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5,11-Bis(4-*tert*-butylphenyl)-6,12-diphenylnaphthacene (form A)

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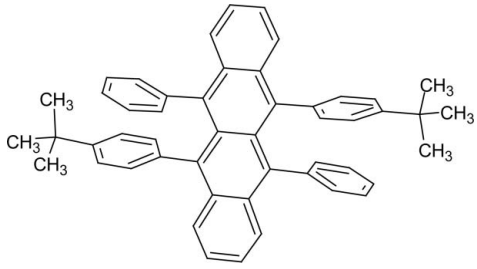
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.007 Å; R factor = 0.098; wR factor = 0.169; data-to-parameter ratio = 12.4.

The title compound, $C_{50}H_{44}$, is a derivative of rubrene where *tert*-butyl side groups are added to two of the pendant aromatic rings. Two polymorphs of this derivative, the title compound (form A) and form B, have been identified. The molecule of form A displays a strongly twisted naphthacene backbone. The in-plane arrangement differs from the classical herringbone structure, resembling a slip–stack structure type with the backbones separated by a minimum 7.0 Å in the direction of possible π-stacking.

Related literature

For related literature, see: Goldmann *et al.* (2004); Haas *et al.* (2007); Kloc *et al.* (1997); Kopranenkov & Luk'yanets (1972); Laudise *et al.* (1998); Mattheus *et al.* (2001); Schuck *et al.* (2007); Strassen *et al.* (2007); Sundar *et al.* (2004).



Experimental

Crystal data

$C_{50}H_{44}$
M_r = 644.85
Monoclinic, $P2_1/c$
a = 23.527 (3) Å
b = 9.0277 (10) Å
c = 17.764 (2) Å
β = 95.928 (4)°
V = 3752.8 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.06 mm^{-1}
T = 292 (1) K
0.36 × 0.16 × 0.04 mm

Data collection

Brucker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)
T_{min} = 0.990, T_{max} = 0.997
31129 measured reflections
6626 independent reflections
3478 reflections with $I > 2\sigma(I)$
R_{int} = 0.100

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.098
$wR(F^2)$ = 0.169
S = 1.11
6626 reflections
536 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The SMART CCD measurements were performed in the group of Professor R. Nesper at the Laboratory of Inorganic Chemistry, ETH Zürich. We acknowledge useful discussions with Michael Wörle (Laboratory of Inorganic Chemistry, ETH Zürich), and thank Oliver Dosenbach for assistance in the synthesis of the title compound.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2402).

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supplementary materials

Acta Cryst. (2007). E**63**, o2894 [**doi:10.1107/S1600536807022490**]

5,11-Bis(4-*tert*-butylphenyl)-6,12-diphenylnaphthacene (form A)

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Comment

The electronic properties of rubrene and rubrene derivatives are of great interest owing to fundamental questions on charge transport and associated applications (Sundar *et al.*, 2004; Goldmann *et al.*, 2004). The electric transport properties of the two polymorphs of the title compound are distinctly different: in polymorph B, the in-plane hole is as high as 12 cm^2/Vs, on par with rubrene, which is known to be the organic semiconductor with the highest hole mobility. In contrast, the title compound, (I), polymorph A is highly resistive and does not show any field-induced electrical transport (Haas *et al.*, 2007, Strassen *et al.*, 2007).

The crystal structure of (I) is monoclinic, with space group $P2_1/c$, with four molecules in the unit cell (Fig. 1). The molecules form a layered structure, similar to linear acenes such as pentacene (Mattheus *et al.*, 2001) with the naphthacene backbone standing upright (see Fig. 2). A particular characteristic of polymorph A is the twist of the naphthalene backbone by 43° (defined as the torsion angle between the two terminal C—C bonds [C1—C2 and C17—C18] at the ends of the backbone).

Polymorph B exclusively grows in the form of ultrathin platelets (Haas *et al.*, 2007). From d-spacing measurements on these samples, a structure closely related to the one found for a constitutional isomer, 5,12-bis-(4-tert-butyl-phenyl)-6,11-diphenyl-naphthacene (Schuck *et al.*, 2007) was assumed for polymorph B. A complete structure determination of form B, however, has not been feasible so far due to the crystal morphology.

Experimental

The title compound was synthesized according to the method of Kopranenkov & Luk'yanets (1972). Physical vapour transport (Kloc *et al.*, 1997, Laudise *et al.*, 1998) at 533 K, using high purity argon as the transport gas made single crystals of both polymorphs at the same time. The morphology (plates typically 0.1-0.2 µm thick), orange colour and transparency of both forms are basically the same. The two forms can only be distinguished by measuring their d-spacings perpendicular to the crystal platelets (form A: d_{100} = 23.4 Å and form B d = 35.1 Å) (Haas *et al.*, 2007).

Only at a slightly higher temperature (and with longer growth time), a few thicker crystals of form A could be grown for full structural characterization with XRD.

Refinement

The H atoms in the aromatic units were located in difference maps and their positions were freely refined with $U_{iso}(H) = 1.2U_{eq}$(carrier). The H atoms of the methyl groups were positioned geometrically (C—H = 0.96 Å) and were refined as riding on the parent C atoms with $U_{iso}(H) = 1.5U_{eq}$(carrier).

Figures

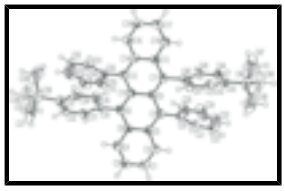

Fig. 1. The molecular structure of (I), showing the atom numbering scheme and displacement ellipsoids at the 50% probability level (arbitrary spheres for the H atoms).

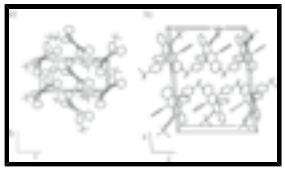

Fig. 2. The crystal packing for (I), viewed (a) down the a axis and (b) viewed down the b axis.

5,11-Bis(4-tert-butyl-phenyl)-6,12-diphenylnaphthacene

Crystal data

$C_{50}H_{44}$	F_{000} = 1376
M_r = 644.85	D_x = 1.141 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3136 reflections
a = 23.527 (3) Å	θ = 3.0–25.0º
b = 9.0277 (10) Å	μ = 0.06 mm^{-1}
c = 17.764 (2) Å	T = 292 (1) K
β = 95.928 (4)º	Plate, translucent orange
V = 3752.8 (8) Å^3	0.36 × 0.16 × 0.04 mm
Z = 4	

Data collection

Brucker SMART CCD diffractometer	6626 independent reflections
Radiation source: fine-focus sealed tube	3478 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.100
T = 292(1) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 0.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996; Blessing, 1995)	h = −27→27
T_{min} = 0.990, T_{max} = 0.997	k = −10→10
31129 measured reflections	l = −21→21

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0241P)^2 + 4.9951P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.098$	$(\Delta/\sigma)_{max} = 0.004$
$wR(F^2) = 0.169$	$\Delta\rho_{max} = 0.29$ e Å^{-3}
$S = 1.11$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
6626 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
536 parameters	Extinction coefficient: 0.0020 (3)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: difmap and geom	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4082 (2)	0.7231 (5)	0.3755 (3)	0.0571 (13)
C2	0.43973 (19)	0.6785 (5)	0.4434 (3)	0.0544 (13)
C3	0.35092 (18)	0.7072 (5)	0.3654 (2)	0.0444 (11)
C4	0.41355 (18)	0.6099 (5)	0.4982 (3)	0.0481 (12)
C5	0.32005 (16)	0.6423 (4)	0.4231 (2)	0.0388 (10)
C6	0.35296 (15)	0.5814 (4)	0.4884 (2)	0.0352 (10)
C7	0.26002 (16)	0.6412 (4)	0.4184 (2)	0.0378 (10)
C8	0.32605 (15)	0.4935 (4)	0.5393 (2)	0.0356 (10)
C9	0.23227 (15)	0.5692 (4)	0.4762 (2)	0.0350 (10)
C10	0.26556 (15)	0.4713 (4)	0.5276 (2)	0.0357 (10)
C11	0.17319 (15)	0.5862 (4)	0.4856 (2)	0.0353 (10)
C12	0.23732 (16)	0.3584 (4)	0.5653 (2)	0.0370 (10)
C13	0.14684 (15)	0.4909 (4)	0.5329 (2)	0.0360 (10)
C14	0.17806 (16)	0.3674 (4)	0.5681 (2)	0.0387 (10)
C15	0.08776 (17)	0.5078 (5)	0.5463 (2)	0.0464 (11)
C16	0.14702 (19)	0.2603 (5)	0.6065 (3)	0.0512 (12)
C17	0.0615 (2)	0.4075 (6)	0.5867 (3)	0.0550 (13)
C18	0.0911 (2)	0.2800 (6)	0.6153 (3)	0.0604 (14)
C20	0.22674 (17)	0.6982 (5)	0.3482 (2)	0.0483 (11)
C21	0.2261 (2)	0.8465 (6)	0.3280 (3)	0.0723 (16)
C22	0.1970 (3)	0.8925 (10)	0.2595 (5)	0.106 (3)

C23	0.1690 (3)	0.7895 (13)	0.2123 (4)	0.120 (4)
C24	0.1700 (3)	0.6451 (11)	0.2308 (3)	0.105 (3)
C25	0.1988 (2)	0.5961 (7)	0.2987 (3)	0.0669 (15)
C30	0.35873 (15)	0.4391 (4)	0.6107 (2)	0.0375 (10)
C31	0.40131 (16)	0.3323 (5)	0.6126 (2)	0.0444 (11)
C32	0.42905 (18)	0.2851 (5)	0.6807 (3)	0.0487 (12)
C33	0.41595 (18)	0.3416 (5)	0.7495 (2)	0.0488 (11)
C34	0.3746 (2)	0.4500 (5)	0.7468 (2)	0.0519 (12)
C35	0.34595 (19)	0.4986 (5)	0.6788 (2)	0.0486 (12)
C36	0.4456 (2)	0.2853 (6)	0.8254 (3)	0.0669 (14)
C37	0.4903 (4)	0.3883 (8)	0.8554 (4)	0.202 (5)
H37A	0.5054	0.3571	0.9052	0.303*
H37B	0.4745	0.4860	0.8580	0.303*
H37C	0.5204	0.3893	0.8228	0.303*
C38	0.4708 (3)	0.1331 (7)	0.8175 (3)	0.146 (3)
H38A	0.5047	0.1407	0.7920	0.219*
H38B	0.4435	0.0710	0.7886	0.219*
H38C	0.4802	0.0908	0.8667	0.219*
C39	0.4024 (4)	0.2652 (12)	0.8809 (4)	0.218 (6)
H39A	0.4184	0.2046	0.9222	0.327*
H39B	0.3689	0.2180	0.8563	0.327*
H39C	0.3922	0.3601	0.8999	0.327*
C40	0.14101 (16)	0.7183 (4)	0.4525 (2)	0.0371 (10)
C41	0.15368 (19)	0.8579 (5)	0.4817 (2)	0.0491 (12)
C42	0.1243 (2)	0.9821 (5)	0.4531 (3)	0.0579 (13)
C43	0.08086 (18)	0.9718 (5)	0.3945 (2)	0.0446 (11)
C44	0.06779 (18)	0.8326 (5)	0.3667 (2)	0.0490 (12)
C45	0.09662 (17)	0.7067 (5)	0.3952 (2)	0.0437 (11)
C46	0.0491 (2)	1.1098 (5)	0.3632 (3)	0.0653 (14)
C47	0.0073 (3)	1.1571 (8)	0.4184 (4)	0.166 (4)
H47A	0.0282	1.1912	0.4645	0.249*
H47B	−0.0161	1.0743	0.4292	0.249*
H47C	−0.0164	1.2357	0.3965	0.249*
C48	0.0899 (3)	1.2343 (6)	0.3525 (4)	0.147 (3)
H48A	0.1074	1.2666	0.4009	0.220*
H48B	0.0695	1.3154	0.3273	0.220*
H48C	0.1190	1.2005	0.3223	0.220*
C49	0.0140 (3)	1.0800 (6)	0.2874 (3)	0.110 (2)
H49A	−0.0043	1.1698	0.2690	0.165*
H49B	−0.0145	1.0063	0.2941	0.165*
H49C	0.0388	1.0450	0.2515	0.165*
C50	0.26843 (17)	0.2211 (5)	0.5919 (3)	0.0473 (11)
C51	0.2768 (2)	0.1763 (6)	0.6668 (3)	0.0656 (15)
C52	0.3053 (2)	0.0437 (8)	0.6856 (4)	0.089 (2)
C53	0.3249 (3)	−0.0439 (7)	0.6305 (6)	0.103 (3)
C54	0.3169 (3)	−0.0008 (7)	0.5560 (5)	0.092 (2)
C55	0.2890 (2)	0.1303 (5)	0.5368 (3)	0.0639 (14)
H1	0.4291 (19)	0.759 (5)	0.335 (2)	0.077*
H2	0.4827 (19)	0.693 (5)	0.454 (2)	0.077*

H3	0.3284 (18)	0.744 (5)	0.317 (2)	0.077*
H4	0.4347 (18)	0.574 (5)	0.547 (2)	0.077*
H15	0.0685 (18)	0.600 (5)	0.524 (2)	0.077*
H16	0.1680 (18)	0.174 (5)	0.630 (2)	0.077*
H17	0.0193 (19)	0.428 (5)	0.596 (2)	0.077*
H18	0.0713 (19)	0.218 (5)	0.644 (2)	0.077*
H21	0.245 (2)	0.918 (6)	0.366 (3)	0.096*
H22	0.197 (2)	0.993 (6)	0.249 (3)	0.096*
H23	0.148 (2)	0.818 (6)	0.163 (3)	0.096*
H24	0.152 (2)	0.564 (6)	0.199 (3)	0.096*
H25	0.201 (2)	0.488 (6)	0.316 (3)	0.096*
H31	0.4121 (18)	0.287 (5)	0.565 (2)	0.077*
H32	0.4602 (19)	0.215 (5)	0.678 (2)	0.077*
H34	0.3639 (18)	0.496 (5)	0.793 (2)	0.077*
H35	0.3160 (18)	0.572 (5)	0.681 (2)	0.077*
H41	0.1844 (18)	0.866 (5)	0.523 (2)	0.077*
H42	0.1385 (18)	1.075 (5)	0.476 (2)	0.077*
H44	0.0400 (18)	0.817 (5)	0.325 (2)	0.077*
H45	0.0856 (18)	0.607 (5)	0.373 (2)	0.077*
H51	0.263 (2)	0.241 (6)	0.706 (3)	0.096*
H52	0.310 (2)	0.018 (6)	0.736 (3)	0.096*
H53	0.346 (2)	−0.140 (6)	0.646 (3)	0.096*
H54	0.329 (2)	−0.069 (6)	0.514 (3)	0.096*
H55	0.281 (2)	0.163 (5)	0.480 (3)	0.096*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.047 (3)	0.065 (3)	0.061 (3)	−0.008 (3)	0.018 (2)	0.010 (3)
C2	0.034 (3)	0.070 (3)	0.058 (3)	−0.011 (3)	0.000 (2)	0.009 (3)
C3	0.043 (3)	0.045 (3)	0.046 (3)	−0.002 (2)	0.009 (2)	0.008 (2)
C4	0.039 (3)	0.056 (3)	0.048 (3)	−0.004 (2)	−0.003 (2)	0.004 (2)
C5	0.039 (2)	0.034 (2)	0.043 (2)	−0.002 (2)	0.0004 (19)	0.0016 (19)
C6	0.028 (2)	0.035 (2)	0.042 (2)	−0.0030 (19)	0.0011 (18)	0.0019 (19)
C7	0.038 (2)	0.038 (2)	0.037 (2)	0.003 (2)	−0.0016 (18)	0.0045 (19)
C8	0.033 (2)	0.034 (2)	0.039 (2)	0.0025 (19)	0.0022 (18)	−0.0026 (19)
C9	0.032 (2)	0.036 (2)	0.036 (2)	0.0012 (19)	−0.0014 (18)	0.0010 (19)
C10	0.031 (2)	0.040 (2)	0.036 (2)	0.0034 (19)	0.0023 (17)	0.0007 (19)
C11	0.031 (2)	0.038 (2)	0.035 (2)	0.0015 (19)	−0.0029 (18)	0.0006 (19)
C12	0.035 (2)	0.040 (3)	0.037 (2)	0.004 (2)	0.0057 (18)	0.0036 (19)
C13	0.030 (2)	0.045 (3)	0.032 (2)	−0.001 (2)	0.0005 (17)	−0.005 (2)
C14	0.039 (2)	0.039 (3)	0.039 (2)	−0.004 (2)	0.0082 (19)	0.002 (2)
C15	0.038 (3)	0.057 (3)	0.045 (3)	−0.001 (2)	0.006 (2)	−0.001 (2)
C16	0.043 (3)	0.056 (3)	0.055 (3)	−0.005 (2)	0.004 (2)	0.008 (2)
C17	0.039 (3)	0.068 (3)	0.059 (3)	0.000 (3)	0.013 (2)	0.004 (3)
C18	0.049 (3)	0.072 (4)	0.063 (3)	−0.011 (3)	0.019 (2)	0.011 (3)
C20	0.041 (3)	0.065 (3)	0.041 (3)	0.010 (2)	0.010 (2)	0.012 (2)
C21	0.059 (3)	0.081 (4)	0.078 (4)	0.012 (3)	0.010 (3)	0.041 (3)

C22	0.079 (5)	0.127 (7)	0.115 (6)	0.033 (5)	0.028 (4)	0.076 (6)
C23	0.094 (6)	0.208 (11)	0.059 (5)	0.061 (7)	0.009 (4)	0.045 (6)
C24	0.088 (5)	0.168 (8)	0.053 (4)	0.050 (5)	−0.019 (3)	−0.023 (4)
C25	0.056 (3)	0.097 (4)	0.046 (3)	0.023 (3)	−0.003 (2)	−0.010 (3)
C30	0.027 (2)	0.043 (3)	0.043 (3)	−0.001 (2)	0.0014 (18)	0.004 (2)
C31	0.031 (2)	0.059 (3)	0.043 (3)	0.009 (2)	0.002 (2)	0.004 (2)
C32	0.037 (3)	0.056 (3)	0.053 (3)	0.010 (2)	0.004 (2)	0.011 (2)
C33	0.051 (3)	0.048 (3)	0.047 (3)	0.001 (2)	0.000 (2)	0.013 (2)
C34	0.065 (3)	0.050 (3)	0.040 (3)	0.008 (3)	0.006 (2)	−0.002 (2)
C35	0.053 (3)	0.046 (3)	0.046 (3)	0.010 (2)	0.002 (2)	0.001 (2)
C36	0.085 (4)	0.061 (3)	0.051 (3)	0.013 (3)	−0.010 (3)	0.016 (3)
C37	0.268 (10)	0.137 (7)	0.160 (7)	−0.100 (7)	−0.174 (8)	0.081 (6)
C38	0.226 (9)	0.095 (5)	0.100 (5)	0.050 (6)	−0.066 (5)	0.025 (4)
C39	0.200 (9)	0.369 (15)	0.095 (6)	0.109 (10)	0.062 (6)	0.141 (8)
C40	0.032 (2)	0.042 (3)	0.037 (2)	0.003 (2)	0.0034 (18)	−0.005 (2)
C41	0.051 (3)	0.050 (3)	0.043 (3)	0.005 (2)	−0.012 (2)	−0.005 (2)
C42	0.077 (3)	0.038 (3)	0.055 (3)	0.002 (3)	−0.015 (3)	−0.010 (2)
C43	0.050 (3)	0.044 (3)	0.040 (2)	0.013 (2)	0.003 (2)	0.001 (2)
C44	0.043 (3)	0.050 (3)	0.051 (3)	0.005 (2)	−0.009 (2)	−0.004 (2)
C45	0.037 (2)	0.040 (3)	0.053 (3)	0.005 (2)	−0.003 (2)	−0.003 (2)
C46	0.086 (4)	0.047 (3)	0.060 (3)	0.024 (3)	−0.005 (3)	0.005 (2)
C47	0.227 (9)	0.165 (8)	0.112 (6)	0.157 (7)	0.044 (6)	0.026 (5)
C48	0.164 (7)	0.055 (4)	0.205 (8)	−0.021 (5)	−0.060 (6)	0.053 (5)
C49	0.152 (6)	0.084 (4)	0.085 (4)	0.042 (4)	−0.029 (4)	0.026 (4)
C50	0.034 (2)	0.041 (3)	0.067 (3)	−0.002 (2)	0.003 (2)	0.011 (2)
C51	0.047 (3)	0.067 (4)	0.082 (4)	0.001 (3)	0.005 (3)	0.035 (3)
C52	0.057 (4)	0.088 (5)	0.118 (6)	0.002 (3)	−0.001 (4)	0.062 (5)
C53	0.075 (5)	0.049 (4)	0.184 (9)	0.016 (3)	0.005 (5)	0.035 (5)
C54	0.081 (4)	0.046 (4)	0.149 (7)	0.012 (3)	0.003 (4)	−0.014 (4)
C55	0.056 (3)	0.044 (3)	0.091 (4)	0.005 (3)	0.003 (3)	−0.008 (3)

Geometric parameters (Å, °)

C1—C3	1.348 (6)	C33—C36	1.539 (6)
C1—C2	1.408 (6)	C34—C35	1.392 (6)
C1—H1	0.97 (4)	C34—H34	0.98 (4)
C2—C4	1.355 (6)	C35—H35	0.97 (4)
C2—H2	1.02 (4)	C36—C37	1.464 (7)
C3—C5	1.439 (5)	C36—C39	1.498 (8)
C3—H3	1.02 (4)	C36—C38	1.508 (7)
C4—C6	1.441 (5)	C37—H37A	0.9600
C4—H4	1.01 (4)	C37—H37B	0.9600
C5—C7	1.406 (5)	C37—H37C	0.9600
C5—C6	1.437 (5)	C38—H38A	0.9600
C6—C8	1.402 (5)	C38—H38B	0.9600
C7—C9	1.428 (5)	C38—H38C	0.9600
C7—C20	1.495 (5)	C39—H39A	0.9600
C8—C10	1.431 (5)	C39—H39B	0.9600
C8—C30	1.498 (5)	C39—H39C	0.9600

C9—C11	1.425 (5)	C40—C45	1.384 (5)
C9—C10	1.443 (5)	C40—C41	1.384 (5)
C10—C12	1.422 (5)	C41—C42	1.386 (6)
C11—C13	1.392 (5)	C41—H41	0.98 (4)
C11—C40	1.499 (5)	C42—C43	1.385 (6)
C12—C14	1.402 (5)	C42—H42	0.98 (4)
C12—C50	1.491 (5)	C43—C44	1.373 (6)
C13—C14	1.442 (5)	C43—C46	1.528 (6)
C13—C15	1.442 (5)	C44—C45	1.392 (6)
C14—C16	1.427 (6)	C44—H44	0.95 (4)
C15—C17	1.346 (6)	C45—H45	1.00 (4)
C15—H15	1.01 (4)	C46—C48	1.504 (7)
C16—C18	1.353 (6)	C46—C47	1.519 (7)
C16—H16	0.99 (4)	C46—C49	1.528 (7)
C17—C18	1.412 (7)	C47—H47A	0.9600
C17—H17	1.04 (4)	C47—H47B	0.9600
C18—H18	0.92 (4)	C47—H47C	0.9600
C20—C21	1.385 (6)	C48—H48A	0.9600
C20—C25	1.391 (6)	C48—H48B	0.9600
C21—C22	1.397 (8)	C48—H48C	0.9600
C21—H21	1.00 (5)	C49—H49A	0.9600
C22—C23	1.373 (11)	C49—H49B	0.9600
C22—H22	0.93 (5)	C49—H49C	0.9600
C23—C24	1.344 (11)	C50—C51	1.386 (6)
C23—H23	1.00 (5)	C50—C55	1.401 (6)
C24—C25	1.392 (8)	C51—C52	1.395 (8)
C24—H24	1.00 (5)	C51—H51	1.00 (5)
C25—H25	1.03 (5)	C52—C53	1.374 (9)
C30—C35	1.384 (5)	C52—H52	0.92 (5)
C30—C31	1.388 (5)	C53—C54	1.373 (9)
C31—C32	1.381 (5)	C53—H53	1.02 (5)
C31—H31	0.99 (4)	C54—C55	1.379 (7)
C32—C33	1.387 (6)	C54—H54	1.04 (5)
C32—H32	0.97 (4)	C55—H55	1.06 (5)
C33—C34	1.378 (6)		
C3—C1—C2	121.0 (4)	C30—C35—C34	120.5 (4)
C3—C1—H1	121 (3)	C30—C35—H35	121 (3)
C2—C1—H1	118 (3)	C34—C35—H35	118 (3)
C4—C2—C1	120.5 (4)	C37—C36—C39	110.3 (7)
C4—C2—H2	117 (2)	C37—C36—C38	109.7 (6)
C1—C2—H2	123 (2)	C39—C36—C38	104.5 (6)
C1—C3—C5	121.3 (4)	C37—C36—C33	110.7 (4)
C1—C3—H3	120 (2)	C39—C36—C33	109.9 (5)
C5—C3—H3	118 (2)	C38—C36—C33	111.5 (4)
C2—C4—C6	120.8 (4)	C36—C37—H37A	109.5
C2—C4—H4	123 (2)	C36—C37—H37B	109.5
C6—C4—H4	116 (2)	H37A—C37—H37B	109.5
C7—C5—C6	119.9 (4)	C36—C37—H37C	109.5
C7—C5—C3	122.6 (4)	H37A—C37—H37C	109.5

C6—C5—C3	117.5 (4)	H37B—C37—H37C	109.5
C8—C6—C5	119.7 (3)	C36—C38—H38A	109.5
C8—C6—C4	122.0 (4)	C36—C38—H38B	109.5
C5—C6—C4	118.2 (4)	H38A—C38—H38B	109.5
C5—C7—C9	119.5 (3)	C36—C38—H38C	109.5
C5—C7—C20	118.8 (4)	H38A—C38—H38C	109.5
C9—C7—C20	121.2 (3)	H38B—C38—H38C	109.5
C6—C8—C10	119.6 (3)	C36—C39—H39A	109.5
C6—C8—C30	120.4 (3)	C36—C39—H39B	109.5
C10—C8—C30	119.5 (3)	H39A—C39—H39B	109.5
C11—C9—C7	124.0 (3)	C36—C39—H39C	109.5
C11—C9—C10	117.7 (3)	H39A—C39—H39C	109.5
C7—C9—C10	118.4 (3)	H39B—C39—H39C	109.5
C12—C10—C8	122.6 (3)	C45—C40—C41	117.5 (4)
C12—C10—C9	119.2 (3)	C45—C40—C11	122.7 (4)
C8—C10—C9	118.2 (3)	C41—C40—C11	119.8 (3)
C13—C11—C9	120.3 (3)	C40—C41—C42	121.3 (4)
C13—C11—C40	119.3 (3)	C40—C41—H41	118 (3)
C9—C11—C40	119.9 (3)	C42—C41—H41	121 (3)
C14—C12—C10	119.3 (3)	C43—C42—C41	121.5 (4)
C14—C12—C50	119.6 (4)	C43—C42—H42	124 (3)
C10—C12—C50	120.5 (3)	C41—C42—H42	114 (3)
C11—C13—C14	120.1 (3)	C44—C43—C42	116.9 (4)
C11—C13—C15	122.1 (4)	C44—C43—C46	122.1 (4)
C14—C13—C15	117.8 (4)	C42—C43—C46	121.0 (4)
C12—C14—C16	122.5 (4)	C43—C44—C45	122.3 (4)
C12—C14—C13	119.6 (4)	C43—C44—H44	122 (3)
C16—C14—C13	117.9 (4)	C45—C44—H44	116 (3)
C17—C15—C13	121.4 (4)	C40—C45—C44	120.5 (4)
C17—C15—H15	123 (3)	C40—C45—H45	120 (3)
C13—C15—H15	115 (3)	C44—C45—H45	120 (3)
C18—C16—C14	121.2 (4)	C48—C46—C47	109.6 (6)
C18—C16—H16	120 (3)	C48—C46—C49	108.3 (5)
C14—C16—H16	119 (3)	C47—C46—C49	107.0 (5)
C15—C17—C18	120.2 (4)	C48—C46—C43	111.1 (4)
C15—C17—H17	118 (2)	C47—C46—C43	108.6 (4)
C18—C17—H17	122 (2)	C49—C46—C43	112.1 (4)
C16—C18—C17	121.0 (5)	C46—C47—H47A	109.5
C16—C18—H18	123 (3)	C46—C47—H47B	109.5
C17—C18—H18	116 (3)	H47A—C47—H47B	109.5
C21—C20—C25	119.0 (5)	C46—C47—H47C	109.5
C21—C20—C7	122.6 (4)	H47A—C47—H47C	109.5
C25—C20—C7	118.2 (4)	H47B—C47—H47C	109.5
C20—C21—C22	120.2 (6)	C46—C48—H48A	109.5
C20—C21—H21	117 (3)	C46—C48—H48B	109.5
C22—C21—H21	123 (3)	H48A—C48—H48B	109.5
C23—C22—C21	119.4 (7)	C46—C48—H48C	109.5
C23—C22—H22	123 (4)	H48A—C48—H48C	109.5
C21—C22—H22	118 (4)	H48B—C48—H48C	109.5

C24—C23—C22	120.8 (7)	C46—C49—H49A	109.5
C24—C23—H23	118 (3)	C46—C49—H49B	109.5
C22—C23—H23	122 (3)	H49A—C49—H49B	109.5
C23—C24—C25	120.9 (7)	C46—C49—H49C	109.5
C23—C24—H24	126 (3)	H49A—C49—H49C	109.5
C25—C24—H24	113 (3)	H49B—C49—H49C	109.5
C20—C25—C24	119.5 (6)	C51—C50—C55	118.4 (5)
C20—C25—H25	116 (3)	C51—C50—C12	124.2 (4)
C24—C25—H25	124 (3)	C55—C50—C12	117.3 (4)
C35—C30—C31	118.0 (4)	C50—C51—C52	119.8 (6)
C35—C30—C8	118.3 (3)	C50—C51—H51	119 (3)
C31—C30—C8	123.6 (4)	C52—C51—H51	121 (3)
C32—C31—C30	120.7 (4)	C53—C52—C51	120.8 (6)
C32—C31—H31	118 (3)	C53—C52—H52	123 (3)
C30—C31—H31	121 (3)	C51—C52—H52	117 (4)
C31—C32—C33	122.0 (4)	C52—C53—C54	120.0 (6)
C31—C32—H32	117 (3)	C52—C53—H53	119 (3)
C33—C32—H32	121 (3)	C54—C53—H53	121 (3)
C34—C33—C32	116.9 (4)	C53—C54—C55	119.8 (6)
C34—C33—C36	121.2 (4)	C53—C54—H54	121 (3)
C32—C33—C36	121.9 (4)	C55—C54—H54	119 (3)
C33—C34—C35	122.0 (4)	C54—C55—C50	121.2 (6)
C33—C34—H34	121 (3)	C54—C55—H55	120 (3)
C35—C34—H34	117 (3)	C50—C55—H55	118 (3)

Fig. 1

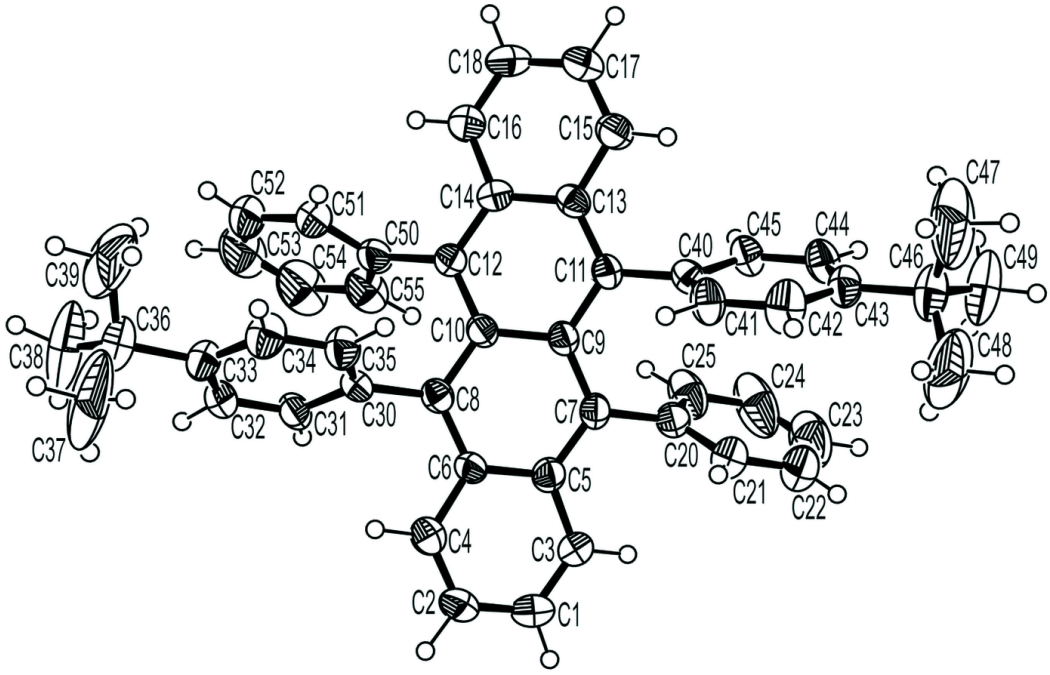
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Fig. 2