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

# 9,9-Dibutyl-9*H*-fluorene-2-carbonitrile

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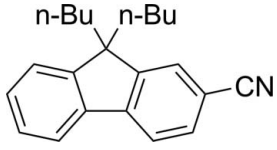
Received 30 April 2012; accepted 18 May 2012

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.068; $wR$ factor = 0.186; data-to-parameter ratio = 16.4.

The fluorene fragment of the title compound, $C_{22}H_{25}N$, is essentially planar, with an r.m.s deviation of the five-membered ring of 0.005 (2) Å. The dihedral angle between this ring and the outer benzene rings are 1.5 (2) and 0.7 (2)° while that between the benzene rings is 2.1 (2)°. The cyano group makes an angle of 0.3 (2)° with the attached benzene ring.

## Related literature

For applications of the title compound, including as a substrate in the synthesis of organic light-emitting materials, see: Jiang *et al.* (2012). For its synthesis, see: Omer *et al.* (2010). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{22}H_{25}N$ $M_r$ = 303.43
Triclinic, $P\overline{1}$
$a$ = 9.2810 (19) Å
$b$ = 9.994 (2) Å
$c$ = 11.885 (2) Å
$\alpha$ = 100.35 (3)°
$\beta$ = 96.73 (3)°
$\gamma$ = 117.42 (3)°
$V$ = 937.0 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.06 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.982, $T_{max}$ = 0.994
3652 measured reflections
3420 independent reflections
1875 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027
3 standard reflections every 200 reflections
intensity decay: 1%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.186
$S$ = 1.00
3420 reflections
208 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.13 e Å$^{-3}$

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *SET4* in *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank the Center of Testing and Analysis, Nanjing University, for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2373).

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# supporting information

*Acta Cryst.* (2012). E**68**, o1903 [doi:10.1107/S1600536812022672]

## 9,9-Dibutyl-9*H*-fluorene-2-carbonitrile

**Dong-dong Zhao, Peng Jiang and Hong-Jun Zhu**

### S1. Comment

The title compound, 2-cyano-9,9-dibutylfluorene, is an important compound which can be used in many fields such as a substrate in the synthesis of organic light-emitting materials (Jiang *et al.*, 2012). We report here the crystal structure of the title compound, (I).

The molecular structure of (I) is shown in Fig. 1. Bond lengths are within normal ranges (Allen *et al.*, 1987).

In the molecule of the title compound, the fluorene fragment of the title compound, $C_{22}H_{25}N$, is essentially planar with a r.m.s deviation of ring A (C1/C6/C7/C12/C13) of 0.005 (2). The dihedral angle between ring A (C1/C6/C7/C12/C13) and the benzene rings B (C1—C6) and C (C7—C12) is 1.5 (2)° and 0.7 (2)°, respectively. The dihedral angle between the benzene rings B and C is 2.1 (2)°. The angle of cyano group with the benzene ring B is 0.3 (2)°.

### S2. Experimental

The title compound,(I) was prepared according to the literature method (Omer *et al.*, 2010). Yellow block-shaped crystals were obtained by dissolving (I) (0.5 g, 1.04 mmol) in a mixed solution (10 ml petroleum ether and 1 ml EtOAc) and evaporating the solvent slowly at room temperature for about 5 d.

### S3. Refinement

All hydrogen atoms were positioned geometrically, with C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{iso}$(H) = $xU_{eq}$ (C), where $x$ = 1.2 for aromatic H, and $x$ = 1.5 for other H.

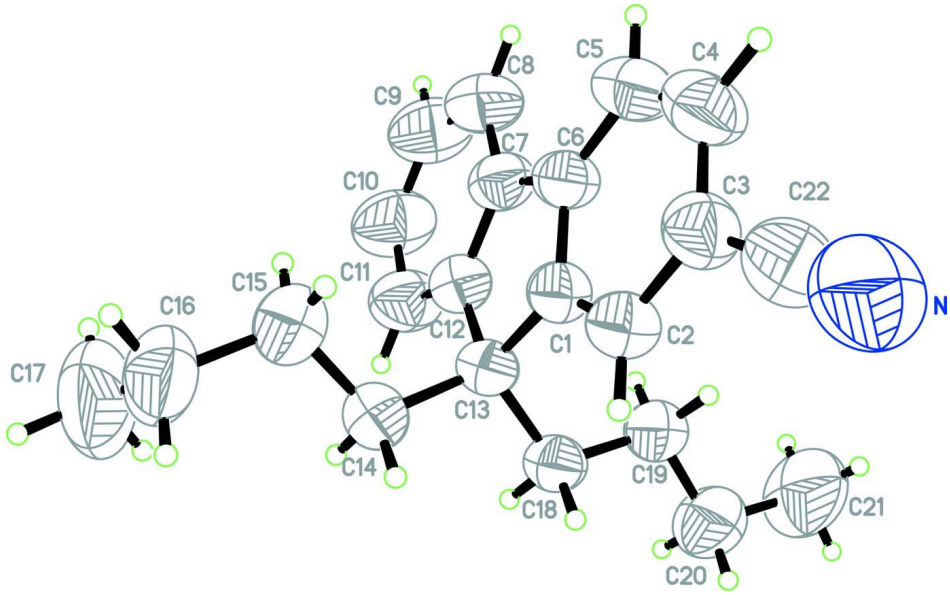


**Figure 1**

The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level.

### 9,9-Dibutyl-9*H*-fluorene-2-carbonitrile

*Crystal data*

$C_{22}H_{25}N$
$M_r = 303.43$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.2810\ (19)$ Å
$b = 9.994\ (2)$ Å
$c = 11.885\ (2)$ Å
$\alpha = 100.35\ (3)°$
$\beta = 96.73\ (3)°$
$\gamma = 117.42\ (3)°$
$V = 937.0\ (3)$ Å$^3$
$Z = 2$
$F(000) = 328$
$D_x = 1.075$ Mg m$^{-3}$
Melting point: 374 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–13°$
$\mu = 0.06$ mm$^{-1}$
$T = 293$ K
Block, yellow
0.30 × 0.20 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min} = 0.982$, $T_{max} = 0.994$
3652 measured reflections
3420 independent reflections
1875 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 25.4°$, $\theta_{min} = 1.8°$
$h = 0\rightarrow11$
$k = -12\rightarrow10$
$l = -14\rightarrow14$
3 standard reflections every 200 reflections
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.186$
$S = 1.00$
3420 reflections
208 parameters
1 restraint

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
$w = 1/[\sigma^2(F_o^2) + (0.070P)^2 + 0.3P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å$^{-3}$
$\Delta\rho_{min} = -0.13$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N | −0.2377 (4) | −0.2430 (4) | 0.3798 (3) | 0.1162 (11) |
| C1 | 0.2296 (3) | 0.0884 (3) | 0.2410 (2) | 0.0587 (7) |
| C2 | 0.1181 (3) | 0.0220 (3) | 0.3086 (2) | 0.0643 (7) |
| H2A | 0.1403 | 0.0698 | 0.3881 | 0.077* |
| C3 | −0.0281 (3) | −0.1178 (3) | 0.2548 (3) | 0.0692 (7) |
| C4 | −0.0608 (4) | −0.1901 (3) | 0.1362 (3) | 0.0816 (9) |
| H4A | −0.1594 | −0.2834 | 0.1014 | 0.098* |
| C5 | 0.0513 (4) | −0.1248 (3) | 0.0704 (3) | 0.0782 (9) |
| H5A | 0.0301 | −0.1742 | −0.0086 | 0.094* |
| C6 | 0.1966 (3) | 0.0153 (3) | 0.1223 (2) | 0.0624 (7) |
| C7 | 0.3335 (3) | 0.1124 (3) | 0.0740 (2) | 0.0658 (7) |
| C8 | 0.3608 (4) | 0.0907 (4) | −0.0388 (3) | 0.0875 (9) |
| H8A | 0.2854 | 0.0015 | −0.0980 | 0.105* |
| C9 | 0.5023 (5) | 0.2045 (5) | −0.0604 (3) | 0.1045 (12) |
| H9A | 0.5215 | 0.1928 | −0.1357 | 0.125* |
| C10 | 0.6160 (5) | 0.3356 (4) | 0.0274 (3) | 0.1079 (12) |
| H10A | 0.7116 | 0.4102 | 0.0110 | 0.130* |
| C11 | 0.5895 (4) | 0.3572 (4) | 0.1397 (3) | 0.0883 (10) |
| H11A | 0.6659 | 0.4461 | 0.1988 | 0.106* |
| C12 | 0.4472 (3) | 0.2443 (3) | 0.1626 (2) | 0.0652 (7) |
| C13 | 0.3936 (3) | 0.2420 (3) | 0.2785 (2) | 0.0587 (7) |
| C14 | 0.5202 (3) | 0.2379 (3) | 0.3724 (2) | 0.0684 (8) |
| H14A | 0.6249 | 0.3348 | 0.3892 | 0.082* |
| H14B | 0.4798 | 0.2341 | 0.4441 | 0.082* |
| C15 | 0.5545 (4) | 0.1028 (4) | 0.3405 (3) | 0.0891 (10) |
| H15A | 0.5793 | 0.0965 | 0.2633 | 0.107* |
| H15B | 0.4544 | 0.0062 | 0.3359 | 0.107* |
| C16 | 0.6984 (5) | 0.1167 (5) | 0.4276 (3) | 0.1128 (13) |
| H16A | 0.6845 | 0.1435 | 0.5066 | 0.135* |

| | | | | |
|---|---|---|---|---|
| H16B | 0.6929 | 0.0156 | 0.4143 | 0.135* |
| C17 | 0.8637 (6) | 0.2332 (7) | 0.4198 (5) | 0.166 (2) |
| H17A | 0.9473 | 0.2382 | 0.4789 | 0.248* |
| H17B | 0.8703 | 0.3337 | 0.4319 | 0.248* |
| H17C | 0.8819 | 0.2042 | 0.3435 | 0.248* |
| C18 | 0.3682 (3) | 0.3808 (3) | 0.3257 (2) | 0.0625 (7) |
| H18A | 0.3309 | 0.3698 | 0.3981 | 0.075* |
| H18B | 0.4755 | 0.4756 | 0.3451 | 0.075* |
| C19 | 0.2465 (4) | 0.4010 (3) | 0.2449 (2) | 0.0739 (8) |
| H19A | 0.1378 | 0.3081 | 0.2269 | 0.089* |
| H19B | 0.2819 | 0.4109 | 0.1718 | 0.089* |
| C20 | 0.2307 (5) | 0.5418 (4) | 0.2962 (3) | 0.1006 (11) |
| H20A | 0.2037 | 0.5355 | 0.3722 | 0.121* |
| H20B | 0.3378 | 0.6351 | 0.3089 | 0.121* |
| C21 | 0.1008 (6) | 0.5581 (6) | 0.2209 (4) | 0.1452 (17) |
| H21A | 0.0981 | 0.6498 | 0.2590 | 0.218* |
| H21B | −0.0064 | 0.4676 | 0.2095 | 0.218* |
| H21C | 0.1279 | 0.5672 | 0.1461 | 0.218* |
| C22 | −0.1465 (4) | −0.1884 (4) | 0.3242 (3) | 0.0849 (9) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N | 0.092 (2) | 0.094 (2) | 0.125 (3) | 0.0158 (18) | 0.039 (2) | 0.0225 (19) |
| C1 | 0.0596 (16) | 0.0563 (15) | 0.0570 (15) | 0.0306 (13) | 0.0061 (13) | 0.0067 (12) |
| C2 | 0.0649 (17) | 0.0584 (16) | 0.0611 (16) | 0.0283 (15) | 0.0085 (14) | 0.0062 (13) |
| C3 | 0.0641 (17) | 0.0559 (16) | 0.079 (2) | 0.0258 (14) | 0.0094 (14) | 0.0128 (14) |
| C4 | 0.074 (2) | 0.0562 (17) | 0.087 (2) | 0.0209 (16) | −0.0050 (18) | 0.0046 (16) |
| C5 | 0.087 (2) | 0.0663 (18) | 0.0619 (17) | 0.0320 (17) | 0.0012 (16) | 0.0007 (14) |
| C6 | 0.0681 (17) | 0.0559 (15) | 0.0562 (16) | 0.0317 (14) | 0.0023 (13) | 0.0031 (13) |
| C7 | 0.0797 (19) | 0.0696 (18) | 0.0539 (16) | 0.0437 (16) | 0.0139 (14) | 0.0105 (14) |
| C8 | 0.107 (3) | 0.083 (2) | 0.0657 (19) | 0.046 (2) | 0.0185 (18) | 0.0053 (16) |
| C9 | 0.134 (3) | 0.107 (3) | 0.076 (2) | 0.058 (3) | 0.047 (2) | 0.022 (2) |
| C10 | 0.118 (3) | 0.100 (3) | 0.097 (3) | 0.042 (2) | 0.053 (2) | 0.021 (2) |
| C11 | 0.084 (2) | 0.084 (2) | 0.080 (2) | 0.0303 (19) | 0.0287 (18) | 0.0086 (17) |
| C12 | 0.0658 (17) | 0.0667 (17) | 0.0613 (16) | 0.0340 (15) | 0.0142 (14) | 0.0091 (14) |
| C13 | 0.0553 (15) | 0.0584 (15) | 0.0524 (14) | 0.0254 (13) | 0.0067 (12) | 0.0032 (12) |
| C14 | 0.0605 (16) | 0.0752 (18) | 0.0640 (17) | 0.0334 (15) | 0.0085 (13) | 0.0092 (14) |
| C15 | 0.093 (2) | 0.094 (2) | 0.093 (2) | 0.060 (2) | 0.0151 (19) | 0.0181 (18) |
| C16 | 0.121 (3) | 0.146 (4) | 0.112 (3) | 0.097 (3) | 0.022 (2) | 0.039 (3) |
| C17 | 0.101 (3) | 0.239 (6) | 0.176 (5) | 0.105 (4) | 0.022 (3) | 0.048 (4) |
| C18 | 0.0583 (16) | 0.0606 (16) | 0.0571 (15) | 0.0246 (13) | 0.0107 (13) | 0.0043 (12) |
| C19 | 0.0756 (19) | 0.0799 (19) | 0.0663 (17) | 0.0441 (17) | 0.0084 (15) | 0.0081 (15) |
| C20 | 0.116 (3) | 0.099 (3) | 0.104 (3) | 0.073 (2) | 0.017 (2) | 0.014 (2) |
| C21 | 0.178 (4) | 0.184 (5) | 0.137 (4) | 0.143 (4) | 0.024 (3) | 0.043 (3) |
| C22 | 0.074 (2) | 0.064 (2) | 0.095 (2) | 0.0224 (17) | 0.0118 (18) | 0.0086 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N—C22 | 1.135 (4) | C13—C14 | 1.544 (3) |
| C1—C2 | 1.382 (3) | C14—C15 | 1.519 (4) |
| C1—C6 | 1.393 (3) | C14—H14A | 0.9700 |
| C1—C13 | 1.522 (3) | C14—H14B | 0.9700 |
| C2—C3 | 1.390 (4) | C15—C16 | 1.525 (4) |
| C2—H2A | 0.9300 | C15—H15A | 0.9700 |
| C3—C4 | 1.390 (4) | C15—H15B | 0.9700 |
| C3—C22 | 1.447 (4) | C16—C17 | 1.464 (5) |
| C4—C5 | 1.366 (4) | C16—H16A | 0.9700 |
| C4—H4A | 0.9300 | C16—H16B | 0.9700 |
| C5—C6 | 1.384 (4) | C17—H17A | 0.9600 |
| C5—H5A | 0.9300 | C17—H17B | 0.9600 |
| C6—C7 | 1.457 (4) | C17—H17C | 0.9600 |
| C7—C12 | 1.385 (4) | C18—C19 | 1.505 (4) |
| C7—C8 | 1.391 (4) | C18—H18A | 0.9700 |
| C8—C9 | 1.376 (4) | C18—H18B | 0.9700 |
| C8—H8A | 0.9300 | C19—C20 | 1.508 (4) |
| C9—C10 | 1.376 (5) | C19—H19A | 0.9700 |
| C9—H9A | 0.9300 | C19—H19B | 0.9700 |
| C10—C11 | 1.383 (4) | C20—C21 | 1.504 (5) |
| C10—H10A | 0.9300 | C20—H20A | 0.9700 |
| C11—C12 | 1.383 (4) | C20—H20B | 0.9700 |
| C11—H11A | 0.9300 | C21—H21A | 0.9600 |
| C12—C13 | 1.519 (3) | C21—H21B | 0.9600 |
| C13—C18 | 1.531 (3) | C21—H21C | 0.9600 |
| | | | |
| C2—C1—C6 | 120.5 (2) | C13—C14—H14B | 108.3 |
| C2—C1—C13 | 128.1 (2) | H14A—C14—H14B | 107.4 |
| C6—C1—C13 | 111.4 (2) | C14—C15—C16 | 113.8 (3) |
| C1—C2—C3 | 118.4 (2) | C14—C15—H15A | 108.8 |
| C1—C2—H2A | 120.8 | C16—C15—H15A | 108.8 |
| C3—C2—H2A | 120.8 | C14—C15—H15B | 108.8 |
| C2—C3—C4 | 120.9 (3) | C16—C15—H15B | 108.8 |
| C2—C3—C22 | 119.0 (3) | H15A—C15—H15B | 107.7 |
| C4—C3—C22 | 120.1 (3) | C17—C16—C15 | 114.2 (3) |
| C5—C4—C3 | 120.3 (3) | C17—C16—H16A | 108.7 |
| C5—C4—H4A | 119.8 | C15—C16—H16A | 108.7 |
| C3—C4—H4A | 119.8 | C17—C16—H16B | 108.7 |
| C4—C5—C6 | 119.5 (3) | C15—C16—H16B | 108.7 |
| C4—C5—H5A | 120.3 | H16A—C16—H16B | 107.6 |
| C6—C5—H5A | 120.3 | C16—C17—H17A | 109.5 |
| C5—C6—C1 | 120.3 (3) | C16—C17—H17B | 109.5 |
| C5—C6—C7 | 131.4 (3) | H17A—C17—H17B | 109.5 |
| C1—C6—C7 | 108.3 (2) | C16—C17—H17C | 109.5 |
| C12—C7—C8 | 120.8 (3) | H17A—C17—H17C | 109.5 |
| C12—C7—C6 | 108.5 (2) | H17B—C17—H17C | 109.5 |

| | | | |
|---|---|---|---|
| C8—C7—C6 | 130.7 (3) | C19—C18—C13 | 116.2 (2) |
| C9—C8—C7 | 118.3 (3) | C19—C18—H18A | 108.2 |
| C9—C8—H8A | 120.9 | C13—C18—H18A | 108.2 |
| C7—C8—H8A | 120.9 | C19—C18—H18B | 108.2 |
| C8—C9—C10 | 121.2 (3) | C13—C18—H18B | 108.2 |
| C8—C9—H9A | 119.4 | H18A—C18—H18B | 107.4 |
| C10—C9—H9A | 119.4 | C18—C19—C20 | 113.2 (2) |
| C9—C10—C11 | 120.6 (3) | C18—C19—H19A | 108.9 |
| C9—C10—H10A | 119.7 | C20—C19—H19A | 108.9 |
| C11—C10—H10A | 119.7 | C18—C19—H19B | 108.9 |
| C12—C11—C10 | 118.8 (3) | C20—C19—H19B | 108.9 |
| C12—C11—H11A | 120.6 | H19A—C19—H19B | 107.7 |
| C10—C11—H11A | 120.6 | C21—C20—C19 | 114.2 (3) |
| C11—C12—C7 | 120.3 (3) | C21—C20—H20A | 108.7 |
| C11—C12—C13 | 128.0 (2) | C19—C20—H20A | 108.7 |
| C7—C12—C13 | 111.7 (2) | C21—C20—H20B | 108.7 |
| C12—C13—C1 | 100.2 (2) | C19—C20—H20B | 108.7 |
| C12—C13—C18 | 112.8 (2) | H20A—C20—H20B | 107.6 |
| C1—C13—C18 | 111.7 (2) | C20—C21—H21A | 109.5 |
| C12—C13—C14 | 111.2 (2) | C20—C21—H21B | 109.5 |
| C1—C13—C14 | 111.3 (2) | H21A—C21—H21B | 109.5 |
| C18—C13—C14 | 109.4 (2) | C20—C21—H21C | 109.5 |
| C15—C14—C13 | 115.9 (2) | H21A—C21—H21C | 109.5 |
| C15—C14—H14A | 108.3 | H21B—C21—H21C | 109.5 |
| C13—C14—H14A | 108.3 | N—C22—C3 | 179.1 (4) |
| C15—C14—H14B | 108.3 | | |

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|---|---|---|---|
| C6—C1—C2—C3 | −0.8 (4) | C8—C7—C12—C13 | −179.0 (3) |
| C13—C1—C2—C3 | 177.7 (3) | C6—C7—C12—C13 | 1.0 (3) |
| C1—C2—C3—C4 | 0.6 (4) | C11—C12—C13—C1 | 179.9 (3) |
| C1—C2—C3—C22 | −179.7 (3) | C7—C12—C13—C1 | −0.8 (3) |
| C2—C3—C4—C5 | 0.3 (4) | C11—C12—C13—C18 | 61.0 (4) |
| C22—C3—C4—C5 | −179.4 (3) | C7—C12—C13—C18 | −119.7 (2) |
| C3—C4—C5—C6 | −1.0 (4) | C11—C12—C13—C14 | −62.3 (4) |
| C4—C5—C6—C1 | 0.8 (4) | C7—C12—C13—C14 | 117.0 (3) |
| C4—C5—C6—C7 | −178.0 (3) | C2—C1—C13—C12 | −178.5 (3) |
| C2—C1—C6—C5 | 0.1 (4) | C6—C1—C13—C12 | 0.2 (3) |
| C13—C1—C6—C5 | −178.7 (2) | C2—C1—C13—C18 | −58.7 (3) |
| C2—C1—C6—C7 | 179.2 (2) | C6—C1—C13—C18 | 119.9 (2) |
| C13—C1—C6—C7 | 0.4 (3) | C2—C1—C13—C14 | 63.9 (3) |
| C5—C6—C7—C12 | 178.1 (3) | C6—C1—C13—C14 | −117.5 (2) |
| C1—C6—C7—C12 | −0.9 (3) | C12—C13—C14—C15 | −56.8 (3) |
| C5—C6—C7—C8 | −1.9 (5) | C1—C13—C14—C15 | 54.0 (3) |
| C1—C6—C7—C8 | 179.1 (3) | C18—C13—C14—C15 | 177.9 (2) |
| C12—C7—C8—C9 | −0.9 (5) | C13—C14—C15—C16 | 171.4 (3) |
| C6—C7—C8—C9 | 179.1 (3) | C14—C15—C16—C17 | −74.2 (4) |
| C7—C8—C9—C10 | 1.2 (5) | C12—C13—C18—C19 | 56.3 (3) |
| C8—C9—C10—C11 | −1.0 (6) | C1—C13—C18—C19 | −55.7 (3) |

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|---|---|---|---|
| C9—C10—C11—C12 | 0.5 (6) | C14—C13—C18—C19 | −179.5 (2) |
| C10—C11—C12—C7 | −0.2 (5) | C13—C18—C19—C20 | −178.8 (3) |
| C10—C11—C12—C13 | 179.1 (3) | C18—C19—C20—C21 | −175.8 (3) |
| C8—C7—C12—C11 | 0.4 (4) | C2—C3—C22—N | −32 (24) |
| C6—C7—C12—C11 | −179.6 (3) | C4—C3—C22—N | 147 (24) |