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

Götz Schuck, Simon Haas, Arno F. Stassen, Hans-Jörg Kirner and Bertram Batlogg

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5,12-Bis(4-*tert*-butylphenyl)-6,11-diphenylnaphthaceneGötz Schuck,^{a*} Simon Haas,^b Arno F. Stassen,^b Hans-Jörg Kirner^c and Bertram Batlogg^b^aLaboratory for Neutron Scattering, ETH Zürich and Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, ^bLaboratory for Solid State Physics, ETH Zürich, Schafmattstrasse 16, CH-8093 Zürich, Switzerland, and ^cCiba Specialty Chemistry Inc., CH-4002 Basel, Switzerland

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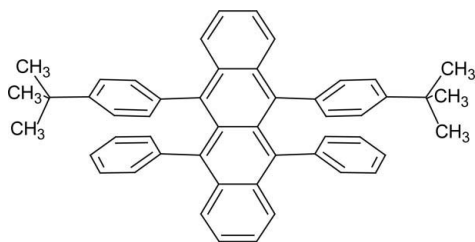
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Key indicators: single-crystal X-ray study; $T = 292$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.074; wR factor = 0.207; data-to-parameter ratio = 12.2.

The title compound, $\text{C}_{50}\text{H}_{44}$, is a derivative of rubrene in which *tert*-butyl side groups are added to two of the pendant aromatic rings. The complete molecule is generated by a mirror plane, and the unsubstituted and substituted pendant aromatic rings are almost perpendicular to the main backbone of the molecule, which is essentially planar.

Related literature

For related literature, see: Dodge *et al.* (1990); Goldmann *et al.* (2004); Jurchescu *et al.* (2006); Kloc *et al.* (1997); Laudise *et al.* (1998); Stassen *et al.* (2007); Sundar *et al.* (2004).



Experimental

Crystal data

$\text{C}_{50}\text{H}_{44}$
 $M_r = 644.90$
 Orthorhombic, $Pnma$
 $a = 14.158$ (2) Å

$b = 35.390$ (5) Å
 $c = 7.2215$ (11) Å
 $V = 3618.4$ (9) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹

$T = 292$ (1) K
 $0.80 \times 0.32 \times 0.06$ mm

Data collection

Siemens SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996; Blessing, 1995)
 $T_{\min} = 0.988$, $T_{\max} = 0.996$

28135 measured reflections
 3446 independent reflections
 2208 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.060$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.074$
 $wR(F^2) = 0.207$
 $S = 1.15$
 3446 reflections
 282 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.44$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.40$ 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 Würle (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: HB2400).

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supplementary materials

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

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Comment

The electronic properties of rubrene and rubrene derivatives are of great interest owing to fundamental questions on electron transport and associated applications (Sundar *et al.*, 2004; Goldmann *et al.*, 2004). The electric transport properties will be published elsewhere (Stassen *et al.*, 2007).

The crystal structure of the title compound is orthorhombic, with space group *Pnma*. The unit cell contains four molecules (Fig. 1). In (I), the in-plane arrangement of the molecules is very similar to that of rubrene (Jurchescu *et al.*, 2006). Noteworthy is the somewhat shorter distance of 3.55 Å between the naphthacene backbones compared to 3.74 Å in rubrene. However, the addition of the *t*-butyl groups increases the inter-layer spacing by 31%. Interestingly, it leaves the backbone almost perfectly planar (Fig. 2). Both the pendant aromatic rings are almost perpendicular to the main backbone of the molecule: atoms C20—C25 and C30—C35 make dihedral angles of 85.04 (13)° and 84.55 (11)°, respectively, with the backbone carbon atoms.

Experimental

The title compound was synthesized according to the method of Dodge *et al.* (1990). Single crystals of (I) were grown by physical vapour transport (Kloc *et al.*, 1997, Laudise *et al.*, 1998) at 533 K using high purity argon as the transport gas.

Refinement

The H atoms in the aromatic units were located in difference maps and were refined freely along with individual isotropic displacement parameters. The H atoms of the methyl groups were positioned geometrically and were refined as riding on the parent C atoms, $U_{\text{iso}}(\text{H})$ values were set at 1.2 U_{eq} of the parent atom.

Figures

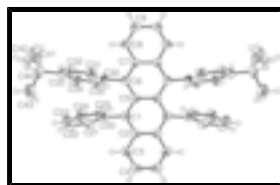


Fig. 1. The molecular structure of (I), showing displacement ellipsoids at the 50% probability level (arbitrary spheres for the H atoms). The unlabelled atoms are generated by the symmetry operation $(x, 3/2-y, z)$.

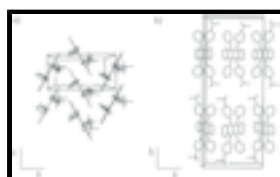


Fig. 2. The crystal packing of the title compound, viewed (a) down the *b* axis and (b) viewed down the *c* axis.

supplementary materials

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

Crystal data

$C_{50}H_{44}$	$F_{000} = 1376$
$M_r = 644.90$	$D_x = 1.184 \text{ Mg m}^{-3}$
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation
Hall symbol: -P 2ac 2n	$\lambda = 0.71073 \text{ \AA}$
$a = 14.158 (2) \text{ \AA}$	Cell parameters from 3136 reflections
$b = 35.390 (5) \text{ \AA}$	$\theta = 3.0\text{--}25.0^\circ$
$c = 7.2215 (11) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$V = 3618.4 (9) \text{ \AA}^3$	$T = 292 (1) \text{ K}$
$Z = 4$	Plate, translucent orange
	$0.80 \times 0.32 \times 0.06 \text{ mm}$

Data collection

Siemens SMART CCD area-detector diffractometer	3446 independent reflections
Radiation source: fine-focus sealed tube	2208 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.060$
$T = 292(1) \text{ K}$	$\theta_{\text{max}} = 25.6^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.2^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996; Blessing, 1995)	$h = -17 \rightarrow 17$
$T_{\text{min}} = 0.988$, $T_{\text{max}} = 0.996$	$k = -42 \rightarrow 42$
28135 measured reflections	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0891P)^2 + 1.9474P]$
$R[F^2 > 2\sigma(F^2)] = 0.074$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.207$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.15$	$\Delta\rho_{\text{max}} = 0.44 \text{ e \AA}^{-3}$
3446 reflections	$\Delta\rho_{\text{min}} = -0.40 \text{ e \AA}^{-3}$
282 parameters	Extinction correction: SHELXL97,
Primary atom site location: structure-invariant direct methods	$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0146 (15)
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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.93705 (17)	0.70977 (7)	0.3527 (4)	0.0340 (6)
C2	0.89917 (17)	0.72967 (7)	0.2033 (3)	0.0350 (6)
C3	0.85410 (19)	0.71093 (9)	0.0504 (4)	0.0424 (7)
C5	0.98466 (18)	0.72940 (7)	0.4982 (3)	0.0317 (6)
C6	1.03201 (17)	0.70973 (7)	0.6438 (4)	0.0326 (6)
C8	1.11360 (19)	0.71085 (9)	0.9468 (4)	0.0396 (7)
C7	1.06983 (17)	0.72991 (7)	0.7940 (3)	0.0320 (6)
C4	0.8150 (2)	0.73005 (9)	-0.0912 (4)	0.0479 (8)
C9	1.1524 (2)	0.73011 (8)	1.0896 (4)	0.0440 (7)
H8	1.1141 (19)	0.6838 (8)	0.942 (4)	0.043 (8)*
H3	0.8547 (19)	0.6831 (8)	0.045 (4)	0.045 (8)*
H31	0.948 (2)	0.6491 (8)	0.807 (4)	0.051 (8)*
H34	1.219 (3)	0.6126 (10)	0.480 (5)	0.074 (11)*
H25	0.798 (2)	0.6770 (9)	0.527 (5)	0.068 (10)*
H32	1.000 (2)	0.5855 (9)	0.807 (5)	0.067 (10)*
H24	0.745 (3)	0.6144 (11)	0.534 (6)	0.092 (13)*
H35	1.171 (2)	0.6769 (8)	0.470 (4)	0.055 (9)*
H21	1.019 (3)	0.6479 (9)	0.194 (5)	0.070 (10)*
H23	0.828 (3)	0.5687 (11)	0.359 (5)	0.081 (11)*
H4	0.787 (2)	0.7156 (8)	-0.197 (4)	0.047 (8)*
H22	0.964 (3)	0.5854 (10)	0.196 (5)	0.082 (12)*
H9	1.179 (2)	0.7171 (8)	1.191 (4)	0.057 (9)*
C20	0.91358 (19)	0.66864 (7)	0.3598 (4)	0.0387 (7)
C30	1.05447 (18)	0.66849 (7)	0.6373 (4)	0.0361 (6)
C31	1.0058 (2)	0.64137 (8)	0.7376 (4)	0.0446 (7)
C21	0.9614 (2)	0.64110 (8)	0.2608 (4)	0.0503 (8)
C35	1.1346 (2)	0.65679 (8)	0.5419 (4)	0.0455 (7)
C25	0.8324 (2)	0.65765 (9)	0.4549 (5)	0.0508 (8)
C24	0.8020 (3)	0.62075 (10)	0.4534 (6)	0.0681 (10)
C34	1.1634 (2)	0.61949 (9)	0.5450 (5)	0.0569 (9)
C32	1.0352 (3)	0.60433 (9)	0.7392 (5)	0.0539 (8)
C33	1.1156 (2)	0.59238 (8)	0.6449 (5)	0.0553 (9)
C22	0.9308 (3)	0.60409 (10)	0.2607 (6)	0.0661 (10)

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C23	0.8510 (3)	0.59405 (11)	0.3566 (6)	0.0745 (11)
C40	1.1464 (3)	0.55077 (10)	0.6420 (6)	0.0786 (12)
C42	1.1059 (6)	0.52857 (12)	0.8005 (9)	0.167 (3)
H42A	1.0383	0.5278	0.7896	0.200*
H42B	1.1229	0.5404	0.9153	0.200*
H42C	1.1305	0.5033	0.7979	0.200*
C41	1.2544 (4)	0.54734 (13)	0.6482 (8)	0.121 (2)
H41A	1.2777	0.5588	0.7596	0.146*
H41B	1.2811	0.5599	0.5427	0.146*
H41C	1.2719	0.5211	0.6463	0.146*
C43	1.1162 (4)	0.53380 (12)	0.4580 (8)	0.129 (2)
H43A	1.1357	0.5078	0.4524	0.155*
H43B	1.1450	0.5476	0.3585	0.155*
H43C	1.0487	0.5352	0.4467	0.155*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0293 (14)	0.0368 (14)	0.0360 (15)	0.0011 (10)	0.0026 (11)	-0.0043 (12)
C2	0.0258 (14)	0.0460 (14)	0.0331 (15)	-0.0011 (11)	0.0012 (11)	-0.0022 (11)
C3	0.0375 (16)	0.0488 (18)	0.0410 (17)	0.0013 (13)	-0.0007 (13)	-0.0089 (14)
C5	0.0271 (12)	0.0350 (13)	0.0331 (13)	0.0012 (11)	0.0014 (10)	0.0001 (12)
C6	0.0292 (13)	0.0346 (14)	0.0339 (14)	-0.0016 (10)	0.0021 (11)	0.0007 (11)
C8	0.0377 (16)	0.0435 (17)	0.0377 (16)	0.0012 (12)	-0.0028 (12)	0.0048 (13)
C7	0.0269 (13)	0.0370 (13)	0.0321 (14)	-0.0001 (10)	0.0018 (11)	0.0020 (11)
C4	0.0404 (17)	0.0676 (19)	0.0359 (16)	-0.0018 (14)	-0.0066 (13)	-0.0082 (14)
C9	0.0391 (16)	0.0563 (17)	0.0365 (16)	0.0014 (13)	-0.0064 (13)	0.0074 (13)
C20	0.0406 (15)	0.0393 (15)	0.0361 (15)	-0.0003 (12)	-0.0070 (12)	-0.0027 (12)
C30	0.0362 (15)	0.0365 (14)	0.0355 (15)	0.0005 (11)	-0.0061 (12)	0.0030 (12)
C31	0.0508 (19)	0.0387 (16)	0.0443 (17)	0.0015 (13)	0.0038 (14)	0.0042 (13)
C21	0.061 (2)	0.0449 (18)	0.0454 (18)	0.0049 (15)	0.0008 (16)	-0.0076 (15)
C35	0.0405 (17)	0.0431 (17)	0.0529 (18)	0.0015 (13)	0.0033 (14)	0.0020 (14)
C25	0.0416 (17)	0.0468 (18)	0.064 (2)	-0.0018 (14)	0.0005 (15)	0.0016 (16)
C24	0.062 (2)	0.054 (2)	0.088 (3)	-0.0155 (18)	-0.002 (2)	0.008 (2)
C34	0.0497 (19)	0.0500 (19)	0.071 (2)	0.0126 (15)	0.0013 (17)	-0.0047 (17)
C32	0.073 (2)	0.0387 (17)	0.0505 (19)	-0.0047 (16)	0.0000 (17)	0.0070 (15)
C33	0.071 (2)	0.0374 (16)	0.058 (2)	0.0110 (15)	-0.0107 (17)	-0.0009 (15)
C22	0.095 (3)	0.0441 (19)	0.060 (2)	0.010 (2)	-0.012 (2)	-0.0107 (18)
C23	0.092 (3)	0.045 (2)	0.087 (3)	-0.020 (2)	-0.018 (2)	0.002 (2)
C40	0.110 (3)	0.0417 (19)	0.084 (3)	0.023 (2)	-0.014 (2)	-0.0067 (19)
C42	0.281 (9)	0.049 (3)	0.171 (6)	0.058 (4)	0.069 (6)	0.049 (3)
C41	0.135 (5)	0.080 (3)	0.150 (5)	0.061 (3)	-0.029 (4)	-0.014 (3)
C43	0.169 (5)	0.060 (3)	0.158 (5)	0.033 (3)	-0.051 (4)	-0.044 (3)

Geometric parameters (\AA , $^\circ$)

C1—C2	1.396 (4)	C35—C34	1.382 (4)
C1—C5	1.429 (4)	C35—H35	1.02 (3)
C1—C20	1.494 (4)	C25—C24	1.375 (4)

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C2—C3	1.437 (4)	C25—H25	0.99 (3)
C2—C2 ⁱ	1.439 (5)	C24—C23	1.365 (6)
C3—C4	1.345 (4)	C24—H24	1.02 (4)
C3—H3	0.99 (3)	C34—C33	1.378 (5)
C5—C6	1.428 (4)	C34—H34	0.95 (4)
C5—C5 ⁱ	1.458 (5)	C32—C33	1.392 (5)
C6—C7	1.405 (4)	C32—H32	0.97 (3)
C6—C30	1.495 (3)	C33—C40	1.536 (4)
C8—C9	1.353 (4)	C22—C23	1.371 (6)
C8—C7	1.434 (4)	C22—H22	0.94 (4)
C8—H8	0.96 (3)	C23—H23	0.96 (4)
C7—C7 ⁱ	1.422 (5)	C40—C42	1.502 (6)
C4—C4 ⁱ	1.412 (6)	C40—C43	1.520 (6)
C4—H4	1.00 (3)	C40—C41	1.534 (6)
C9—C9 ⁱ	1.408 (6)	C42—H42A	0.9600
C9—H9	0.95 (3)	C42—H42B	0.9600
C20—C21	1.385 (4)	C42—H42C	0.9600
C20—C25	1.395 (4)	C41—H41A	0.9600
C30—C31	1.386 (4)	C41—H41B	0.9600
C30—C35	1.390 (4)	C41—H41C	0.9600
C31—C32	1.376 (4)	C43—H43A	0.9600
C31—H31	1.00 (3)	C43—H43B	0.9600
C21—C22	1.380 (5)	C43—H43C	0.9600
C21—H21	0.98 (4)		
C2—C1—C5	120.3 (2)	C20—C25—H25	117.9 (19)
C2—C1—C20	115.6 (2)	C23—C24—C25	120.2 (4)
C5—C1—C20	123.6 (2)	C23—C24—H24	123 (2)
C1—C2—C3	122.1 (2)	C25—C24—H24	117 (2)
C1—C2—C2 ⁱ	120.30 (15)	C33—C34—C35	121.9 (3)
C3—C2—C2 ⁱ	117.48 (16)	C33—C34—H34	119 (2)
C4—C3—C2	122.3 (3)	C35—C34—H34	119 (2)
C4—C3—H3	118.4 (17)	C31—C32—C33	122.2 (3)
C2—C3—H3	119.3 (17)	C31—C32—H32	120 (2)
C6—C5—C1	121.7 (2)	C33—C32—H32	117.5 (19)
C6—C5—C5 ⁱ	119.17 (14)	C34—C33—C32	116.5 (3)
C1—C5—C5 ⁱ	119.09 (14)	C34—C33—C40	121.4 (3)
C7—C6—C5	120.0 (2)	C32—C33—C40	122.0 (3)
C7—C6—C30	116.1 (2)	C23—C22—C21	120.3 (4)
C5—C6—C30	123.6 (2)	C23—C22—H22	119 (2)
C9—C8—C7	121.7 (3)	C21—C22—H22	121 (2)
C9—C8—H8	121.8 (17)	C24—C23—C22	119.9 (3)
C7—C8—H8	116.6 (17)	C24—C23—H23	118 (2)
C6—C7—C7 ⁱ	120.55 (14)	C22—C23—H23	122 (2)
C6—C7—C8	121.3 (2)	C42—C40—C43	110.6 (4)
C7 ⁱ —C7—C8	118.05 (16)	C42—C40—C41	108.5 (5)
C3—C4—C4 ⁱ	120.20 (18)	C43—C40—C41	106.0 (4)

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C3—C4—H4	119.0 (16)	C42—C40—C33	112.5 (4)
C4 ⁱ —C4—H4	120.8 (16)	C43—C40—C33	108.1 (3)
C8—C9—C9 ⁱ	120.26 (18)	C41—C40—C33	111.0 (4)
C8—C9—H9	120.8 (19)	C40—C42—H42A	109.5
C9 ⁱ —C9—H9	119.0 (18)	C40—C42—H42B	109.5
C21—C20—C25	117.4 (3)	H42A—C42—H42B	109.5
C21—C20—C1	124.0 (3)	C40—C42—H42C	109.5
C25—C20—C1	118.2 (2)	H42A—C42—H42C	109.5
C31—C30—C35	117.3 (3)	H42B—C42—H42C	109.5
C31—C30—C6	123.7 (2)	C40—C41—H41A	109.5
C35—C30—C6	118.7 (2)	C40—C41—H41B	109.5
C32—C31—C30	120.9 (3)	H41A—C41—H41B	109.5
C32—C31—H31	120.2 (16)	C40—C41—H41C	109.5
C30—C31—H31	118.9 (16)	H41A—C41—H41C	109.5
C22—C21—C20	121.0 (3)	H41B—C41—H41C	109.5
C22—C21—H21	120 (2)	C40—C43—H43A	109.5
C20—C21—H21	119 (2)	C40—C43—H43B	109.5
C34—C35—C30	121.2 (3)	H43A—C43—H43B	109.5
C34—C35—H35	121.8 (17)	C40—C43—H43C	109.5
C30—C35—H35	117.1 (16)	H43A—C43—H43C	109.5
C24—C25—C20	121.2 (3)	H43B—C43—H43C	109.5
C24—C25—H25	121 (2)		

Symmetry codes: (i) $x, -y+3/2, z$.

Fig. 1

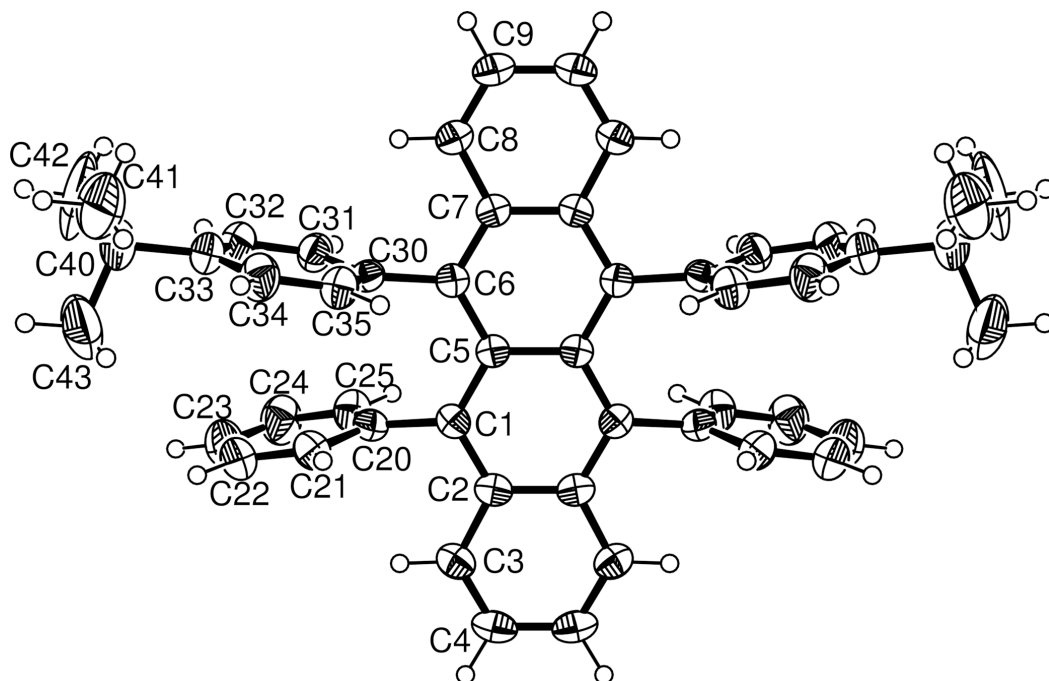


Fig. 2

