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2,6-Bis(4-methoxyphenyl)-4-phenylpyridine

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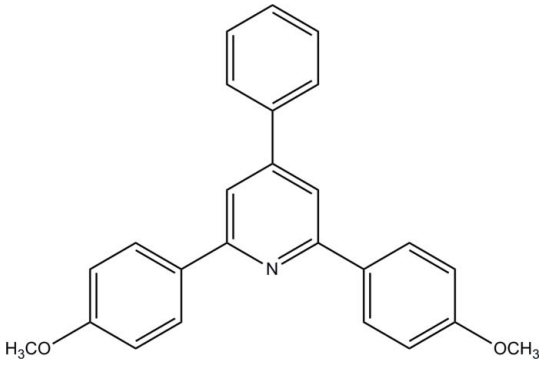
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.099; wR factor = 0.191; data-to-parameter ratio = 14.0.

In the title compound, $C_{25}H_{21}NO_2$, which was synthesized by the condensation of 2,6-bis(4-methoxyphenyl)-4-phenylpyridinium tetrafluoroborate with ammonia under microwave irradiation and solvent-free conditions, the angles between the central pyridine ring and the three benzene rings are 22.3 (2), 35.3 (2) and 19.8 (2)°. In the crystal, intermolecular C—H$\cdots\pi$ hydrogen-bond interactions link the molecules.

Related literature

For the biological properties of pyridines, see Keys & Hamilton (1987); Chen *et al.*(1995). For related structures, see: Ondráček *et al.* (1994).



Experimental

Crystal data

$C_{25}H_{21}NO_2$
M_r = 367.43
Monoclinic, $P2_1/n$
a = 6.379 (3) Å
b = 15.538 (8) Å
c = 20.51 (1) Å
β = 94.281 (7)°
V = 2027.3 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.41 × 0.18 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.994
10098 measured reflections
3566 independent reflections
1522 reflections with $I > 2\sigma(I)$
R_{int} = 0.109

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.099
$wR(F^2)$ = 0.191
S = 1.04
3566 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C25—H25$C\cdots Cg1^{i}$	0.96	2.82	3.605	140

Symmetry code: (i) $-x, -y, -z$. $Cg1$ is the centroid of the C19–C24 ring.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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 author acknowledges the support of the Foundation of Tianshui Normal University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2177).

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supporting information

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2,6-Bis(4-methoxyphenyl)-4-phenylpyridine

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S1. Comment

It was well known that pyridine ring systems have represented an important class of compounds not only for their theoretical interest but also because they displayed strong biological activity (Keys, *et al.*, 1987). Moreover, pyridine derivatives have remarkable versatility in synthetic organic chemistry as intermediates in the preparation of nature products and as ligands recently used in asymmetric synthesis (Chen, *et al.*, 1995).

In this paper, we present a new crystal, 2,6-bis(4′-methoxyphenyl)-4-phenylpyridine, (I), which was synthesized using benzaldehyde and 4-methoxylacetophenone as starting material.

In (I) (Fig. 1), the bond lengths and angles are normal and comparable to those observed in reported the compound (Ondráček *et al.*, 1994). The angles between the center pyridine ring and benzene rings (c6 - *c*11), (*c*13 - *c*18) and (*c*19 - *c*24) are 22.28 (19)°, 35.29 (18)° and 19.81 (20)°, respectively, which show the pyridine ring and three benzene rings aren't coplanar. Moreover, the crystal supramolecular structure was built from the connections of C—H···π hydrogen bonding interactions, as shown in Table 1 and Fig. 2.

S2. Experimental

Benzaldehyde (0.3 mmol) and 4-methoxylacetophenone (0.6 mmol), ammonia (1.0 mmol) under boron trifluoride ether (0.1 mmol) catalyzed, the mixture were mixed in 50 ml flash. After eradiating 3 min at 375 W, the mixture then cooled slowly to room temperature affording the title compound, then recrystallized from ethanol, affording the title compound as a colorless crystalline solid. Elemental analysis: calculated for $C_{25}H_{21}NO_2$: C 81.72, H 5.76, N 3.81%; found: C 81.68, H 5.75, N 3.72%.

S3. Refinement

All H atoms were positioned geometrically, with C—H=0.93- 0.96 Å, and refined as riding, with U_{iso}(H)=1.2–1.5U_{eq}(C).

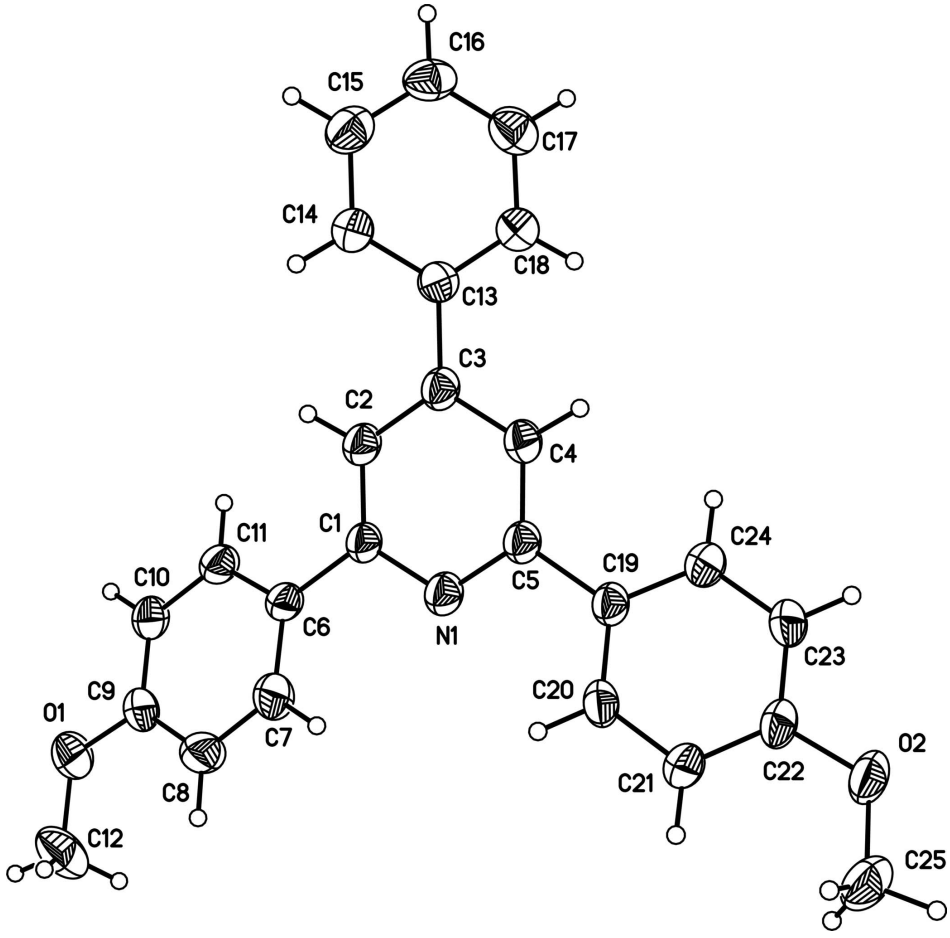

Figure 1

ORTEP drawing of the title complex with atomic numbering scheme and thermal ellipsoids at 30% probability level.

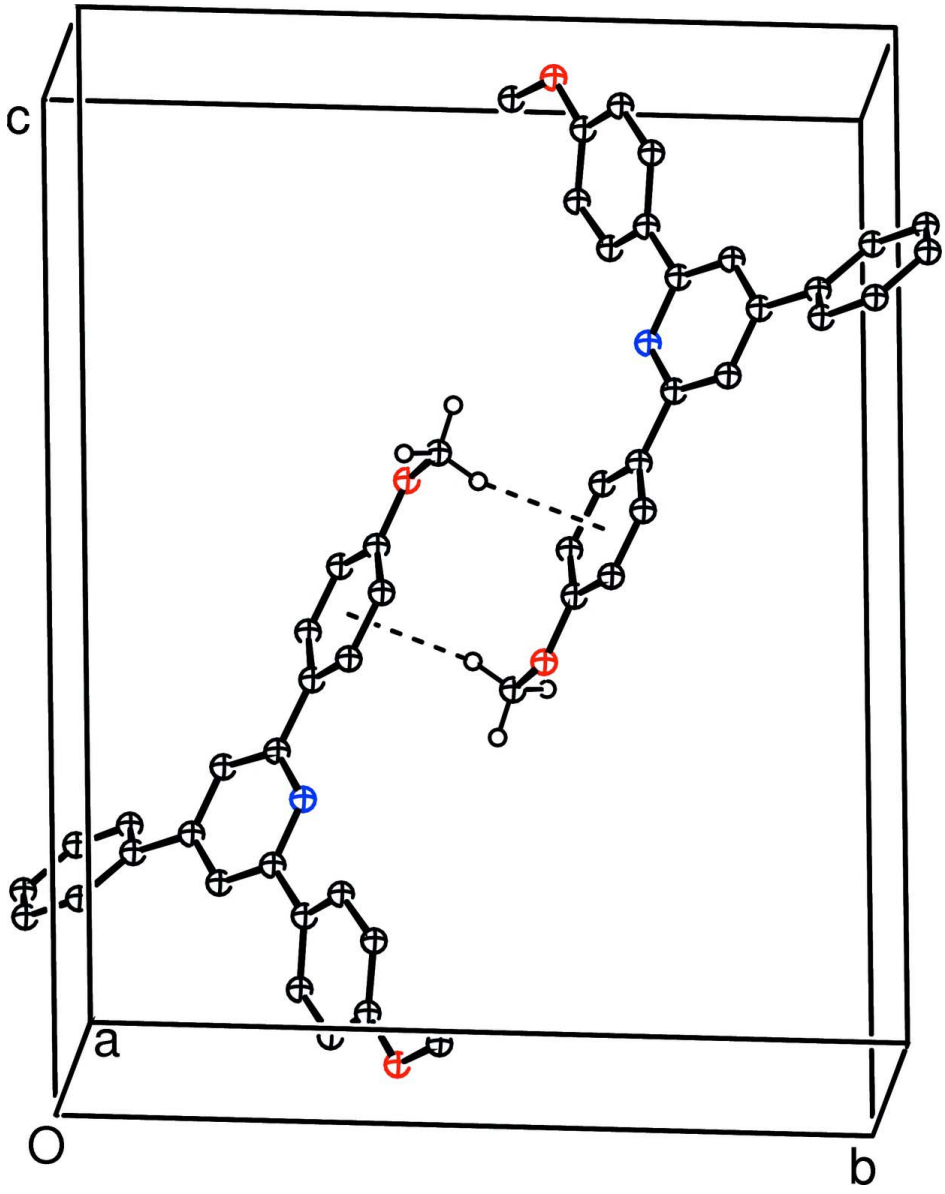

Figure 2

The one-dimensional chain structure was built by the C—H···π H-bond interactions (dashed lines).

2,6-Bis(4-methoxyphenyl)-4-phenylpyridine

Crystal data

$C_{25}H_{21}NO_2$
M_r = 367.43
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 6.379 (3) Å
b = 15.538 (8) Å
c = 20.51 (1) Å
β = 94.281 (7)°
V = 2027.3 (17) Å^3
Z = 4

$F(000)$ = 776
D_x = 1.204 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 964 reflections
θ = 2.6–25.1°
μ = 0.08 mm^{-1}
T = 298 K
Needle, colourless
0.41 × 0.18 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.994
10098 measured reflections
3566 independent reflections
1522 reflections with $I > 2\sigma(I)$
R_{int} = 0.109
θ_{max} = 25.0°, θ_{min} = 1.7°
$h = -7 \rightarrow 7$
$k = -18 \rightarrow 16$
$l = -24 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.099
$wR(F^2)$ = 0.191
S = 1.04
3566 reflections
255 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
$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2 + 0.3542P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 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}
N1	0.2077 (6)	0.7947 (2)	0.20968 (17)	0.0595 (10)
O1	−0.0669 (6)	0.8942 (2)	0.49408 (14)	0.0804 (11)
O2	−0.0509 (6)	0.9151 (2)	−0.08307 (14)	0.0762 (10)
C1	0.2860 (7)	0.7601 (3)	0.2683 (2)	0.0539 (12)
C2	0.4486 (7)	0.7015 (3)	0.2720 (2)	0.0608 (13)
H2	0.4984	0.6806	0.3127	0.073*
C3	0.5412 (7)	0.6725 (3)	0.2161 (2)	0.0569 (12)
C4	0.4592 (7)	0.7086 (3)	0.1567 (2)	0.0602 (13)
H4	0.5156	0.6927	0.1180	0.072*
C5	0.2955 (7)	0.7675 (3)	0.1551 (2)	0.0550 (12)
C6	0.1864 (7)	0.7938 (3)	0.3266 (2)	0.0542 (12)
C7	−0.0101 (8)	0.8304 (3)	0.3224 (2)	0.0724 (15)
H7	−0.0854	0.8318	0.2817	0.087*
C8	−0.1032 (8)	0.8657 (3)	0.3762 (2)	0.0759 (16)
H8	−0.2356	0.8909	0.3712	0.091*
C9	0.0074 (8)	0.8620 (3)	0.4375 (2)	0.0613 (13)

C10	0.2024 (8)	0.8247 (3)	0.4432 (2)	0.0637 (14)
H10	0.2753	0.8216	0.4841	0.076*
C11	0.2932 (7)	0.7916 (3)	0.3894 (2)	0.0619 (13)
H11	0.4268	0.7675	0.3947	0.074*
C12	−0.2641 (9)	0.9374 (4)	0.4904 (2)	0.105 (2)
H12A	−0.2614	0.9843	0.4600	0.157*
H12B	−0.2906	0.9592	0.5328	0.157*
H12C	−0.3734	0.8978	0.4759	0.157*
C13	0.7134 (7)	0.6082 (3)	0.2196 (2)	0.0548 (12)
C14	0.7190 (8)	0.5414 (3)	0.2660 (2)	0.0671 (14)
H14	0.6117	0.5367	0.2940	0.081*
C15	0.8826 (9)	0.4826 (3)	0.2703 (2)	0.0787 (16)
H15	0.8830	0.4387	0.3011	0.094*
C16	1.0438 (9)	0.4878 (3)	0.2299 (3)	0.0758 (16)
H16	1.1541	0.4486	0.2335	0.091*
C17	1.0390 (9)	0.5529 (4)	0.1837 (3)	0.0803 (16)
H17	1.1473	0.5573	0.1560	0.096*
C18	0.8745 (8)	0.6116 (3)	0.1782 (2)	0.0685 (14)
H18	0.8727	0.6539	0.1462	0.082*
C19	0.2008 (8)	0.8072 (3)	0.0924 (2)	0.0543 (12)
C20	0.0029 (8)	0.8437 (3)	0.0891 (2)	0.0613 (13)
H20	−0.0715	0.8438	0.1264	0.074*
C21	−0.0899 (7)	0.8807 (3)	0.0316 (2)	0.0645 (13)
H21	−0.2233	0.9050	0.0307	0.077*
C22	0.0210 (8)	0.8803 (3)	−0.0238 (2)	0.0605 (13)
C23	0.2184 (8)	0.8437 (3)	−0.0216 (2)	0.0661 (14)
H23	0.2922	0.8432	−0.0590	0.079*
C24	0.3083 (7)	0.8077 (3)	0.0356 (2)	0.0641 (13)
H24	0.4419	0.7835	0.0362	0.077*
C25	−0.2637 (9)	0.9444 (4)	−0.0914 (2)	0.0928 (18)
H25A	−0.3566	0.8985	−0.0813	0.139*
H25B	−0.2949	0.9623	−0.1359	0.139*
H25C	−0.2826	0.9921	−0.0627	0.139*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.071 (3)	0.063 (3)	0.045 (2)	0.004 (2)	0.001 (2)	0.001 (2)
O1	0.098 (3)	0.090 (3)	0.056 (2)	0.012 (2)	0.022 (2)	−0.0092 (19)
O2	0.093 (3)	0.089 (3)	0.045 (2)	0.004 (2)	−0.0074 (18)	0.0110 (17)
C1	0.068 (3)	0.055 (3)	0.039 (3)	0.007 (3)	0.005 (2)	0.001 (2)
C2	0.076 (4)	0.063 (3)	0.042 (3)	0.011 (3)	0.001 (2)	0.002 (2)
C3	0.068 (3)	0.058 (3)	0.044 (3)	0.002 (3)	0.001 (2)	0.000 (2)
C4	0.074 (4)	0.065 (3)	0.042 (3)	0.007 (3)	0.008 (3)	−0.002 (2)
C5	0.065 (3)	0.058 (3)	0.042 (3)	0.002 (3)	0.003 (2)	0.000 (2)
C6	0.059 (3)	0.059 (3)	0.044 (3)	0.009 (3)	0.000 (2)	0.002 (2)
C7	0.076 (4)	0.098 (4)	0.042 (3)	0.010 (3)	0.001 (3)	−0.002 (3)
C8	0.068 (4)	0.101 (4)	0.058 (3)	0.022 (3)	0.000 (3)	−0.002 (3)

C9	0.069 (4)	0.072 (4)	0.045 (3)	0.002 (3)	0.013 (3)	−0.001 (3)
C10	0.077 (4)	0.076 (4)	0.037 (3)	0.007 (3)	0.001 (3)	−0.001 (2)
C11	0.069 (3)	0.066 (3)	0.049 (3)	0.013 (3)	−0.002 (3)	0.003 (3)
C12	0.092 (5)	0.138 (5)	0.089 (4)	0.011 (4)	0.033 (4)	−0.029 (4)
C13	0.063 (3)	0.054 (3)	0.046 (3)	0.004 (3)	−0.002 (2)	−0.008 (2)
C14	0.072 (4)	0.072 (4)	0.057 (3)	0.010 (3)	0.006 (3)	0.006 (3)
C15	0.092 (5)	0.073 (4)	0.070 (4)	0.008 (4)	−0.007 (4)	0.005 (3)
C16	0.082 (4)	0.066 (4)	0.077 (4)	0.015 (3)	−0.011 (3)	−0.016 (3)
C17	0.076 (4)	0.091 (4)	0.074 (4)	0.004 (3)	0.007 (3)	−0.015 (3)
C18	0.074 (4)	0.068 (4)	0.064 (3)	0.008 (3)	0.010 (3)	0.002 (3)
C19	0.064 (3)	0.059 (3)	0.040 (3)	0.001 (2)	0.003 (2)	0.000 (2)
C20	0.068 (4)	0.076 (4)	0.041 (3)	0.000 (3)	0.011 (2)	0.004 (2)
C21	0.069 (3)	0.076 (4)	0.047 (3)	0.009 (3)	−0.004 (3)	0.004 (3)
C22	0.078 (4)	0.065 (3)	0.037 (3)	−0.002 (3)	−0.002 (3)	0.001 (2)
C23	0.073 (4)	0.084 (4)	0.041 (3)	0.007 (3)	0.006 (3)	−0.002 (3)
C24	0.065 (3)	0.077 (4)	0.049 (3)	0.006 (3)	−0.003 (3)	0.003 (3)
C25	0.089 (5)	0.114 (5)	0.070 (4)	0.009 (4)	−0.024 (3)	0.015 (3)

Geometric parameters (Å, º)

N1—C5	1.356 (5)	C12—H12B	0.9600
N1—C1	1.376 (5)	C12—H12C	0.9600
O1—C9	1.379 (5)	C13—C18	1.381 (6)
O1—C12	1.423 (5)	C13—C14	1.406 (6)
O2—C22	1.378 (5)	C14—C15	1.385 (6)
O2—C25	1.430 (5)	C14—H14	0.9300
C1—C2	1.378 (5)	C15—C16	1.370 (6)
C1—C6	1.491 (5)	C15—H15	0.9300
C2—C3	1.402 (5)	C16—C17	1.384 (6)
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.406 (5)	C17—C18	1.388 (6)
C3—C13	1.483 (6)	C17—H17	0.9300
C4—C5	1.387 (5)	C18—H18	0.9300
C4—H4	0.9300	C19—C20	1.381 (6)
C5—C19	1.512 (6)	C19—C24	1.394 (5)
C6—C7	1.373 (6)	C20—C21	1.403 (5)
C6—C11	1.412 (5)	C20—H20	0.9300
C7—C8	1.404 (6)	C21—C22	1.382 (6)
C7—H7	0.9300	C21—H21	0.9300
C8—C9	1.396 (5)	C22—C23	1.379 (6)
C8—H8	0.9300	C23—C24	1.385 (5)
C9—C10	1.369 (6)	C23—H23	0.9300
C10—C11	1.383 (5)	C24—H24	0.9300
C10—H10	0.9300	C25—H25A	0.9600
C11—H11	0.9300	C25—H25B	0.9600
C12—H12A	0.9600	C25—H25C	0.9600
C5—N1—C1	117.0 (4)	C18—C13—C14	117.4 (4)

C9—O1—C12	119.0 (4)	C18—C13—C3	121.8 (4)
C22—O2—C25	118.8 (4)	C14—C13—C3	120.7 (4)
N1—C1—C2	121.9 (4)	C15—C14—C13	120.7 (5)
N1—C1—C6	114.5 (4)	C15—C14—H14	119.6
C2—C1—C6	123.5 (4)	C13—C14—H14	119.6
C1—C2—C3	121.9 (4)	C16—C15—C14	121.2 (5)
C1—C2—H2	119.1	C16—C15—H15	119.4
C3—C2—H2	119.1	C14—C15—H15	119.4
C2—C3—C4	115.3 (4)	C15—C16—C17	118.5 (5)
C2—C3—C13	122.2 (4)	C15—C16—H16	120.7
C4—C3—C13	122.4 (4)	C17—C16—H16	120.7
C5—C4—C3	121.0 (4)	C16—C17—C18	120.9 (5)
C5—C4—H4	119.5	C16—C17—H17	119.6
C3—C4—H4	119.5	C18—C17—H17	119.6
N1—C5—C4	122.8 (4)	C13—C18—C17	121.2 (5)
N1—C5—C19	114.4 (4)	C13—C18—H18	119.4
C4—C5—C19	122.8 (4)	C17—C18—H18	119.4
C7—C6—C11	116.3 (4)	C20—C19—C24	117.5 (4)
C7—C6—C1	122.4 (4)	C20—C19—C5	121.0 (4)
C11—C6—C1	121.2 (4)	C24—C19—C5	121.5 (4)
C6—C7—C8	123.3 (4)	C19—C20—C21	122.4 (4)
C6—C7—H7	118.3	C19—C20—H20	118.8
C8—C7—H7	118.3	C21—C20—H20	118.8
C9—C8—C7	118.5 (4)	C22—C21—C20	118.6 (5)
C9—C8—H8	120.7	C22—C21—H21	120.7
C7—C8—H8	120.7	C20—C21—H21	120.7
C10—C9—O1	116.7 (4)	O2—C22—C23	115.7 (4)
C10—C9—C8	119.3 (4)	O2—C22—C21	124.5 (5)
O1—C9—C8	124.1 (5)	C23—C22—C21	119.8 (4)
C9—C10—C11	121.4 (4)	C22—C23—C24	120.9 (4)
C9—C10—H10	119.3	C22—C23—H23	119.5
C11—C10—H10	119.3	C24—C23—H23	119.5
C10—C11—C6	121.1 (4)	C23—C24—C19	120.7 (4)
C10—C11—H11	119.4	C23—C24—H24	119.6
C6—C11—H11	119.4	C19—C24—H24	119.6
O1—C12—H12A	109.5	O2—C25—H25A	109.5
O1—C12—H12B	109.5	O2—C25—H25B	109.5
H12A—C12—H12B	109.5	H25A—C25—H25B	109.5
O1—C12—H12C	109.5	O2—C25—H25C	109.5
H12A—C12—H12C	109.5	H25A—C25—H25C	109.5
H12B—C12—H12C	109.5	H25B—C25—H25C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C25—H25*C*···*Cg*1^{i}	0.96	2.82	3.605	140

Symmetry code: (i) −*x*, −*y*, −*z*.