Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

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

**Götz Schuck,[a]* Simon Haas,[b] Arno F. Stassen,[b] Hans-Jörg Kirner[c] and Bertram Batlogg[b]**

[a]Laboratory for Neutron Scattering, ETH Zürich and Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, [b]Laboratory for Solid State Physics, ETH Zürich, Schafmattstrasse 16, CH-8093 Zürich, Switzerland, and [c]Ciba Specialty Chemistry Inc., CH-4002 Basel, Switzerland
Correspondence e-mail: goetz.schuck@psi.ch

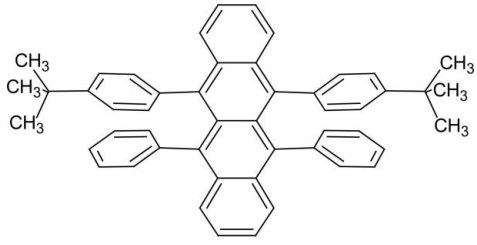
Received 27 April 2007; accepted 7 May 2007

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

The title compound, $C_{50}H_{44}$, 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*

$C_{50}H_{44}$
$M_r$ = 644.90
Orthorhombic, *Pnma*
$a$ = 14.158 (2) Å
$b$ = 35.390 (5) Å
$c$ = 7.2215 (11) Å
$V$ = 3618.4 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 292 (1) K
0.80 × 0.32 × 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 $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.44 e Å$^{-3}$
$\Delta\rho_{min}$ = −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 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: HB2400).

## References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (2000). *SAINT* (Version 6.02a) and *SMART* (Version 5.55). Bruker AXS Inc., Madison, Wisconsin, USA.
Dodge, J. A., Bain, J. D. & Chamberlin, A. R. (1990). *J. Org. Chem.* **55**, 4190–4198.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Goldmann, C., Haas, S., Krellner, C., Pernstich, K. P., Gundlach, D. J. & Batlogg, B. (2004). *J. Appl. Phys.* **96**, 2080–2086.
Jurchescu, O. D., Meetsma, A. & Palstra, T. T. M. (2006). *Acta Cryst.* B**62**, 330–334.
Kloc, C., Simpkins, P. G., Siegrist, T. & Laudise, R. A. (1997). *J. Cryst. Growth*, **182**, 416–427.
Laudise, R. A., Kloc, C., Simpkins, P. G. & Siegrist, T. (1998). *J. Cryst. Growth*, **187**, 449–454.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stassen, A. F., Haas, S., Schuck, G. & Batlogg, B. (2007). Unpublished results.
Sundar, V. C., Zaumseil, J., Podzorov, V., Menard, E., Willett, R. L., Someya, T., Gershenson, M. E. & Rogers, J. A. (2004). *Science*, **303**, 1644–1646.

# supplementary materials

*Acta Cryst.* (2007). E**63**, o2893 [ **doi:10.1107/S1600536807022489** ]

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

**G. Schuck, S. Haas, A. F. Stassen, H.-J. Kirner and B. Batlogg**

## 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 orthorombic, 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 mehthod 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, $U_{iso}$(H) values were set at 1.2$U_{eq}$ of the parent atom.

## Figures

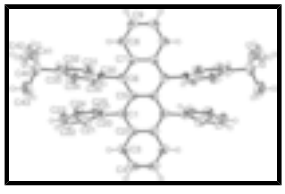


Fig. 1. The molecular structure of (I), showing displacement ellipsoids at the 50% probability level (arbitrary spheres for the H atoms). The unlabelled atoms are generated by the symmetry operation (x, 3/2-y, z).

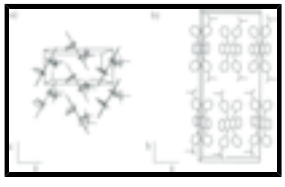


Fig. 2. The crystal packing of the title compound, viewed (a) down the b axis and (b) viewed down the c axis.

### 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 Mg m$^{-3}$ |
| Orthorhombic, *Pnma* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ac 2n | Cell parameters from 3136 reflections |
| *a* = 14.158 (2) Å | θ = 3.0–25.0º |
| *b* = 35.390 (5) Å | μ = 0.07 mm$^{-1}$ |
| *c* = 7.2215 (11) Å | *T* = 292 (1) K |
| *V* = 3618.4 (9) Å$^3$ | Plate, translucent orange |
| *Z* = 4 | 0.80 × 0.32 × 0.06 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 | $R_{int}$ = 0.060 |
| *T* = 292(1) K | $\theta_{max}$ = 25.6º |
| φ and ω scans | $\theta_{min}$ = 1.2º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996; Blessing, 1995) | *h* = −17→17 |
| $T_{min}$ = 0.988, $T_{max}$ = 0.996 | *k* = −42→42 |
| 28135 measured reflections | *l* = −8→8 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | H atoms treated by a mixture of independent and constrained refinement |
| Least-squares matrix: full | $w = 1/[\sigma^2(F_o^2) + (0.0891P)^2 + 1.9474P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.074 | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2)$ = 0.207 | $\Delta\rho_{max}$ = 0.44 e Å$^{-3}$ |
| *S* = 1.15 | $\Delta\rho_{min}$ = −0.40 e Å$^{-3}$ |
| 3446 reflections | Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| 282 parameters | Extinction coefficient: 0.0146 (15) |
| 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 | 0.93705 (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) |

| | | | | |
|---|---|---|---|---|
| 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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 (Å, °)*

| | | | |
|---|---|---|---|
| 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) |

| | | | |
|---|---|---|---|
| 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) |

| | | | |
|---|---|---|---|
| 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**

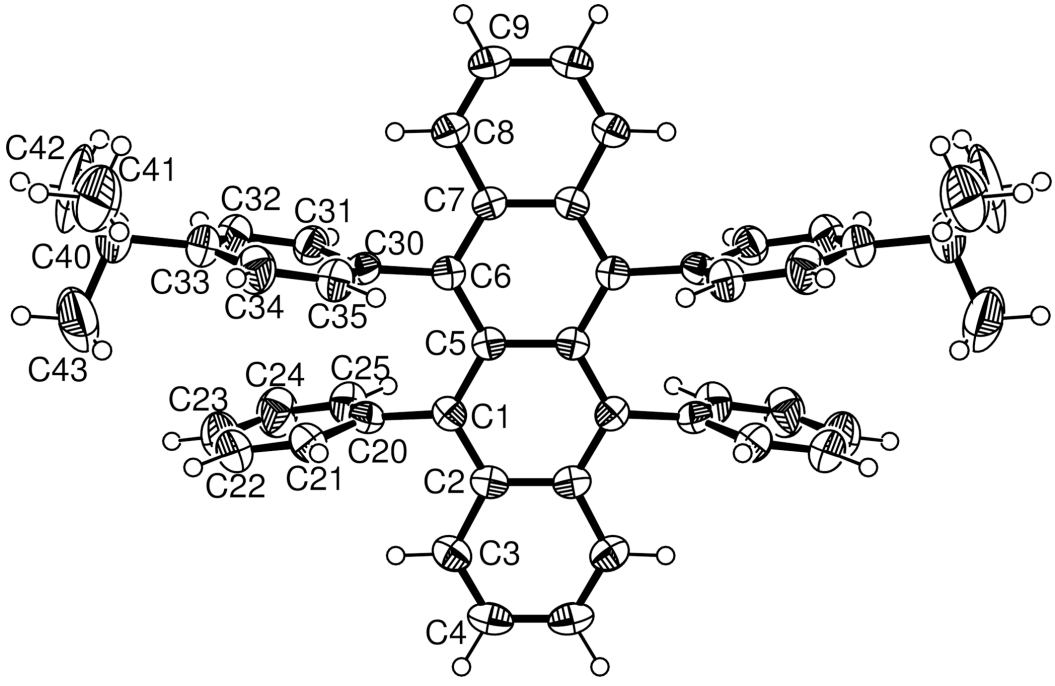

C9
C8
C42
C41
C32
C31
C7
C40
C30
C33
C6
C34
C35
C5
C43
C24
C25
C23
C1
C20
C22
C21
C2
C3
C4

**Fig. 2**