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

# 4-(4-Chlorophenyl)-2,6-diphenylpyridine

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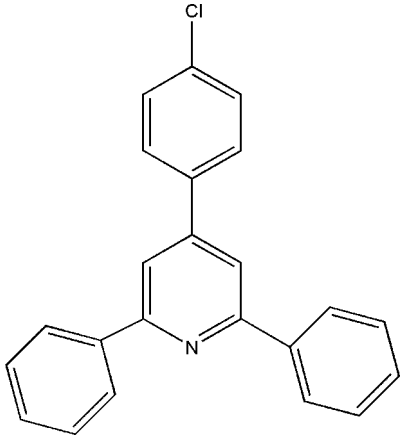
Received 22 November 2007; accepted 29 November 2007

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.048; $wR$ factor = 0.135; data-to-parameter ratio = 13.6.

In the title compound, $C_{23}H_{16}ClN$, the crystal packing exhibits no significantly short intermolecular contacts. The benzene rings show a disrotatory arrangement and the angles between them and the pyridine ring range from 20.80 (3) to 37.56 (4)°. The Cl atom deviates by 0.01 (3) Å from the plane of the benzene ring to which it is attached.

## Related literature

For the structure of 2,4,6-triphenylpyridine, see: Ondracek *et al.* (1994).




## Experimental

### Crystal data

$C_{23}H_{16}ClN$
$M_r$ = 341.82
Monoclinic, $P2_1/c$
$a$ = 9.3995 (11) Å
$b$ = 20.621 (2) Å
$c$ = 9.5362 (12) Å
$\beta$ = 108.146 (2)°
$V$ = 1756.4 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.22 mm$^{-1}$
$T$ = 298 (2) K
0.42 × 0.37 × 0.15 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.913, $T_{max}$ = 0.968
8674 measured reflections
3078 independent reflections
1752 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.135
$S$ = 1.02
3078 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the support of the National Natural Science Foundation of Liaocheng University (No. X051040).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AV2004).

## References

Ondrácek, J., Novotný, J., Petru, M., Lhoták, P. & Kuthan, J. (1994). *Acta Cryst.* C**50**, 1809–1811.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

# supporting information

*Acta Cryst.* (2008). E**64**, o186 [https://doi.org/10.1107/S1600536807064380]

## 4-(4-Chlorophenyl)-2,6-diphenylpyridine

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### S1. Comment

In this paper,we present a new crystal, 4-(4′-chlorophenyl)-2,6-diphenylpyridine, (I). In (I) (Fig. 1), the bond lengths and angles are normal and comparable to those observed in reported the compound (Ondracek *et al.*, 1994).

The three phenyl rings display a disrotatory conformation and form different angles with the pyridine ring. The phenyl ring attached at C1 forms the smallest angle with the heterocycle, 20.8°, because there is only the free electron pair of the N atom and one H atom in the *ortho* positions. The angle formed by the phenyl ring attached at C5 is slightly larger - 22.39°. The remaining phenyl ring forms the largest angle with the heterocycle, 37.56°. Meanwhile,the crystal packing demonstrates no significantly short intermolecular contacts.

### S2. Experimental

4-chlorobenzaldehyde (0.3 mmol) and acetophenone (0.6 mmol) under boron trifluoride ether (0.1 mmol) as a catalyst, the mixture was mixed in 50 ml flask. After irradiating for 3 min at 375 W, the mixture was cooled slowly to room temperature and the title compound was then recrystallized from ethanol, affording the title compound as a colorless crystalline solid. Elemental analysis: calculated for $C_{23}H_{16}ClN$: C 80.81, H 4.72, N 4.10%; found: C 80.68, H 4.75, N 4.14%.

### S3. Refinement

All H atoms were positioned geometrically, with C—H=0.93- 0.98 Å, and refined as riding, with $U_{iso}$(H)=1.2$U_{eq}$(C).

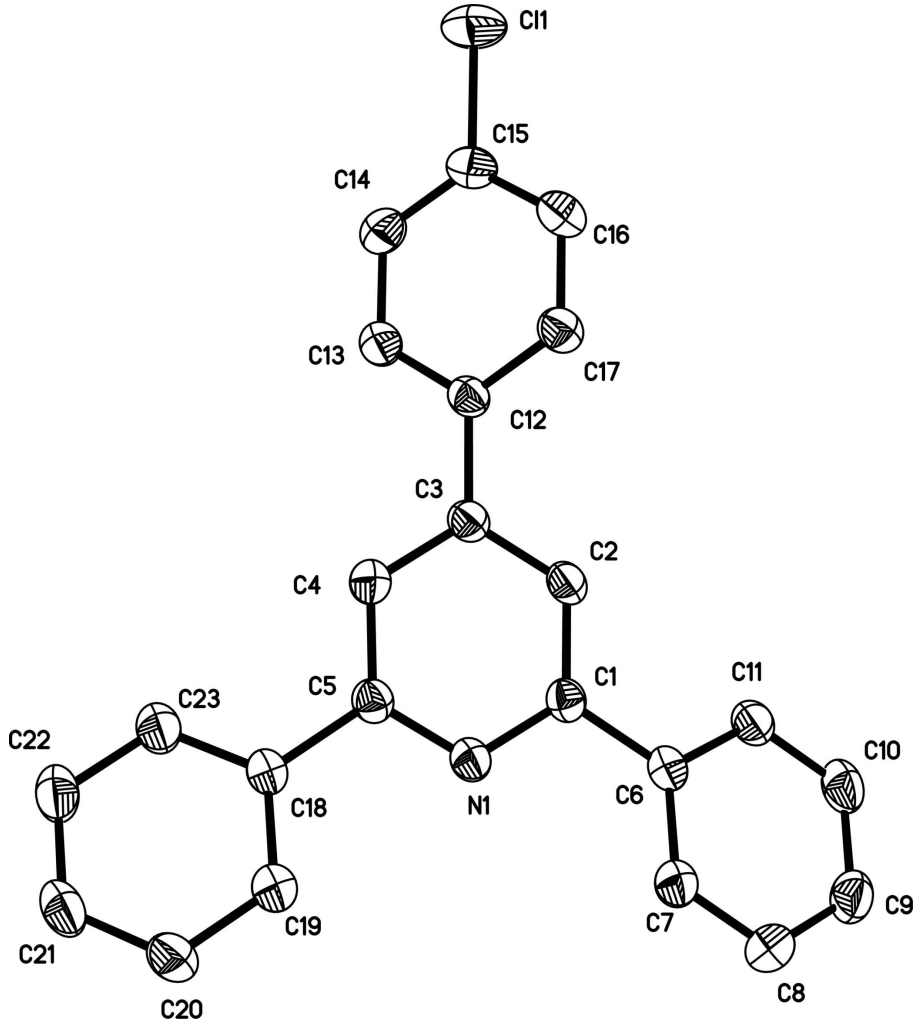


**Figure 1**

*ORTEP* drawing of the title compound with atom numbering scheme and thermal ellipsoids at 30% probability level.

**4-(4-Chlorophenyl)-2,6-diphenylpyridine**

*Crystal data*

$C_{23}H_{16}ClN$
$M_r = 341.82$
Monoclinic, $P2_1/c$
$a = 9.3995$ (11) Å
$b = 20.621$ (2) Å
$c = 9.5362$ (12) Å
$\beta = 108.146$ (2)°
$V = 1756.4$ (3) Å$^3$
$Z = 4$
$F(000) = 712$
$D_x = 1.293$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1970 reflections
$\theta = 2.3$–25.2°
$\mu = 0.22$ mm$^{-1}$
$T = 298$ K
Block, colourless
0.42 × 0.37 × 0.15 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.913$, $T_{max} = 0.968$

8674 measured reflections
3078 independent reflections
1752 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -7 \rightarrow 11$
$k = -24 \rightarrow 24$
$l = -11 \rightarrow 11$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.135$
$S = 1.02$
3078 reflections
226 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
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.2473P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å$^{-3}$
$\Delta\rho_{min} = -0.24$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.16106 (10) | 0.55491 (4) | 0.64505 (11) | 0.0785 (4) |
| N1 | 0.5484 (2) | 0.17758 (10) | 0.9845 (2) | 0.0446 (6) |
| C1 | 0.4223 (3) | 0.18225 (12) | 0.8698 (3) | 0.0416 (7) |
| C2 | 0.3630 (3) | 0.24170 (13) | 0.8142 (3) | 0.0448 (7) |
| H2 | 0.2764 | 0.2434 | 0.7337 | 0.054* |
| C3 | 0.4310 (3) | 0.29874 (12) | 0.8770 (3) | 0.0431 (7) |
| C4 | 0.5590 (3) | 0.29302 (13) | 0.9955 (3) | 0.0480 (7) |
| H4 | 0.6078 | 0.3301 | 1.0417 | 0.058* |
| C5 | 0.6160 (3) | 0.23244 (13) | 1.0465 (3) | 0.0438 (7) |
| C6 | 0.3495 (3) | 0.12018 (13) | 0.8094 (3) | 0.0438 (7) |
| C7 | 0.4301 (3) | 0.06274 (13) | 0.8358 (3) | 0.0527 (8) |
| H7 | 0.5311 | 0.0635 | 0.8906 | 0.063* |
| C8 | 0.3629 (4) | 0.00434 (15) | 0.7821 (4) | 0.0632 (9) |
| H8 | 0.4184 | −0.0338 | 0.8006 | 0.076* |
| C9 | 0.2147 (4) | 0.00284 (16) | 0.7020 (4) | 0.0645 (9) |
| H9 | 0.1695 | −0.0364 | 0.6656 | 0.077* |
| C10 | 0.1321 (3) | 0.05869 (16) | 0.6747 (3) | 0.0624 (9) |
| H10 | 0.0312 | 0.0573 | 0.6200 | 0.075* |
| C11 | 0.1988 (3) | 0.11723 (14) | 0.7284 (3) | 0.0526 (8) |
| H11 | 0.1420 | 0.1550 | 0.7100 | 0.063* |
| C12 | 0.3669 (3) | 0.36252 (12) | 0.8200 (3) | 0.0427 (7) |

| | | | | |
|---|---|---|---|---|
| C13 | 0.3699 (3) | 0.41388 (13) | 0.9151 (3) | 0.0508 (8) |
| H13 | 0.4152 | 0.4085 | 1.0160 | 0.061* |
| C14 | 0.3061 (3) | 0.47293 (14) | 0.8612 (4) | 0.0546 (8) |
| H14 | 0.3076 | 0.5070 | 0.9256 | 0.066* |
| C15 | 0.2407 (3) | 0.48093 (13) | 0.7123 (4) | 0.0500 (8) |
| C16 | 0.2377 (3) | 0.43147 (14) | 0.6161 (3) | 0.0532 (8) |
| H16 | 0.1939 | 0.4376 | 0.5152 | 0.064* |
| C17 | 0.3001 (3) | 0.37246 (13) | 0.6697 (3) | 0.0491 (8) |
| H17 | 0.2973 | 0.3387 | 0.6042 | 0.059* |
| C18 | 0.7568 (3) | 0.22443 (13) | 1.1695 (3) | 0.0441 (7) |
| C19 | 0.8387 (3) | 0.16759 (14) | 1.1839 (3) | 0.0563 (8) |
| H19 | 0.8018 | 0.1336 | 1.1187 | 0.068* |
| C20 | 0.9737 (3) | 0.16067 (15) | 1.2933 (4) | 0.0633 (9) |
| H20 | 1.0271 | 0.1221 | 1.3016 | 0.076* |
| C21 | 1.0291 (3) | 0.21002 (16) | 1.3893 (4) | 0.0622 (9) |
| H21 | 1.1217 | 0.2057 | 1.4614 | 0.075* |
| C22 | 0.9486 (4) | 0.26599 (16) | 1.3800 (4) | 0.0684 (10) |
| H22 | 0.9851 | 0.2993 | 1.4472 | 0.082* |
| C23 | 0.8133 (3) | 0.27280 (15) | 1.2707 (4) | 0.0651 (9) |
| H23 | 0.7591 | 0.3109 | 1.2652 | 0.078* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0786 (6) | 0.0582 (5) | 0.1004 (8) | 0.0210 (4) | 0.0301 (5) | 0.0221 (5) |
| N1 | 0.0400 (14) | 0.0478 (14) | 0.0423 (14) | 0.0003 (11) | 0.0075 (11) | −0.0008 (11) |
| C1 | 0.0391 (17) | 0.0479 (17) | 0.0373 (17) | 0.0008 (13) | 0.0112 (13) | −0.0030 (13) |
| C2 | 0.0404 (17) | 0.0510 (17) | 0.0380 (17) | 0.0031 (13) | 0.0050 (13) | 0.0015 (13) |
| C3 | 0.0408 (17) | 0.0454 (17) | 0.0411 (18) | 0.0035 (13) | 0.0098 (14) | 0.0015 (13) |
| C4 | 0.0449 (18) | 0.0458 (17) | 0.0489 (19) | −0.0022 (13) | 0.0080 (15) | −0.0029 (13) |
| C5 | 0.0387 (17) | 0.0480 (17) | 0.0432 (18) | 0.0008 (13) | 0.0106 (13) | −0.0014 (14) |
| C6 | 0.0407 (17) | 0.0517 (17) | 0.0369 (17) | −0.0026 (13) | 0.0091 (13) | 0.0008 (13) |
| C7 | 0.0480 (18) | 0.0540 (19) | 0.051 (2) | −0.0004 (15) | 0.0078 (14) | −0.0045 (15) |
| C8 | 0.072 (2) | 0.0497 (19) | 0.066 (2) | 0.0011 (16) | 0.0181 (19) | −0.0051 (16) |
| C9 | 0.074 (3) | 0.056 (2) | 0.057 (2) | −0.0182 (18) | 0.0115 (18) | −0.0064 (16) |
| C10 | 0.0508 (19) | 0.075 (2) | 0.052 (2) | −0.0160 (18) | 0.0023 (15) | 0.0003 (17) |
| C11 | 0.0493 (19) | 0.0562 (19) | 0.0466 (19) | −0.0013 (15) | 0.0069 (15) | 0.0036 (14) |
| C12 | 0.0371 (16) | 0.0458 (16) | 0.0428 (18) | 0.0012 (12) | 0.0090 (13) | 0.0042 (13) |
| C13 | 0.0524 (19) | 0.0510 (18) | 0.0454 (19) | 0.0024 (14) | 0.0100 (15) | −0.0012 (14) |
| C14 | 0.058 (2) | 0.0468 (18) | 0.061 (2) | 0.0002 (14) | 0.0202 (17) | −0.0057 (15) |
| C15 | 0.0457 (18) | 0.0511 (18) | 0.057 (2) | 0.0067 (13) | 0.0215 (16) | 0.0108 (15) |
| C16 | 0.0532 (19) | 0.063 (2) | 0.0435 (19) | 0.0119 (15) | 0.0147 (15) | 0.0077 (15) |
| C17 | 0.0497 (18) | 0.0534 (18) | 0.0438 (19) | 0.0077 (14) | 0.0140 (14) | 0.0008 (14) |
| C18 | 0.0391 (17) | 0.0496 (17) | 0.0411 (18) | −0.0013 (13) | 0.0087 (13) | −0.0008 (13) |
| C19 | 0.051 (2) | 0.0526 (19) | 0.057 (2) | 0.0014 (14) | 0.0049 (16) | −0.0033 (15) |
| C20 | 0.047 (2) | 0.062 (2) | 0.070 (2) | 0.0055 (15) | 0.0033 (17) | 0.0071 (18) |
| C21 | 0.0426 (19) | 0.078 (2) | 0.055 (2) | −0.0050 (17) | 0.0003 (15) | 0.0055 (18) |
| C22 | 0.060 (2) | 0.074 (2) | 0.058 (2) | −0.0034 (18) | 0.0004 (17) | −0.0150 (18) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C23 | 0.056 (2) | 0.062 (2) | 0.064 (2) | 0.0083 (16) | 0.0000 (17) | −0.0129 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C15 | 1.732 (3) | C11—H11 | 0.9300 |
| N1—C5 | 1.341 (3) | C12—C17 | 1.389 (4) |
| N1—C1 | 1.343 (3) | C12—C13 | 1.389 (4) |
| C1—C2 | 1.382 (3) | C13—C14 | 1.384 (4) |
| C1—C6 | 1.481 (4) | C13—H13 | 0.9300 |
| C2—C3 | 1.382 (4) | C14—C15 | 1.370 (4) |
| C2—H2 | 0.9300 | C14—H14 | 0.9300 |
| C3—C4 | 1.375 (4) | C15—C16 | 1.366 (4) |
| C3—C12 | 1.478 (3) | C16—C17 | 1.378 (4) |
| C4—C5 | 1.386 (3) | C16—H16 | 0.9300 |
| C4—H4 | 0.9300 | C17—H17 | 0.9300 |
| C5—C18 | 1.479 (4) | C18—C23 | 1.374 (4) |
| C6—C7 | 1.386 (4) | C18—C19 | 1.385 (4) |
| C6—C11 | 1.387 (3) | C19—C20 | 1.376 (4) |
| C7—C8 | 1.382 (4) | C19—H19 | 0.9300 |
| C7—H7 | 0.9300 | C20—C21 | 1.359 (4) |
| C8—C9 | 1.365 (4) | C20—H20 | 0.9300 |
| C8—H8 | 0.9300 | C21—C22 | 1.368 (4) |
| C9—C10 | 1.368 (4) | C21—H21 | 0.9300 |
| C9—H9 | 0.9300 | C22—C23 | 1.378 (4) |
| C10—C11 | 1.383 (4) | C22—H22 | 0.9300 |
| C10—H10 | 0.9300 | C23—H23 | 0.9300 |
| | | | |
| C5—N1—C1 | 118.4 (2) | C17—C12—C3 | 120.8 (2) |
| N1—C1—C2 | 121.6 (2) | C13—C12—C3 | 121.0 (3) |
| N1—C1—C6 | 116.0 (2) | C14—C13—C12 | 120.7 (3) |
| C2—C1—C6 | 122.4 (2) | C14—C13—H13 | 119.7 |
| C1—C2—C3 | 120.8 (3) | C12—C13—H13 | 119.7 |
| C1—C2—H2 | 119.6 | C15—C14—C13 | 119.6 (3) |
| C3—C2—H2 | 119.6 | C15—C14—H14 | 120.2 |
| C4—C3—C2 | 116.8 (2) | C13—C14—H14 | 120.2 |
| C4—C3—C12 | 122.0 (2) | C16—C15—C14 | 121.0 (3) |
| C2—C3—C12 | 121.2 (2) | C16—C15—Cl1 | 119.5 (2) |
| C3—C4—C5 | 120.6 (3) | C14—C15—Cl1 | 119.5 (2) |
| C3—C4—H4 | 119.7 | C15—C16—C17 | 119.5 (3) |
| C5—C4—H4 | 119.7 | C15—C16—H16 | 120.3 |
| N1—C5—C4 | 121.8 (3) | C17—C16—H16 | 120.3 |
| N1—C5—C18 | 116.1 (2) | C16—C17—C12 | 121.1 (3) |
| C4—C5—C18 | 122.1 (2) | C16—C17—H17 | 119.4 |
| C7—C6—C11 | 118.0 (2) | C12—C17—H17 | 119.4 |
| C7—C6—C1 | 120.5 (2) | C23—C18—C19 | 117.6 (3) |
| C11—C6—C1 | 121.5 (2) | C23—C18—C5 | 122.0 (3) |
| C8—C7—C6 | 121.1 (3) | C19—C18—C5 | 120.4 (2) |
| C8—C7—H7 | 119.5 | C20—C19—C18 | 121.0 (3) |

| | | | |
|---|---|---|---|
| C6—C7—H7 | 119.5 | C20—C19—H19 | 119.5 |
| C9—C8—C7 | 119.8 (3) | C18—C19—H19 | 119.5 |
| C9—C8—H8 | 120.1 | C21—C20—C19 | 120.1 (3) |
| C7—C8—H8 | 120.1 | C21—C20—H20 | 119.9 |
| C8—C9—C10 | 120.5 (3) | C19—C20—H20 | 119.9 |
| C8—C9—H9 | 119.8 | C20—C21—C22 | 120.0 (3) |
| C10—C9—H9 | 119.8 | C20—C21—H21 | 120.0 |
| C9—C10—C11 | 120.0 (3) | C22—C21—H21 | 120.0 |
| C9—C10—H10 | 120.0 | C21—C22—C23 | 119.8 (3) |
| C11—C10—H10 | 120.0 | C21—C22—H22 | 120.1 |
| C10—C11—C6 | 120.7 (3) | C23—C22—H22 | 120.1 |
| C10—C11—H11 | 119.6 | C18—C23—C22 | 121.4 (3) |
| C6—C11—H11 | 119.6 | C18—C23—H23 | 119.3 |
| C17—C12—C13 | 118.1 (2) | C22—C23—H23 | 119.3 |