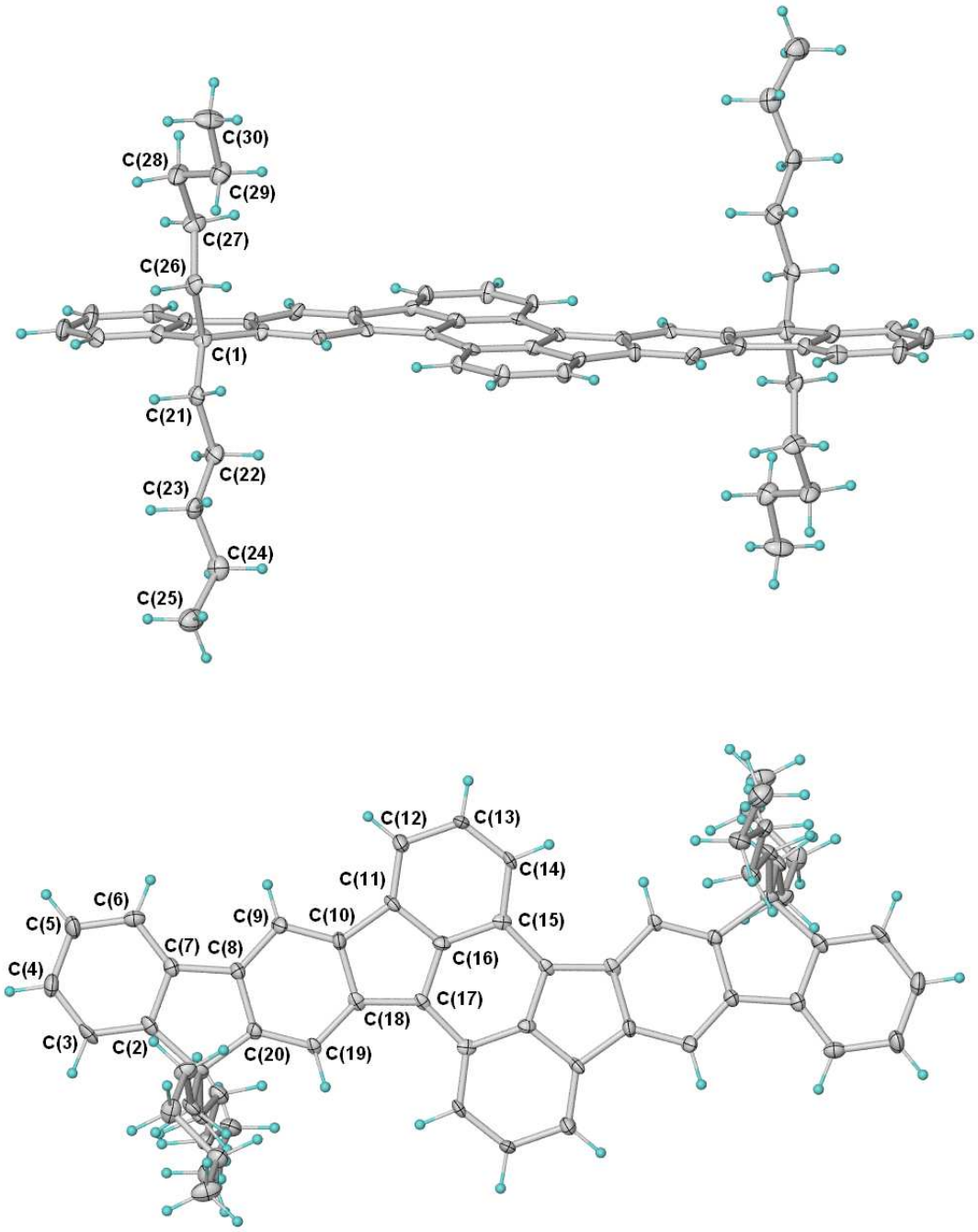


Figure 1. Molecular diagram of molecule 1 as shown with 50% thermal ellipsoids and hydrogen atoms as spheres of arbitrary size (a) side view (b) top view. Unlabeled atoms are generated by symmetry –x, -y, -z.

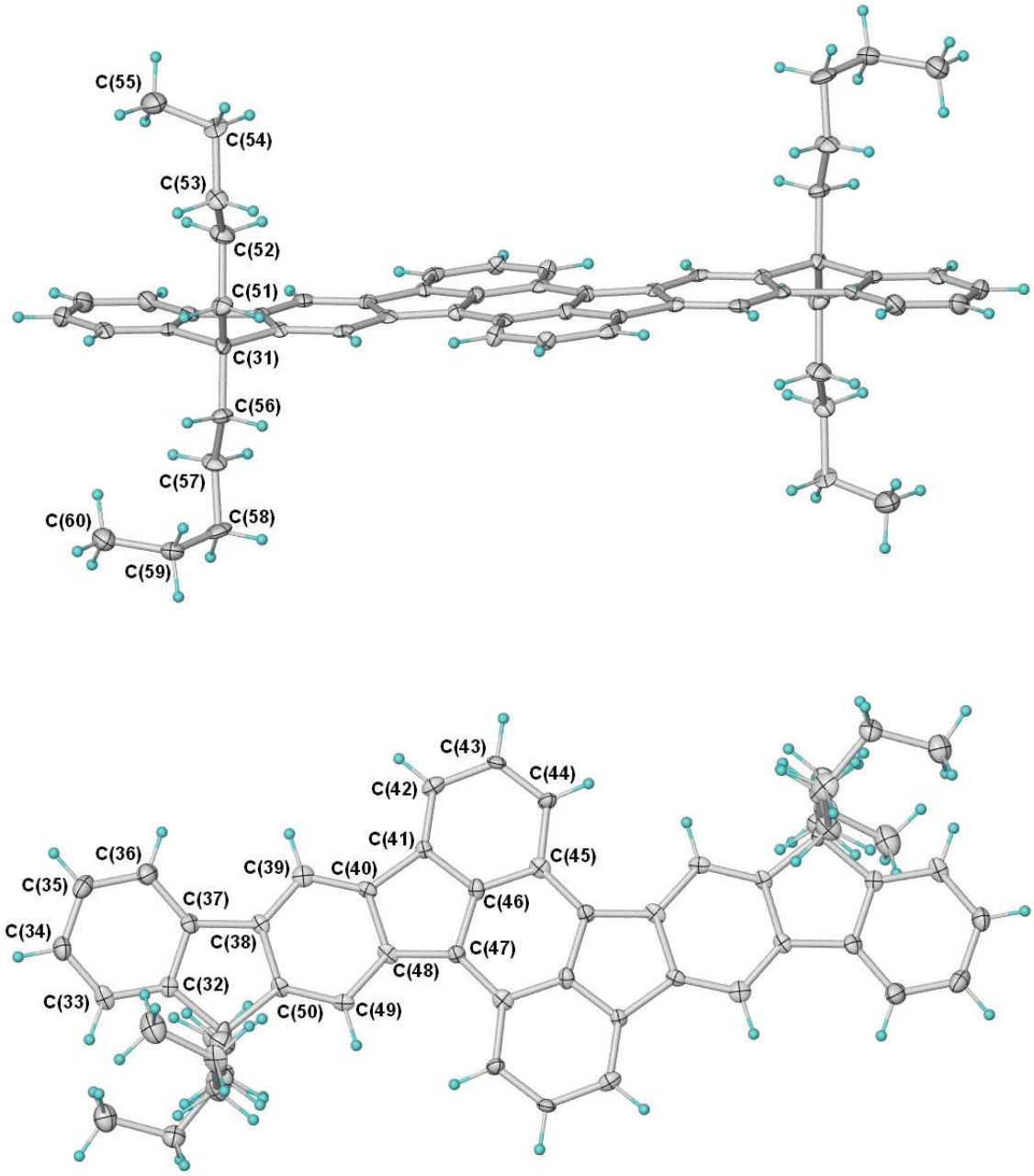


Figure 2. Molecular diagram of molecule 2 as shown with 50% thermal ellipsoids and hydrogen atoms as spheres of arbitrary size (a) side view (b) top view. Unlabeled atoms are generated by symmetry 1-x, 1-y, 1-z.

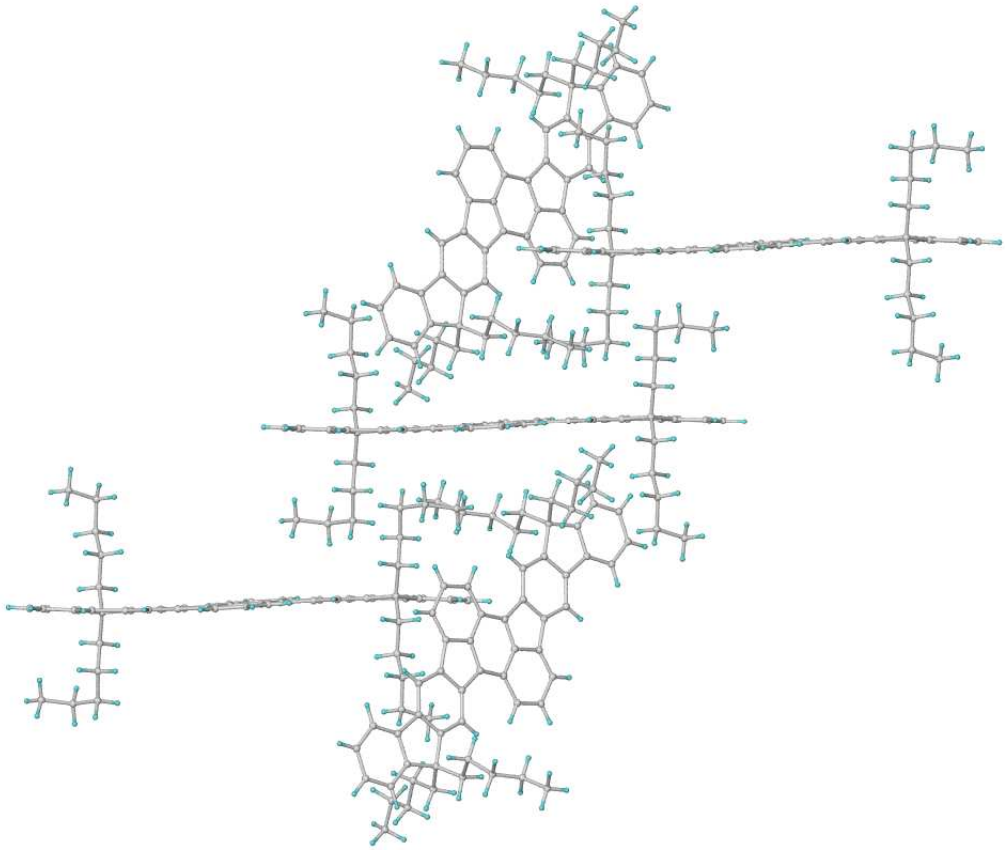


Figure 3. Ball and stick representation showing the packing of adjacent molecules (a) the interplanar angle between neighbouring polycyclic cores is 85.1(1)°(b) the interplanar distance between parallel polycyclic cores is *ca* 7.5Å.

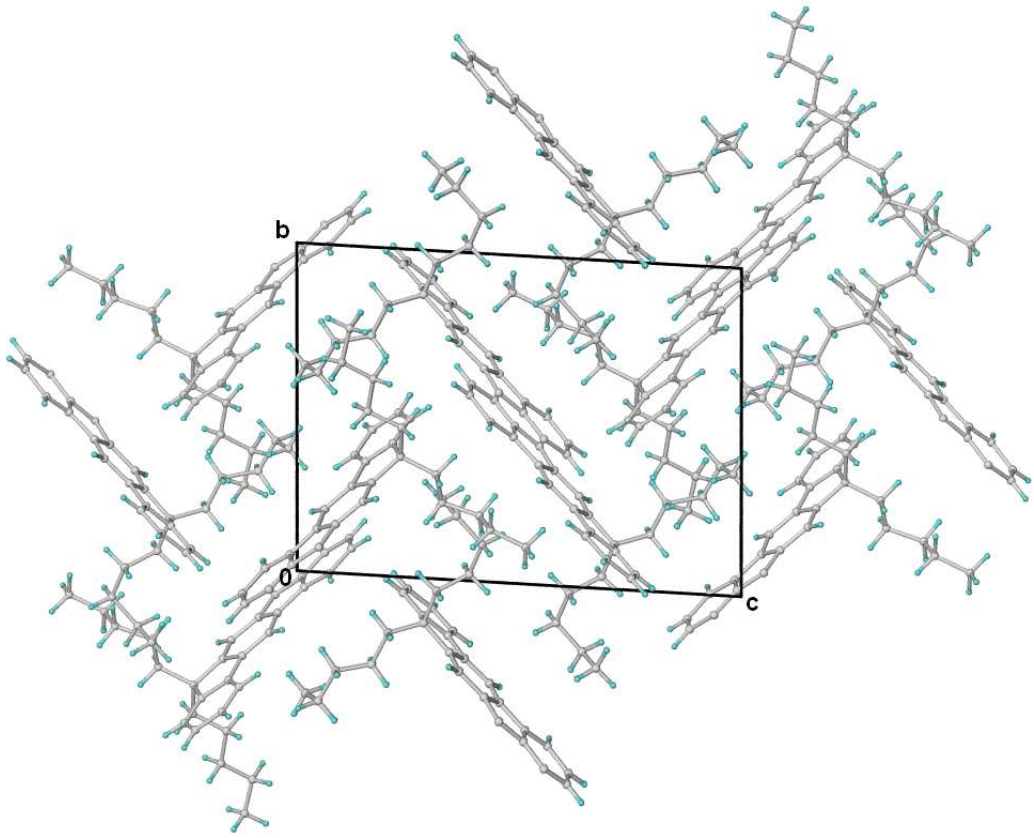


Figure 4. Cell contents as viewed down the ‘a’ axis direction.

Table 1. Crystal data and structure refinement for A7TWIN5.

Identification code	twin5
Empirical formula	C60 H62
Formula weight	783.10
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.8829(19) A alpha = 91.449(6) deg. b = 13.629(3) A beta = 94.875(9) deg. c = 17.419(3) A gamma = 109.933(6) deg.
Volume	2194.0(7) A^3
Z, Calculated density	2, 1.185 Mg/m^3
Absorption coefficient	0.066 mm^-1
F(000)	844
Crystal size	0.20 x 0.18 x 0.12 mm
Theta range for data collection	2.20 to 25.00 deg.
Limiting indices	-11<=h<=11, -16<=k<=16, 0<=l<=20
Reflections collected / unique	16463 / 8167 [R(int) = 0.066]
Completeness to theta = 25.00	97.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0 and 0.68
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8167 / 0 / 543
Goodness-of-fit on F^2	0.956
Final R indices [I>2sigma(I)]	R1 = 0.0781, wR2 = 0.1909
R indices (all data)	R1 = 0.1406, wR2 = 0.2512
Extinction coefficient	0.030(3)
Largest diff. peak and hole	0.492 and -0.396 e.A^-3

Table 2. Bond lengths [A] and angles [deg] for A7TWIN5.

C(1)-C(2)	1.515(7)
C(1)-C(20)	1.534(7)
C(1)-C(21)	1.538(7)
C(1)-C(26)	1.555(7)
C(2)-C(3)	1.396(7)
C(2)-C(7)	1.412(7)
C(3)-C(4)	1.374(7)
C(4)-C(5)	1.395(8)
C(5)-C(6)	1.402(7)
C(6)-C(7)	1.358(7)
C(7)-C(8)	1.487(7)
C(8)-C(20)	1.399(7)
C(8)-C(9)	1.401(7)
C(9)-C(10)	1.389(7)
C(10)-C(18)	1.414(7)
C(10)-C(11)	1.461(7)
C(11)-C(12)	1.366(7)
C(11)-C(16)	1.432(7)
C(12)-C(13)	1.436(7)
C(13)-C(14)	1.381(7)
C(14)-C(15)	1.394(7)
C(15)-C(16)	1.434(7)
C(15)-C(17)#1	1.443(7)
C(16)-C(17)	1.389(7)
C(17)-C(15)#1	1.443(7)
C(17)-C(18)	1.474(7)
C(18)-C(19)	1.400(7)
C(19)-C(20)	1.372(7)
C(21)-C(22)	1.525(7)
C(22)-C(23)	1.525(7)
C(23)-C(24)	1.506(7)
C(24)-C(25)	1.526(8)
C(26)-C(27)	1.505(7)
C(27)-C(28)	1.543(7)
C(28)-C(29)	1.497(7)
C(29)-C(30)	1.534(8)
C(31)-C(32)	1.513(7)
C(31)-C(50)	1.530(7)
C(31)-C(51)	1.542(7)
C(31)-C(56)	1.549(7)
C(32)-C(33)	1.386(7)
C(32)-C(37)	1.417(7)
C(33)-C(34)	1.377(7)
C(34)-C(35)	1.390(7)
C(35)-C(36)	1.385(7)
C(36)-C(37)	1.385(7)
C(37)-C(38)	1.496(7)
C(38)-C(39)	1.373(7)
C(38)-C(50)	1.397(7)
C(39)-C(40)	1.386(7)

C(40)-C(48)	1.434(7)
C(40)-C(41)	1.477(7)
C(41)-C(42)	1.366(6)
C(41)-C(46)	1.411(7)
C(42)-C(43)	1.428(7)
C(43)-C(44)	1.367(7)
C(44)-C(45)	1.430(7)
C(45)-C(47)#2	1.389(7)
C(45)-C(46)	1.420(7)
C(46)-C(47)	1.440(7)
C(47)-C(45)#2	1.389(7)
C(47)-C(48)	1.459(7)
C(48)-C(49)	1.401(7)
C(49)-C(50)	1.387(7)
C(51)-C(52)	1.534(7)
C(52)-C(53)	1.516(7)
C(53)-C(54)	1.527(8)
C(54)-C(55)	1.498(8)
C(56)-C(57)	1.521(7)
C(57)-C(58)	1.508(7)
C(58)-C(59)	1.535(8)
C(59)-C(60)	1.511(7)

C(2)-C(1)-C(20)	101.3(4)
C(2)-C(1)-C(21)	112.7(4)
C(20)-C(1)-C(21)	114.6(4)
C(2)-C(1)-C(26)	110.1(4)
C(20)-C(1)-C(26)	110.9(4)
C(21)-C(1)-C(26)	107.3(4)
C(3)-C(2)-C(7)	118.2(5)
C(3)-C(2)-C(1)	129.8(5)
C(7)-C(2)-C(1)	111.9(4)
C(4)-C(3)-C(2)	119.4(5)
C(3)-C(4)-C(5)	122.0(5)
C(4)-C(5)-C(6)	118.8(5)
C(7)-C(6)-C(5)	119.3(6)
C(6)-C(7)-C(2)	122.3(5)
C(6)-C(7)-C(8)	130.8(5)
C(2)-C(7)-C(8)	106.9(5)
C(20)-C(8)-C(9)	121.6(5)
C(20)-C(8)-C(7)	109.2(5)
C(9)-C(8)-C(7)	129.2(5)
C(10)-C(9)-C(8)	117.8(5)
C(9)-C(10)-C(18)	120.6(5)
C(9)-C(10)-C(11)	129.6(5)
C(18)-C(10)-C(11)	109.8(4)
C(12)-C(11)-C(16)	120.7(5)
C(12)-C(11)-C(10)	134.0(5)
C(16)-C(11)-C(10)	105.3(4)
C(11)-C(12)-C(13)	117.8(5)
C(14)-C(13)-C(12)	122.1(5)
C(13)-C(14)-C(15)	121.2(5)
C(14)-C(15)-C(16)	117.3(5)
C(14)-C(15)-C(17)#1	129.3(5)
C(16)-C(15)-C(17)#1	113.4(4)

C(17)-C(16)-C(11)	110.7(5)
C(17)-C(16)-C(15)	128.5(5)
C(11)-C(16)-C(15)	120.9(5)
C(16)-C(17)-C(15)#1	118.0(5)
C(16)-C(17)-C(18)	108.1(5)
C(15)#1-C(17)-C(18)	133.8(5)
C(19)-C(18)-C(10)	120.4(5)
C(19)-C(18)-C(17)	133.4(5)
C(10)-C(18)-C(17)	106.2(4)
C(20)-C(19)-C(18)	119.0(5)
C(19)-C(20)-C(8)	120.5(5)
C(19)-C(20)-C(1)	129.0(5)
C(8)-C(20)-C(1)	110.4(4)
C(22)-C(21)-C(1)	118.0(4)
C(23)-C(22)-C(21)	112.2(4)
C(24)-C(23)-C(22)	116.5(5)
C(23)-C(24)-C(25)	112.5(5)
C(27)-C(26)-C(1)	116.8(5)
C(26)-C(27)-C(28)	112.0(5)
C(29)-C(28)-C(27)	113.3(4)
C(28)-C(29)-C(30)	112.0(5)
C(32)-C(31)-C(50)	101.1(4)
C(32)-C(31)-C(51)	112.2(4)
C(50)-C(31)-C(51)	112.6(4)
C(32)-C(31)-C(56)	111.2(4)
C(50)-C(31)-C(56)	111.7(4)
C(51)-C(31)-C(56)	107.9(4)
C(33)-C(32)-C(37)	118.1(5)
C(33)-C(32)-C(31)	130.3(5)
C(37)-C(32)-C(31)	111.6(4)
C(34)-C(33)-C(32)	120.9(5)
C(33)-C(34)-C(35)	120.4(5)
C(36)-C(35)-C(34)	120.2(5)
C(35)-C(36)-C(37)	119.3(5)
C(36)-C(37)-C(32)	121.1(5)
C(36)-C(37)-C(38)	131.6(5)
C(32)-C(37)-C(38)	107.3(4)
C(39)-C(38)-C(50)	121.6(5)
C(39)-C(38)-C(37)	130.4(5)
C(50)-C(38)-C(37)	108.0(4)
C(38)-C(39)-C(40)	118.9(5)
C(39)-C(40)-C(48)	120.4(5)
C(39)-C(40)-C(41)	132.3(5)
C(48)-C(40)-C(41)	107.3(4)
C(42)-C(41)-C(46)	119.0(5)
C(42)-C(41)-C(40)	133.8(5)
C(46)-C(41)-C(40)	107.2(4)
C(41)-C(42)-C(43)	119.0(5)
C(44)-C(43)-C(42)	121.8(5)
C(43)-C(44)-C(45)	121.4(5)
C(47)#2-C(45)-C(46)	116.6(5)
C(47)#2-C(45)-C(44)	128.6(5)
C(46)-C(45)-C(44)	114.8(5)
C(41)-C(46)-C(45)	123.9(5)
C(41)-C(46)-C(47)	110.4(4)

C(45)-C(46)-C(47)	125.7(5)
C(45)#2-C(47)-C(46)	117.7(5)
C(45)#2-C(47)-C(48)	135.9(5)
C(46)-C(47)-C(48)	106.4(4)
C(49)-C(48)-C(40)	119.5(5)
C(49)-C(48)-C(47)	131.8(5)
C(40)-C(48)-C(47)	108.7(4)
C(50)-C(49)-C(48)	118.8(5)
C(49)-C(50)-C(38)	120.8(5)
C(49)-C(50)-C(31)	127.6(4)
C(38)-C(50)-C(31)	111.6(4)
C(52)-C(51)-C(31)	114.9(4)
C(53)-C(52)-C(51)	111.2(4)
C(52)-C(53)-C(54)	112.9(4)
C(55)-C(54)-C(53)	113.4(5)
C(57)-C(56)-C(31)	115.6(4)
C(58)-C(57)-C(56)	114.2(5)
C(57)-C(58)-C(59)	115.5(5)
C(60)-C(59)-C(58)	113.9(5)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z #2 -x+1,-y+1,-z+1

C56H54 **4d**

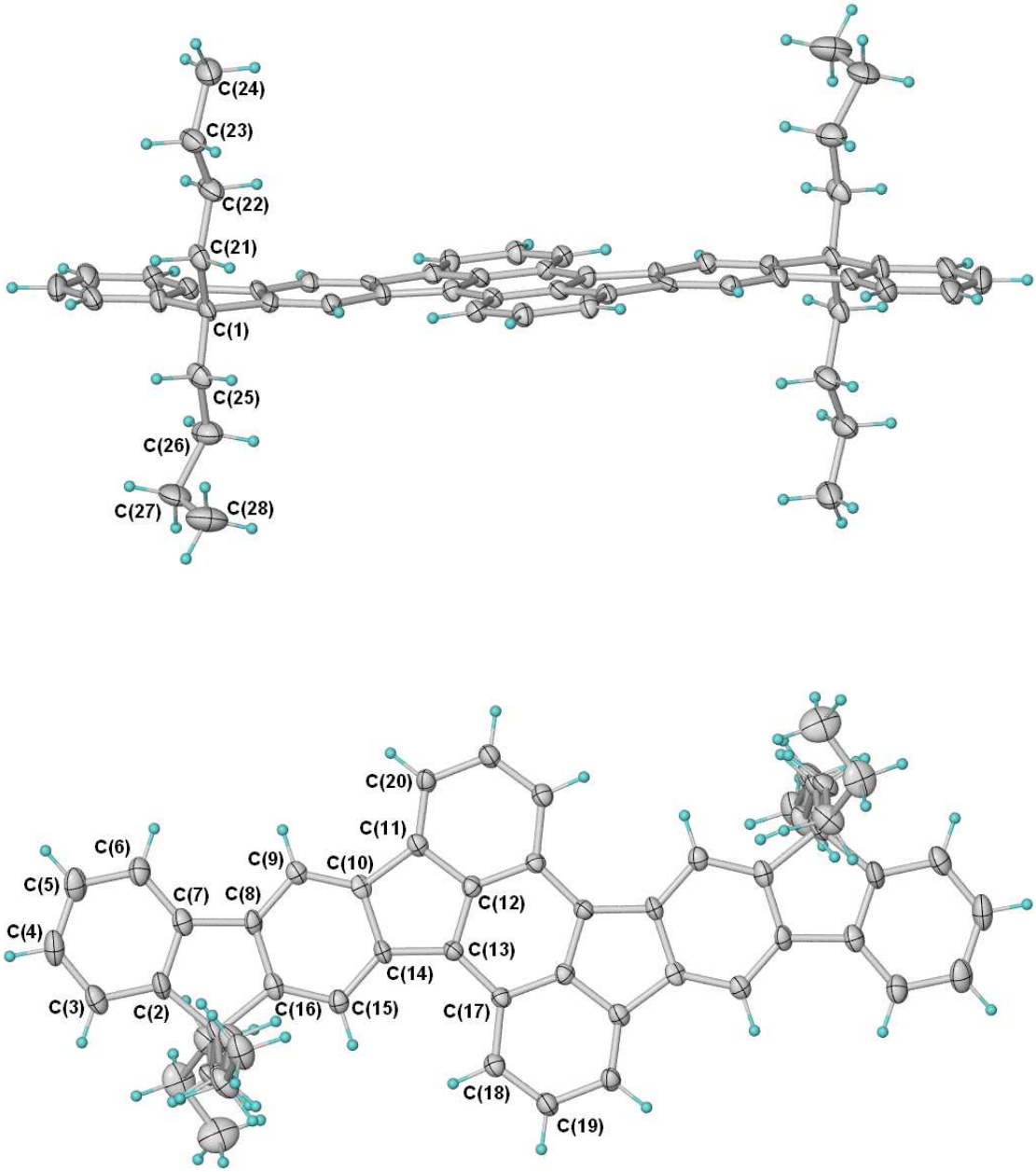


Figure 1. Molecular diagram as shown with 50% thermal ellipsoids and hydrogen atoms as spheres of arbitrary size. Only one component of the disordered butyl chain (C20-24) is shown.

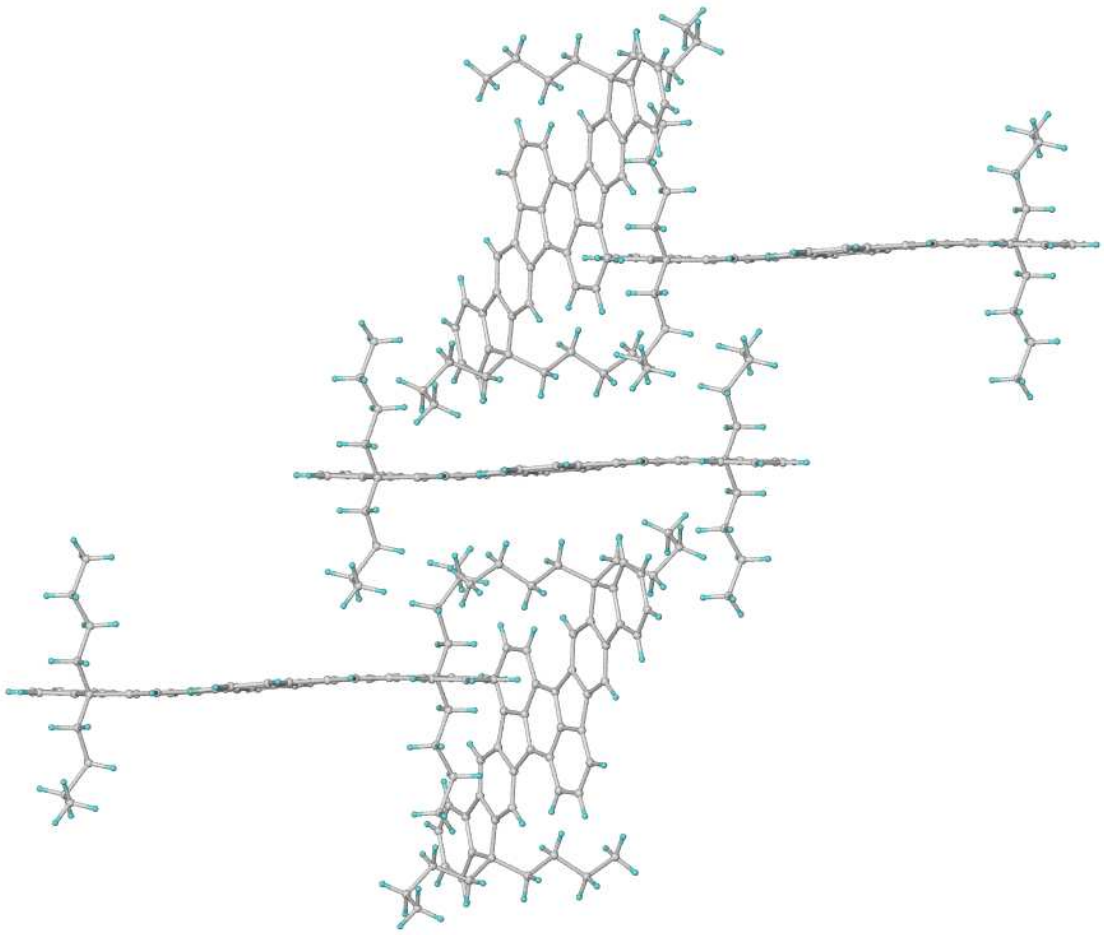


Figure 2. Ball and stick representation showing packing of adjacent molecules and subsequent extended packing motif. The interplanar separation of parallel polycyclic cores is ca 7.7Å.

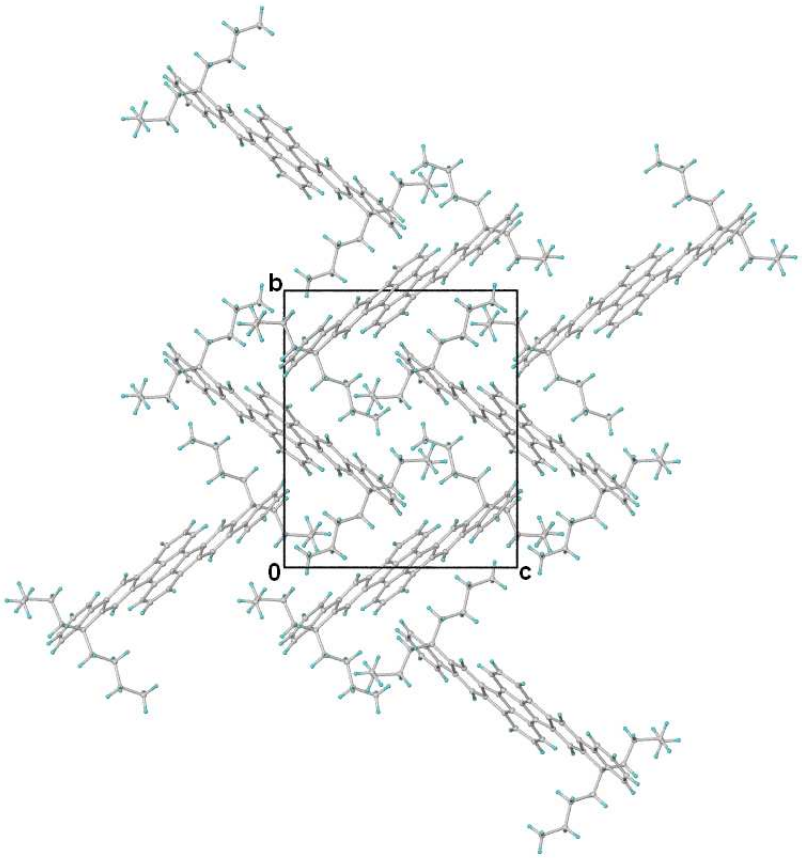


Figure 3. Cell contents as viewed down the ‘a’ axis direction.

Table 1. Crystal data and structure refinement for A10_10M.

Identification code	a10_10m
Empirical formula	C56 H54
Formula weight	726.99
Temperature	123(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 9.7315(12) A alpha = 90 deg. b = 15.9446(19) A beta = 109.908(4) deg. c = 14.2036(18) A gamma = 90 deg.
Volume	2072.2(4) A^3
Z, Calculated density	2, 1.165 Mg/m^3
Absorption coefficient	0.065 mm^-1
F(000)	780
Crystal size	0.20 x 0.10 x 0.08 mm
Theta range for data collection	2.57 to 25.00 deg.
Limiting indices	-10<=h<=11, -18<=k<=18, -16<=l<=12
Reflections collected / unique	6032 / 3591 [R(int) = 0.0788]
Completeness to theta = 25.00	98.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0 and 0.59
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3591 / 1 / 271
Goodness-of-fit on F^2	0.934
Final R indices [I>2sigma(I)]	R1 = 0.0711, wR2 = 0.1404
R indices (all data)	R1 = 0.1991, wR2 = 0.1928
Largest diff. peak and hole	0.219 and -0.259 e.A^-3

Table 2. Bond lengths [A] and angles [deg] for A10_10M.

C(13)-C(12)	1.397(6)
C(13)-C(17)	1.406(5)
C(13)-C(14)	1.473(5)
C(12)-C(17)#1	1.418(5)
C(12)-C(11)	1.428(5)
C(10)-C(9)	1.380(5)
C(10)-C(14)	1.429(5)
C(10)-C(11)	1.467(6)
C(17)-C(12)#1	1.418(5)
C(17)-C(18)	1.420(5)
C(11)-C(20)#1	1.355(5)
C(1)-C(2)	1.521(6)
C(1)-C(16)	1.530(6)
C(1)-C(25)	1.538(6)
C(1)-C(21)	1.547(6)
C(8)-C(9)	1.378(5)
C(8)-C(16)	1.405(6)
C(8)-C(7)	1.485(5)
C(18)-C(19)	1.375(5)
C(14)-C(15)	1.394(6)
C(19)-C(20)	1.423(5)
C(20)-C(11)#1	1.355(5)
C(16)-C(15)	1.394(5)
C(7)-C(6)	1.392(6)
C(7)-C(2)	1.401(6)
C(6)-C(5)	1.373(6)
C(23)-C(24)	1.515(6)
C(23)-C(22)	1.518(6)
C(25)-C(26)	1.528(6)
C(22)-C(21)	1.517(6)
C(3)-C(4)	1.396(6)
C(3)-C(2)	1.396(6)
C(4)-C(5)	1.400(6)
C(26)-C(27)	1.550(11)
C(28)-C(27)	1.444(14)
C(28')-C(27')	1.628(19)

C(12)-C(13)-C(17)	118.0(4)
C(12)-C(13)-C(14)	107.2(4)
C(17)-C(13)-C(14)	134.8(4)
C(13)-C(12)-C(17)#1	126.9(4)
C(13)-C(12)-C(11)	111.0(4)
C(17)#1-C(12)-C(11)	122.1(4)
C(9)-C(10)-C(14)	120.5(4)
C(9)-C(10)-C(11)	131.3(4)
C(14)-C(10)-C(11)	108.2(3)
C(13)-C(17)-C(12)#1	115.1(4)
C(13)-C(17)-C(18)	128.6(4)
C(12)#1-C(17)-C(18)	116.3(4)
C(20)#1-C(11)-C(12)	119.9(4)

C(20)#1-C(11)-C(10)	134.0(4)
C(12)-C(11)-C(10)	106.2(4)
C(2)-C(1)-C(16)	100.9(3)
C(2)-C(1)-C(25)	111.7(3)
C(16)-C(1)-C(25)	112.1(4)
C(2)-C(1)-C(21)	111.2(4)
C(16)-C(1)-C(21)	111.7(3)
C(25)-C(1)-C(21)	109.1(4)
C(9)-C(8)-C(16)	121.2(4)
C(9)-C(8)-C(7)	130.9(4)
C(16)-C(8)-C(7)	107.9(4)
C(19)-C(18)-C(17)	120.8(4)
C(15)-C(14)-C(10)	120.3(4)
C(15)-C(14)-C(13)	132.3(4)
C(10)-C(14)-C(13)	107.4(4)
C(18)-C(19)-C(20)	122.0(4)
C(11)#1-C(20)-C(19)	118.9(4)
C(15)-C(16)-C(8)	120.8(4)
C(15)-C(16)-C(1)	127.7(4)
C(8)-C(16)-C(1)	111.4(4)
C(6)-C(7)-C(2)	121.1(4)
C(6)-C(7)-C(8)	130.8(4)
C(2)-C(7)-C(8)	108.1(4)
C(8)-C(9)-C(10)	119.0(4)
C(14)-C(15)-C(16)	118.2(4)
C(5)-C(6)-C(7)	118.9(5)
C(24)-C(23)-C(22)	115.1(4)
C(26)-C(25)-C(1)	115.8(4)
C(21)-C(22)-C(23)	112.5(4)
C(4)-C(3)-C(2)	117.3(5)
C(3)-C(2)-C(7)	120.5(4)
C(3)-C(2)-C(1)	127.7(4)
C(7)-C(2)-C(1)	111.7(4)
C(3)-C(4)-C(5)	122.0(4)
C(22)-C(21)-C(1)	115.6(4)
C(6)-C(5)-C(4)	120.1(5)
C(25)-C(26)-C(27)	113.5(6)
C(28)-C(27)-C(26)	110.9(11)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1