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## 1,3-Bis(propan-2-yl)naphthalene

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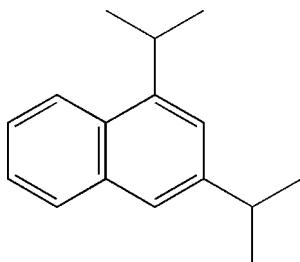
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Key indicators: single-crystal X-ray study;  $T = 150$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.046;  $wR$  factor = 0.108; data-to-parameter ratio = 19.0.

In the title compound,  $\text{C}_{16}\text{H}_{20}$ , one of the isopropyl groups shows almost equal displacements [1.252 (1) and  $-1.270$  (1) Å] of its methyl-C atoms from the mean plane of the naphthalene ring system, while the other shows asymmetric displacements [1.586 (2) and  $-0.315$  (1) Å]. In the crystal, the molecules are linked into sheets lying in the  $ab$  plane by three  $\text{C}-\text{H}\cdots\pi$  contacts, two involving donors belonging to the isopropyl groups and the third a donor atom from the naphthalene ring system. The different orientations of the isopropyl groups might be attributed to the fact that the  $\text{C}-\text{H}\cdots\pi$  interaction involving one of them is enhanced by the  $\text{C}-\text{H}\cdots\pi$  interaction involving the aromatic ring.

## Related literature

For background to diisopropylnaphthalenes, see: Addison (1983); Brzozowski *et al.* (2001); Collin *et al.* (2003).



## Experimental

## Crystal data

$\text{C}_{16}\text{H}_{20}$   
 $M_r = 212.32$   
Orthorhombic,  $Pbca$

$a = 16.1044$  (12) Å  
 $b = 8.2099$  (5) Å  
 $c = 19.0303$  (13) Å

$V = 2516.1$  (3) Å<sup>3</sup>  
 $Z = 8$   
Mo  $K\alpha$  radiation

$\mu = 0.06$  mm<sup>-1</sup>  
 $T = 150$  K  
 $0.22 \times 0.20 \times 0.04$  mm

## Data collection

Bruker SMART APEX CCD diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)  
 $T_{\min} = 0.986$ ,  $T_{\max} = 0.998$

12847 measured reflections  
2751 independent reflections  
2240 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.036$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.108$   
 $S = 1.04$   
2751 reflections

145 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.19$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.21$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$C_{g1}$  and  $C_{g2}$  are the centroids of the C1–C4/C9/C10 and C5–C10 rings, respectively.

| $D-H\cdots A$               | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------|-------|-------------|-------------|---------------|
| $C8-H8\cdots C_{g2}^i$      | 0.95  | 2.88        | 3.7399 (15) | 151           |
| $C11-H11\cdots C_{g1}^i$    | 1.00  | 2.98        | 3.8289 (13) | 144           |
| $C31-H31\cdots C_{g2}^{ii}$ | 1.00  | 2.68        | 3.6048 (14) | 155           |

Symmetry codes: (i)  $x, -y - \frac{3}{2}, z - \frac{1}{2}$ ; (ii)  $x + \frac{3}{2}, -y + \frac{1}{2}, -z$ .

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6496).

## References

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Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

## supporting information

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## 1,3-Bis(propan-2-yl)naphthalene

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### S1. Comment

Alkylated naphthalenes have a wide spectrum of applications, ranging from solvents, insulating material, heat transfer fluids, dye works auxiliary and specialty lubricants, (Collin *et al.*, 2003). Due to a variety of novel applications, diisopropyl naphthalene isomers have recently become of interest; they are used in the food packaging industry and as a plant growth regulator; furthermore, they have been introduced as PCB replacement fluids, (Addison, 1983). The application of diisopropyl naphthalene isomer mixtures as solvents for carbonless copy paper, in its formulation known as KMC - Kureha Micro Capsule Oil - is of special importance. Some aromatic surfactants are partially based on propylated naphthalenes whose isomeric mixtures are used as water repelling agents for a variety of applications, such as corrosion protections, marine paints, resins, inks, coatings, plasticizers, or electrical, electronic and mechanical applications.

The main components of diisopropyl naphthalene isomer mixtures are 2,6-diisopropyl naphthalene and 2,7-diisopropyl naphthalene, contributing each with *ca* 40% to the mixture, while a few percent are made of the 1,3-, 1,6- and 1,7-diisopropyl naphthalenes, (Brzozowski *et al.*, 2001). Diisopropyl naphthalenes with isopropyl groups positioned in adjacent ring positions are usually not detected in the mixtures. Separating all isomers or synthesizing them in pure form remains a challenging task.

The 1,3-isomer (I) is shown in Figure 1. The isopropyl methyl groups are oriented *cis* with respect to atom C2. The naphthalene-isopropyl torsion angles show that the orientations of the isopropyl groups around the C1—C11 and C3—C31 bonds with respect to the naphthalene ring is different in each case, *e.g.* C2—C1—C11—C111/C112 - 23.24 (17)°/100.54 (14)° and C2—C3—C31—C311/C312 64.27 (16)°/-60.14 (15)°. The orientation of the isopropyl group attached to C1 is unexpected in that unlike the group attached to C3 in which the hydrogen atom attached to C31 lies in the plane of the plane of the naphthalene ring that attached to C11 does not do so.

These orientations position the hydrogen atoms attached to C11 and C31 so that the molecules are linked by three C—H $\cdots\pi$  contacts to form a sheet lying in the *ab* plane, Table 1, Figure 2.

### S2. Experimental

Crystal of C<sub>16</sub>H<sub>20</sub> were obtained from Rütgers Novares GmbH, Duisburg, Germany, with a stated purity greater than 98 percent and used as such.

### S3. Refinement

Molecule (I) crystallized in the orthorhombic system; space group *Pbca* from the systematic absences. H atoms were treated as riding atoms with C—H(aromatic), 0.95 Å, C—H(aliphatic), 1.00 Å, with  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ , C—H(methyl), 0.98 Å, with  $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$ . The positions of the hydrogen atoms were confirmed in a final difference map.

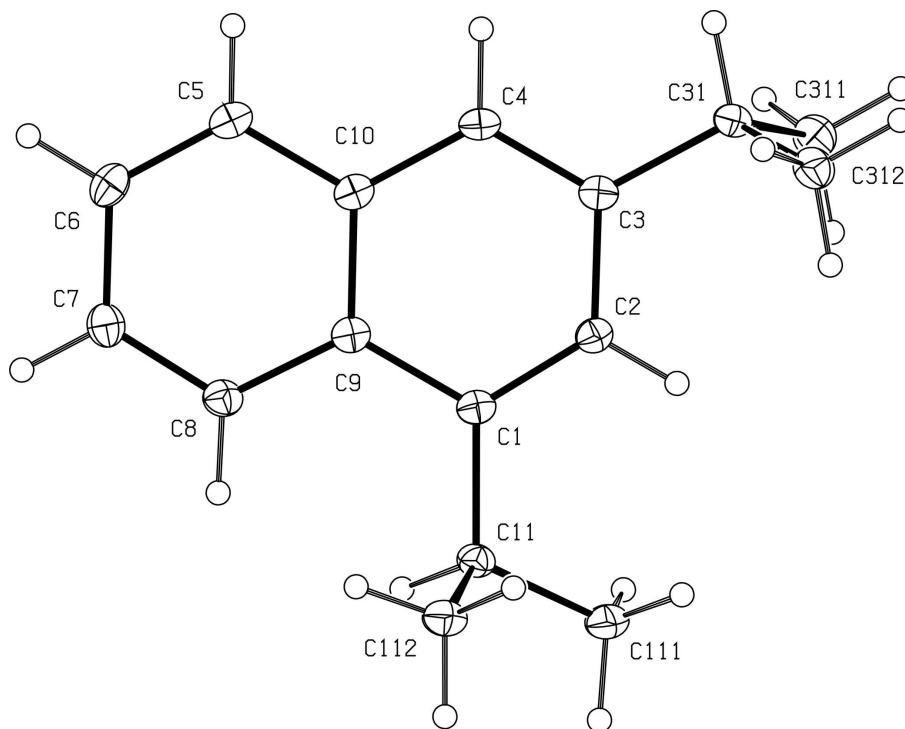


Figure 1

A view of (I) with displacement ellipsoids drawn at the 30% probability level.

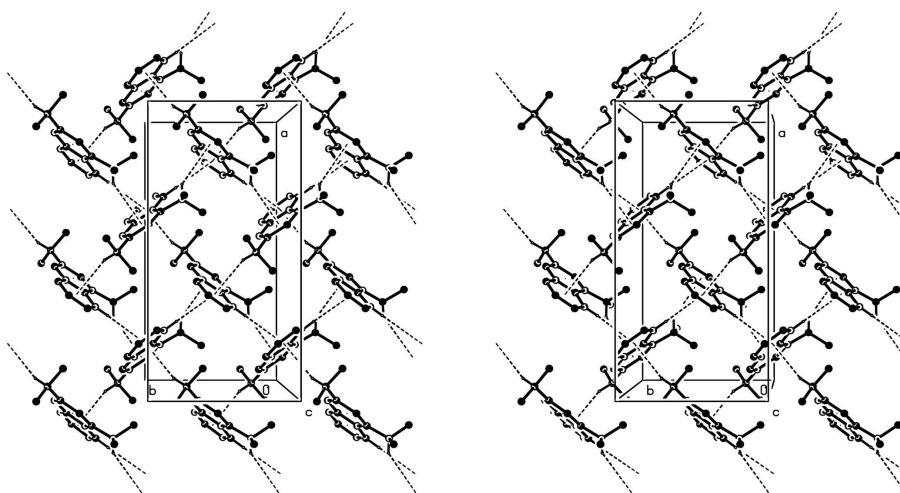


Figure 2

Stereoview of the sheet formed by C—H... $\pi$  interactions. Hydrogen atoms not involved in the motifs are not included.

### 1,3-Bis(propan-2-yl)naphthalene

#### Crystal data

$C_{16}H_{20}$

$M_r = 212.32$

Orthorhombic,  $Pbca$

$a = 16.1044$  (12) Å

$b = 8.2099$  (5) Å

$c = 19.0303$  (13) Å

$V = 2516.1$  (3) Å<sup>3</sup>

$Z = 8$

$F(000) = 928$

$D_x = 1.121$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 421 reflections  
 $\theta = 3.9\text{--}23.6^\circ$   
 $\mu = 0.06 \text{ mm}^{-1}$

$T = 150 \text{ K}$   
 Block, colourless  
 $0.22 \times 0.20 \times 0.04 \text{ mm}$

*Data collection*

Bruker SMART APEX CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 2003)  
 $T_{\min} = 0.986$ ,  $T_{\max} = 0.998$

12847 measured reflections  
 2751 independent reflections  
 2240 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.036$   
 $\theta_{\max} = 27.1^\circ$ ,  $\theta_{\min} = 2.5^\circ$   
 $h = -12 \rightarrow 20$   
 $k = -10 \rightarrow 8$   
 $l = -24 \rightarrow 18$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.108$   
 $S = 1.04$   
 2751 reflections  
 145 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 0.9272P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.19 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.21 \text{ e \AA}^{-3}$

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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  $F^2 > \sigma(F^2)$  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 ( $\text{\AA}^2$ )*

|      | <i>x</i>    | <i>y</i>     | <i>z</i>    | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|--------------|-------------|----------------------------------|
| C1   | 0.35224 (7) | 0.39257 (16) | 0.18964 (7) | 0.0211 (3)                       |
| C11  | 0.30803 (7) | 0.23796 (16) | 0.16559 (7) | 0.0230 (3)                       |
| H11  | 0.2519      | 0.2366       | 0.1881      | 0.028*                           |
| C111 | 0.29530 (9) | 0.22710 (18) | 0.08610 (7) | 0.0321 (3)                       |
| H11A | 0.2666      | 0.1252       | 0.0746      | 0.048*                           |
| H11B | 0.3494      | 0.2295       | 0.0625      | 0.048*                           |
| H11C | 0.2617      | 0.3196       | 0.0702      | 0.048*                           |
| C112 | 0.35537 (8) | 0.08727 (17) | 0.19147 (8) | 0.0288 (3)                       |
| H11D | 0.3266      | -0.0114      | 0.1758      | 0.043*                           |
| H11E | 0.3580      | 0.0885       | 0.2429      | 0.043*                           |
| H11F | 0.4118      | 0.0884       | 0.1722      | 0.043*                           |
| C2   | 0.40246 (7) | 0.47957 (16) | 0.14496 (7) | 0.0223 (3)                       |

|      |             |              |             |            |
|------|-------------|--------------|-------------|------------|
| H2   | 0.4066      | 0.4450       | 0.0974      | 0.027*     |
| C3   | 0.44854 (7) | 0.61884 (15) | 0.16637 (7) | 0.0221 (3) |
| C31  | 0.50394 (8) | 0.70740 (16) | 0.11426 (7) | 0.0250 (3) |
| H31  | 0.5322      | 0.7979       | 0.1400      | 0.030*     |
| C311 | 0.45361 (9) | 0.78327 (18) | 0.05444 (8) | 0.0332 (3) |
| H31A | 0.4912      | 0.8394       | 0.0220      | 0.050*     |
| H31B | 0.4138      | 0.8616       | 0.0738      | 0.050*     |
| H31C | 0.4236      | 0.6975       | 0.0292      | 0.050*     |
| C312 | 0.57143 (8) | 0.59413 (18) | 0.08548 (8) | 0.0314 (3) |
| H31D | 0.6061      | 0.6539       | 0.0519      | 0.047*     |
| H31E | 0.5454      | 0.5013       | 0.0618      | 0.047*     |
| H31F | 0.6060      | 0.5548       | 0.1243      | 0.047*     |
| C4   | 0.44313 (7) | 0.66789 (16) | 0.23492 (7) | 0.0225 (3) |
| H4   | 0.4738      | 0.7604       | 0.2500      | 0.027*     |
| C5   | 0.38868 (8) | 0.63261 (16) | 0.35543 (7) | 0.0257 (3) |
| H5   | 0.4211      | 0.7224       | 0.3708      | 0.031*     |
| C6   | 0.33889 (8) | 0.55295 (18) | 0.40250 (7) | 0.0283 (3) |
| H6   | 0.3372      | 0.5871       | 0.4502      | 0.034*     |
| C7   | 0.29021 (8) | 0.42038 (17) | 0.38021 (7) | 0.0274 (3) |
| H7   | 0.2546      | 0.3671       | 0.4127      | 0.033*     |
| C8   | 0.29370 (8) | 0.36748 (17) | 0.31199 (7) | 0.0245 (3) |
| H8   | 0.2609      | 0.2769       | 0.2981      | 0.029*     |
| C9   | 0.34551 (7) | 0.44543 (16) | 0.26157 (7) | 0.0211 (3) |
| C10  | 0.39261 (7) | 0.58325 (16) | 0.28397 (7) | 0.0216 (3) |

*Atomic displacement parameters (Å<sup>2</sup>)*

|      | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|------|------------|------------|------------|-------------|-------------|-------------|
| C1   | 0.0173 (6) | 0.0207 (6) | 0.0253 (7) | 0.0017 (5)  | -0.0029 (5) | -0.0020 (5) |
| C11  | 0.0196 (6) | 0.0224 (7) | 0.0270 (7) | -0.0032 (5) | 0.0008 (5)  | -0.0018 (6) |
| C111 | 0.0374 (8) | 0.0291 (8) | 0.0297 (8) | -0.0099 (6) | -0.0043 (6) | -0.0038 (6) |
| C112 | 0.0272 (7) | 0.0230 (7) | 0.0360 (8) | -0.0018 (6) | -0.0002 (6) | -0.0029 (6) |
| C2   | 0.0211 (6) | 0.0224 (7) | 0.0232 (6) | 0.0006 (5)  | -0.0012 (5) | -0.0023 (6) |
| C3   | 0.0198 (6) | 0.0203 (7) | 0.0261 (7) | 0.0007 (5)  | -0.0028 (5) | 0.0000 (5)  |
| C31  | 0.0275 (6) | 0.0212 (7) | 0.0261 (7) | -0.0054 (5) | -0.0002 (5) | -0.0001 (6) |
| C311 | 0.0401 (8) | 0.0279 (8) | 0.0317 (8) | 0.0006 (6)  | -0.0002 (6) | 0.0036 (6)  |
| C312 | 0.0277 (7) | 0.0324 (8) | 0.0342 (8) | -0.0036 (6) | 0.0050 (6)  | -0.0010 (7) |
| C4   | 0.0204 (6) | 0.0191 (6) | 0.0280 (7) | -0.0004 (5) | -0.0041 (5) | -0.0030 (5) |
| C5   | 0.0250 (6) | 0.0243 (7) | 0.0280 (7) | 0.0024 (5)  | -0.0045 (5) | -0.0052 (6) |
| C6   | 0.0276 (7) | 0.0324 (8) | 0.0248 (7) | 0.0061 (6)  | -0.0003 (5) | -0.0050 (6) |
| C7   | 0.0230 (6) | 0.0314 (8) | 0.0279 (7) | 0.0023 (6)  | 0.0032 (5)  | 0.0015 (6)  |
| C8   | 0.0193 (6) | 0.0257 (7) | 0.0285 (7) | -0.0005 (5) | -0.0005 (5) | -0.0017 (6) |
| C9   | 0.0164 (6) | 0.0212 (6) | 0.0257 (7) | 0.0035 (5)  | -0.0020 (5) | -0.0012 (5) |
| C10  | 0.0182 (6) | 0.0211 (7) | 0.0253 (7) | 0.0042 (5)  | -0.0035 (5) | -0.0024 (5) |

*Geometric parameters (Å, °)*

|                |             |                |             |
|----------------|-------------|----------------|-------------|
| C1—C2          | 1.3738 (18) | C311—H31A      | 0.9800      |
| C1—C9          | 1.4400 (18) | C311—H31B      | 0.9800      |
| C1—C11         | 1.5256 (18) | C311—H31C      | 0.9800      |
| C11—C111       | 1.5291 (19) | C312—H31D      | 0.9800      |
| C11—C112       | 1.5344 (19) | C312—H31E      | 0.9800      |
| C11—H11        | 1.0000      | C312—H31F      | 0.9800      |
| C111—H11A      | 0.9800      | C4—C10         | 1.4199 (18) |
| C111—H11B      | 0.9800      | C4—H4          | 0.9500      |
| C111—H11C      | 0.9800      | C5—C6          | 1.369 (2)   |
| C112—H11D      | 0.9800      | C5—C10         | 1.4203 (18) |
| C112—H11E      | 0.9800      | C5—H5          | 0.9500      |
| C112—H11F      | 0.9800      | C6—C7          | 1.407 (2)   |
| C2—C3          | 1.4228 (17) | C6—H6          | 0.9500      |
| C2—H2          | 0.9500      | C7—C8          | 1.3701 (19) |
| C3—C4          | 1.3680 (18) | C7—H7          | 0.9500      |
| C3—C31         | 1.5193 (18) | C8—C9          | 1.4236 (18) |
| C31—C311       | 1.5299 (19) | C8—H8          | 0.9500      |
| C31—C312       | 1.5318 (19) | C9—C10         | 1.4273 (18) |
| C31—H31        | 1.0000      |                |             |
| C2—C1—C9       | 118.42 (12) | C31—C311—H31A  | 109.5       |
| C2—C1—C11      | 121.44 (12) | C31—C311—H31B  | 109.5       |
| C9—C1—C11      | 120.05 (11) | H31A—C311—H31B | 109.5       |
| C1—C11—C111    | 114.07 (11) | C31—C311—H31C  | 109.5       |
| C1—C11—C112    | 110.04 (10) | H31A—C311—H31C | 109.5       |
| C111—C11—C112  | 109.70 (11) | H31B—C311—H31C | 109.5       |
| C1—C11—H11     | 107.6       | C31—C312—H31D  | 109.5       |
| C111—C11—H11   | 107.6       | C31—C312—H31E  | 109.5       |
| C112—C11—H11   | 107.6       | H31D—C312—H31E | 109.5       |
| C11—C111—H11A  | 109.5       | C31—C312—H31F  | 109.5       |
| C11—C111—H11B  | 109.5       | H31D—C312—H31F | 109.5       |
| H11A—C111—H11B | 109.5       | H31E—C312—H31F | 109.5       |
| C11—C111—H11C  | 109.5       | C3—C4—C10      | 121.29 (12) |
| H11A—C111—H11C | 109.5       | C3—C4—H4       | 119.4       |
| H11B—C111—H11C | 109.5       | C10—C4—H4      | 119.4       |
| C11—C112—H11D  | 109.5       | C6—C5—C10      | 121.09 (13) |
| C11—C112—H11E  | 109.5       | C6—C5—H5       | 119.5       |
| H11D—C112—H11E | 109.5       | C10—C5—H5      | 119.5       |
| C11—C112—H11F  | 109.5       | C5—C6—C7       | 119.93 (13) |
| H11D—C112—H11F | 109.5       | C5—C6—H6       | 120.0       |
| H11E—C112—H11F | 109.5       | C7—C6—H6       | 120.0       |
| C1—C2—C3       | 123.20 (12) | C8—C7—C6       | 120.54 (13) |
| C1—C2—H2       | 118.4       | C8—C7—H7       | 119.7       |
| C3—C2—H2       | 118.4       | C6—C7—H7       | 119.7       |
| C4—C3—C2       | 118.45 (12) | C7—C8—C9       | 121.34 (13) |
| C4—C3—C31      | 121.27 (12) | C7—C8—H8       | 119.3       |

|                |              |               |              |
|----------------|--------------|---------------|--------------|
| C2—C3—C31      | 120.26 (12)  | C9—C8—H8      | 119.3        |
| C3—C31—C311    | 111.68 (11)  | C8—C9—C10     | 117.81 (12)  |
| C3—C31—C312    | 111.07 (11)  | C8—C9—C1      | 123.32 (12)  |
| C311—C31—C312  | 110.93 (12)  | C10—C9—C1     | 118.87 (11)  |
| C3—C31—H31     | 107.7        | C4—C10—C5     | 121.02 (12)  |
| C311—C31—H31   | 107.7        | C4—C10—C9     | 119.74 (12)  |
| C312—C31—H31   | 107.7        | C5—C10—C9     | 119.24 (12)  |
|                |              |               |              |
| C2—C1—C11—C111 | -23.24 (17)  | C6—C7—C8—C9   | -0.8 (2)     |
| C9—C1—C11—C111 | 160.20 (12)  | C7—C8—C9—C10  | -1.32 (18)   |
| C2—C1—C11—C112 | 100.54 (14)  | C7—C8—C9—C1   | 178.96 (12)  |
| C9—C1—C11—C112 | -76.03 (14)  | C2—C1—C9—C8   | 178.25 (12)  |
| C9—C1—C2—C3    | 0.37 (18)    | C11—C1—C9—C8  | -5.08 (18)   |
| C11—C1—C2—C3   | -176.25 (11) | C2—C1—C9—C10  | -1.47 (17)   |
| C1—C2—C3—C4    | 0.52 (19)    | C11—C1—C9—C10 | 175.20 (11)  |
| C1—C2—C3—C31   | 179.01 (12)  | C3—C4—C10—C5  | 178.59 (12)  |
| C4—C3—C31—C311 | -117.29 (14) | C3—C4—C10—C9  | -0.82 (18)   |
| C2—C3—C31—C311 | 64.27 (16)   | C6—C5—C10—C4  | 178.83 (12)  |
| C4—C3—C31—C312 | 118.31 (14)  | C6—C5—C10—C9  | -1.76 (19)   |
| C2—C3—C31—C312 | -60.14 (15)  | C8—C9—C10—C4  | -178.04 (11) |
| C2—C3—C4—C10   | -0.29 (18)   | C1—C9—C10—C4  | 1.70 (17)    |
| C31—C3—C4—C10  | -178.76 (11) | C8—C9—C10—C5  | 2.54 (17)    |
| C10—C5—C6—C7   | -0.3 (2)     | C1—C9—C10—C5  | -177.73 (11) |
| C5—C6—C7—C8    | 1.6 (2)      |               |              |

#### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

Cg1 and Cg2 are the centroids of the C1—C4/C9/C10 and C5—C10 rings, respectively.

| $D-H\cdots A$                      | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------------|-------|-------------|-------------|---------------|
| C8—H8 $\cdots$ Cg2 <sup>i</sup>    | 0.95  | 2.88        | 3.7399 (15) | 151           |
| C11—H11 $\cdots$ Cg1 <sup>i</sup>  | 1.00  | 2.98        | 3.8289 (13) | 144           |
| C31—H31 $\cdots$ Cg2 <sup>ii</sup> | 1.00  | 2.68        | 3.6048 (14) | 155           |

Symmetry codes: (i)  $x, -y-3/2, z-1/2$ ; (ii)  $x+3/2, -y+1/2, -z$ .