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6-(4-Aminophenyl)-2-methoxy-4-phenyl-nicotinonitrile

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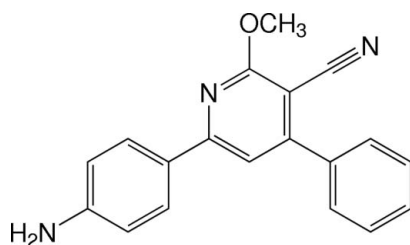
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.046; wR factor = 0.143; data-to-parameter ratio = 17.0.

In the structure of the title nicotinonitrile derivative, $\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}$, the pyridine ring makes dihedral angles of 11.50 (7) and 43.36 (8)° with the 4-aminophenyl and phenyl rings, respectively, and the dihedral angle between the phenyl rings is 36.28°. In the crystal, molecules are linked by $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds into wave-like sheets parallel to (10 $\bar{2}$). These sheets are stacked by $\pi-\pi$ interactions between the 4-aminophenyl rings of adjacent sheets, with centroid-centroid distances of 3.7499 (9) Å. $\text{C}-\text{H}\cdots\pi$ interactions are also present.

Related literature

For the synthesis and applications of nicotinonitrile derivatives, see: Al-Jaber *et al.* (2012); Brandt *et al.* (2010); El-Sayed *et al.* (2011); Ji *et al.* (2007); Kim *et al.* (2005); Koner *et al.* (2012); Raghukumar *et al.* (2003); Zhou *et al.* (2006). For bond-length data, see: Allen *et al.* (1987). For related structures, see: Chantrapromma *et al.* (2013); Suwunwong *et al.* (2012, 2013).



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Experimental

Crystal data

$\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}$
 $M_r = 301.34$
 Monoclinic, $P2_1/c$
 $a = 10.9448$ (12) Å
 $b = 18.960$ (2) Å
 $c = 7.4738$ (8) Å
 $\beta = 94.743$ (2)°
 $V = 1545.6$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 100$ K
 $0.56 \times 0.17 \times 0.06$ mm

Data collection

Bruker APEX DUO CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.955$, $T_{\max} = 0.995$
 14200 measured reflections
 3696 independent reflections
 2689 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.143$
 $S = 1.07$
 3696 reflections
 217 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.30$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.28$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg2 and Cg3 are the centroids of the C1–C6 and C10–C15 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H2N1}\cdots\text{N3}^i$	0.915 (19)	2.338 (19)	3.2416 (18)	169.5 (19)
$\text{N1}-\text{H1N1}\cdots\text{N3}^{ii}$	0.91 (2)	2.28 (2)	3.1773 (19)	168 (2)
$\text{C11}-\text{H11A}\cdots\text{Cg3}^{iii}$	0.95	2.87	3.7667 (17)	158
$\text{C19}-\text{H19C}\cdots\text{Cg2}^{iv}$	0.98	2.69	3.5156 (17)	142

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PLATON (Spek, 2009), Mercury (Macrae *et al.*, 2006) and publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5368).

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supplementary materials

Acta Cryst. (2013). E69, o1816–o1817 [doi:10.1107/S1600536813031437]

6-(4-Aminophenyl)-2-methoxy-4-phenylnicotinonitrile**Thitipone Suwunwong, Suchada Chantrapromma, Ching Kheng Quah and Hoong-Kun Fun****1. Comment**

Nicotinonitrile derivatives are substituted pyridines synthesized from the condensation of α,β -unsaturated ketones with malononitrile (Al-Jaber *et al.*, 2012; Zhou *et al.*, 2006). They have a wide range of bioactivities including antitumor, antimicrobial, analgesic, anti-hyperglycemic and antiproliferative activities (Brandt *et al.*, 2010; El-Sayed *et al.*, 2011; Ji *et al.*, 2007; Kim *et al.*, 2005). Nicotinonitriles also find applications as non-linear optical (Raghukumar *et al.*, 2003) and fluorescent materials (Koner *et al.*, 2012). Continuing our ongoing research on fluorescent materials (Chantrapromma *et al.*, 2013; Suwunwong *et al.*, 2012; 2013), the title compound (I) was synthesized and its fluorescent properties were studied. Our results found that (I) possesses significant fluorescent properties that will be discussed elsewhere, together with those of other closely related compounds. Herein the crystal structure of (I) is reported.

The title compound (I), $C_{19}H_{15}N_3O$, is a non-planar molecule (Fig. 1). The pyridine ring makes dihedral angles of $11.50(7)^\circ$ and $43.36(8)^\circ$ with the 4-aminophenyl and phenyl rings, respectively, and the dihedral angle between the two phenyl rings is 36.28° . The methoxy group lies in the plane of the pyridine ring with an rms deviation of $0.0102(1) \text{ \AA}$ for the eight non-H atoms (C7–C9/C16–C17/C19/N2/O1) and the torsion angle C19–O1–C16–N2 = $-1.2(2)^\circ$. The cyano group is also roughly co-planar with the pyridine ring with an rms deviation of $0.0406(1) \text{ \AA}$ from the ring plane. The bond distances in (I) agree with the literature values (Allen *et al.*, 1987) and are comparable to those found in closely related structures (Chantrapromma *et al.*, 2013 and Suwunwong *et al.*, 2012; 2013).

In the crystal structure (Fig. 2), molecules are linked by intermolecular N—H \cdots N hydrogen bonds (Table 1) forming screw chains. These chains are further linked by N—H \cdots N hydrogen bonds into a two dimensional structure as wave-like sheets parallel to the (1 0 - 2) plane (Fig. 3). These sheets are stacked by $\pi\cdots\pi$ interactions between 4-aminophenyl rings of the adjacent sheets with $Cg_1\cdots Cg_1^{iii,iv}$ distances of $3.7499(9) \text{ \AA}$; Cg_1 is the centroid of the N2/C7–C9/C16–C17 pyridine ring. The crystal is further stabilized by C—H $\cdots\pi$ interactions (Table 1).

2. Experimental

The title compound (I) was synthesized by stirring a solution of (*E*)-1-(4-aminophenyl)-3-phenylprop-2-en-1-one (0.22 g, 1 mmol) in methanol (10 ml) with freshly prepared sodium methoxide (1.0 mmol of sodium in 20 ml of methanol). An excess of malononitrile (0.13 g, 2 mmol) was then added with continuous stirring at room temperature until a precipitate was obtained. The resulting solid was filtered. Yellow plate-shaped single crystals of the title compound suitable for *X*-ray structure determination was recrystallized from ethanol/methanol (1:1 v/v) by slow evaporation of the solvent at room temperature over several days. Mp. 475–476 K.

3. Refinement

The amino H atoms were located from difference maps and refined isotropically. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with $d(C-H) = 0.95 \text{ \AA}$ for aromatic and 0.98 \AA for CH_3 atoms.

The U_{iso} values were constrained to be $1.5U_{\text{eq}}$ of the carrier atom for methyl H atoms and $1.2U_{\text{eq}}$ for the remaining H atoms. A rotating group model was used for the methyl groups.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *PLATON* (Spek, 2009), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

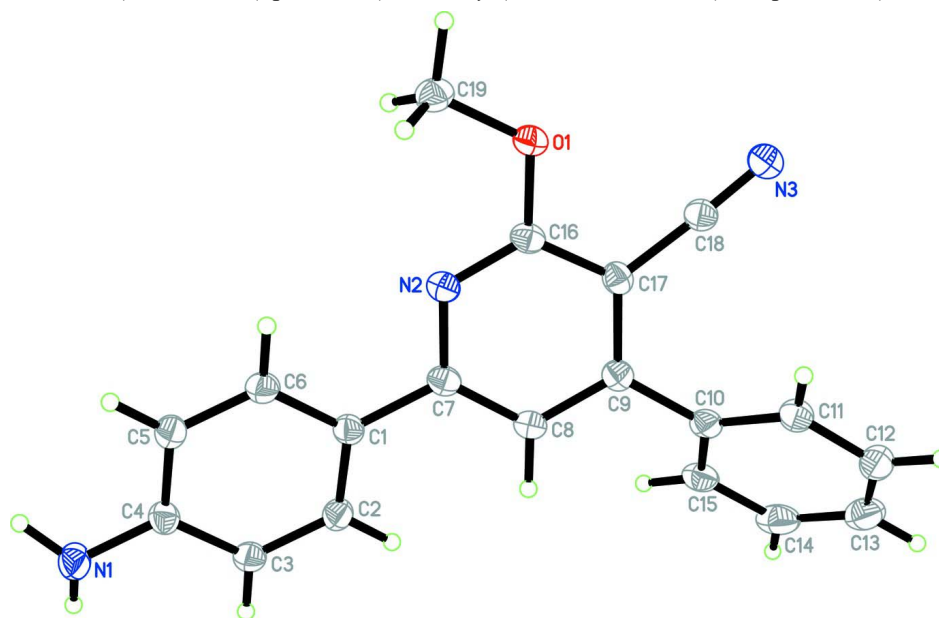


Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

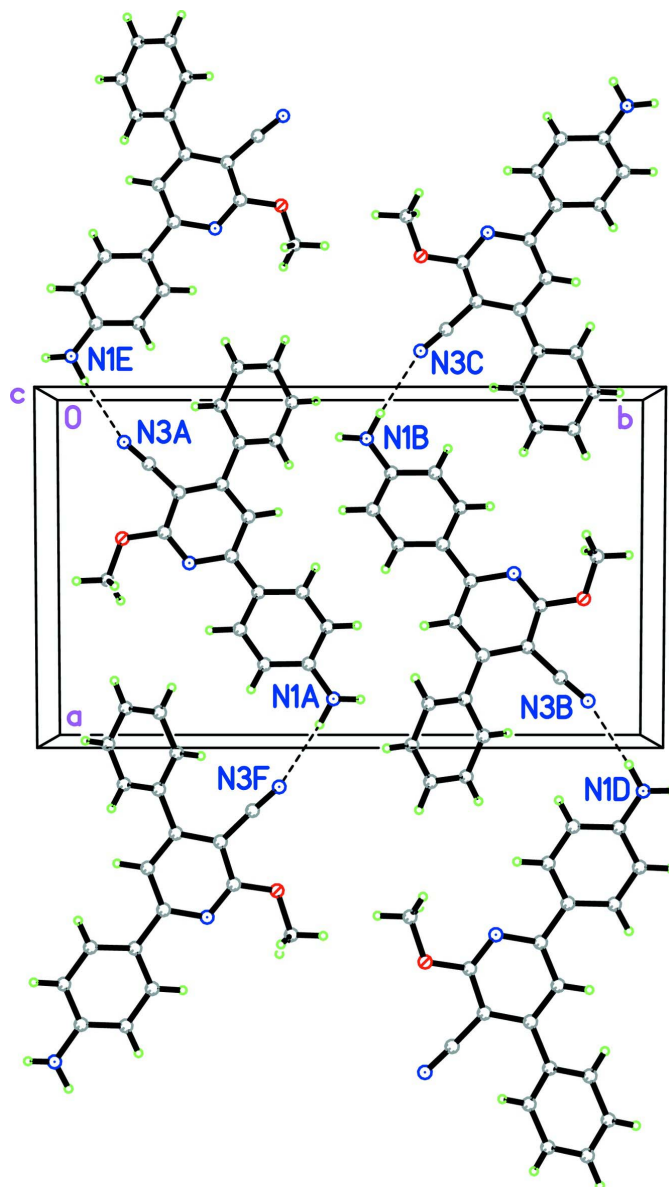
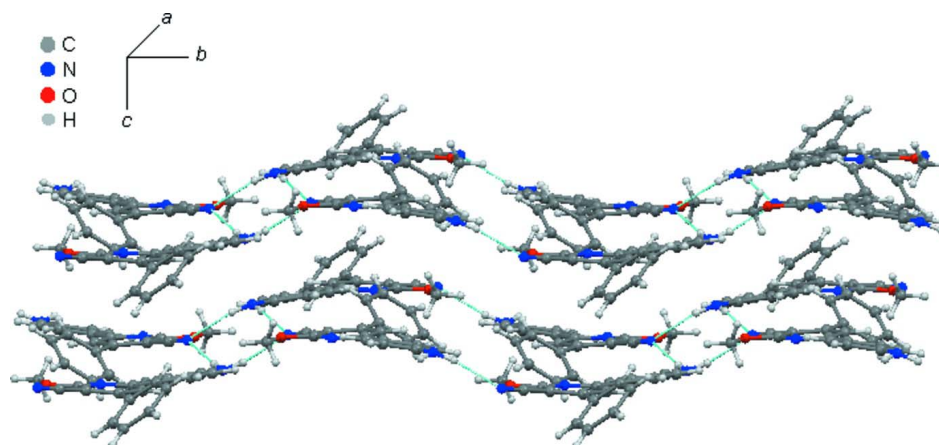


Figure 2

The crystal packing of the title compound viewed approximately along the *c* axis. N—H...N hydrogen bonds are shown as dashed lines.


Figure 3

Wave-like sheets of the title compound viewed approximately along the *a* axis. N—H···N hydrogen bonds are shown as dashed lines.

6-(4-Aminophenyl)-2-methoxy-4-phenylnicotinonitrile

Crystal data

$C_{19}H_{15}N_3O$

$M_r = 301.34$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 10.9448\ (12)\ \text{\AA}$

$b = 18.960\ (2)\ \text{\AA}$

$c = 7.4738\ (8)\ \text{\AA}$

$\beta = 94.743\ (2)^\circ$

$V = 1545.6\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 632$

$D_x = 1.295\ \text{Mg m}^{-3}$

Melting point = 475–476 K

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3696 reflections

$\theta = 2.2\text{--}28.0^\circ$

$\mu = 0.08\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Plate, yellow

$0.56 \times 0.17 \times 0.06\ \text{mm}$

Data collection

Bruker APEX DUO CCD area-detector
diffractometer

Radiation source: sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.955$, $T_{\max} = 0.995$

14200 measured reflections

3696 independent reflections

2689 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\max} = 28.0^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -14 \rightarrow 14$

$k = -24 \rightarrow 25$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.143$

$S = 1.07$

3696 reflections

217 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 atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0815P)^2 + 0.0098P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.30\ \text{e \AA}^{-3}$

$\Delta\rho_{\min} = -0.28\ \text{e \AA}^{-3}$

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.41334 (9)	0.11886 (5)	0.32484 (15)	0.0232 (3)
N1	0.87443 (12)	0.47258 (7)	0.5990 (2)	0.0275 (3)
H2N1	0.9480 (17)	0.4498 (10)	0.619 (3)	0.036 (5)*
H1N1	0.8776 (17)	0.5170 (11)	0.554 (3)	0.043 (6)*
N2	0.48483 (11)	0.23181 (6)	0.37739 (17)	0.0197 (3)
N3	0.12753 (11)	0.11690 (6)	0.1173 (2)	0.0262 (3)
C1	0.56914 (12)	0.34757 (7)	0.4295 (2)	0.0188 (3)
C2	0.56860 (13)	0.42059 (7)	0.4009 (2)	0.0211 (3)
H2A	0.4974	0.4421	0.3435	0.025*
C3	0.66877 (13)	0.46216 (7)	0.4540 (2)	0.0222 (3)
H3A	0.6659	0.5115	0.4320	0.027*
C4	0.77484 (13)	0.43173 (7)	0.5405 (2)	0.0211 (3)
C5	0.77592 (13)	0.35885 (8)	0.5715 (2)	0.0231 (3)
H5A	0.8465	0.3374	0.6310	0.028*
C6	0.67552 (13)	0.31784 (7)	0.5163 (2)	0.0218 (3)
H6A	0.6785	0.2684	0.5375	0.026*
C7	0.46428 (12)	0.30246 (7)	0.3692 (2)	0.0191 (3)
C8	0.34949 (13)	0.32942 (7)	0.3085 (2)	0.0193 (3)
H8A	0.3365	0.3790	0.3080	0.023*
C9	0.25383 (12)	0.28457 (7)	0.2485 (2)	0.0188 (3)
C10	0.13113 (13)	0.31369 (7)	0.1898 (2)	0.0205 (3)
C11	0.02459 (13)	0.28273 (8)	0.2451 (2)	0.0245 (3)
H11A	0.0301	0.2420	0.3193	0.029*
C12	-0.08913 (14)	0.31153 (9)	0.1918 (2)	0.0315 (4)
H12A	-0.1613	0.2909	0.2313	0.038*
C13	-0.09812 (16)	0.37035 (9)	0.0810 (3)	0.0366 (5)
H13A	-0.1763	0.3894	0.0432	0.044*
C14	0.00695 (16)	0.40117 (8)	0.0257 (3)	0.0336 (4)
H14A	0.0008	0.4413	-0.0506	0.040*
C15	0.12153 (14)	0.37363 (8)	0.0814 (2)	0.0253 (4)
H15A	0.1935	0.3957	0.0455	0.030*
C16	0.39525 (12)	0.18928 (7)	0.3197 (2)	0.0192 (3)
C17	0.27805 (12)	0.21180 (7)	0.2504 (2)	0.0196 (3)
C18	0.19270 (13)	0.16011 (7)	0.1769 (2)	0.0207 (3)
C19	0.53384 (14)	0.09527 (8)	0.3919 (2)	0.0253 (4)

H19A	0.5373	0.0437	0.3870	0.038*
H19B	0.5509	0.1109	0.5164	0.038*
H19C	0.5952	0.1152	0.3179	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0235 (5)	0.0159 (5)	0.0299 (7)	-0.0003 (4)	-0.0009 (5)	-0.0005 (4)
N1	0.0209 (7)	0.0207 (6)	0.0401 (9)	-0.0028 (5)	-0.0015 (6)	0.0034 (6)
N2	0.0220 (6)	0.0173 (6)	0.0195 (7)	-0.0007 (4)	0.0010 (5)	-0.0008 (5)
N3	0.0258 (7)	0.0226 (6)	0.0298 (8)	-0.0015 (5)	0.0006 (6)	-0.0012 (6)
C1	0.0190 (7)	0.0201 (7)	0.0172 (8)	-0.0004 (5)	0.0018 (6)	-0.0022 (6)
C2	0.0190 (7)	0.0212 (7)	0.0231 (8)	0.0017 (5)	0.0009 (6)	0.0008 (6)
C3	0.0223 (7)	0.0166 (6)	0.0277 (9)	0.0001 (5)	0.0020 (6)	0.0003 (6)
C4	0.0192 (7)	0.0213 (7)	0.0230 (8)	-0.0025 (5)	0.0033 (6)	-0.0010 (6)
C5	0.0197 (7)	0.0207 (7)	0.0285 (9)	0.0004 (5)	-0.0010 (6)	0.0004 (6)
C6	0.0226 (7)	0.0169 (6)	0.0260 (9)	0.0004 (5)	0.0023 (6)	0.0006 (6)
C7	0.0231 (7)	0.0183 (6)	0.0161 (8)	-0.0008 (5)	0.0029 (6)	-0.0010 (6)
C8	0.0225 (7)	0.0163 (6)	0.0190 (8)	0.0000 (5)	0.0017 (6)	-0.0013 (6)
C9	0.0208 (7)	0.0202 (7)	0.0155 (8)	-0.0011 (5)	0.0028 (5)	-0.0011 (6)
C10	0.0225 (7)	0.0214 (7)	0.0169 (8)	0.0010 (5)	-0.0021 (6)	-0.0056 (6)
C11	0.0241 (7)	0.0260 (7)	0.0233 (9)	-0.0008 (6)	0.0010 (6)	-0.0077 (7)
C12	0.0229 (8)	0.0363 (8)	0.0348 (10)	0.0010 (6)	-0.0002 (7)	-0.0150 (8)
C13	0.0314 (9)	0.0347 (9)	0.0414 (11)	0.0114 (7)	-0.0105 (8)	-0.0154 (8)
C14	0.0424 (9)	0.0238 (7)	0.0323 (10)	0.0099 (7)	-0.0101 (8)	-0.0056 (7)
C15	0.0316 (8)	0.0200 (7)	0.0235 (9)	0.0010 (6)	-0.0023 (7)	-0.0052 (6)
C16	0.0240 (7)	0.0163 (6)	0.0177 (8)	-0.0014 (5)	0.0041 (6)	0.0006 (6)
C17	0.0197 (7)	0.0212 (7)	0.0179 (8)	-0.0025 (5)	0.0015 (6)	-0.0011 (6)
C18	0.0224 (7)	0.0194 (6)	0.0201 (8)	0.0001 (5)	0.0016 (6)	0.0005 (6)
C19	0.0280 (8)	0.0199 (7)	0.0277 (9)	0.0030 (6)	0.0004 (6)	0.0026 (6)

Geometric parameters (Å, °)

O1—C16	1.3498 (16)	C8—C9	1.3937 (18)
O1—C19	1.4427 (17)	C8—H8A	0.9500
N1—C4	1.3786 (18)	C9—C17	1.405 (2)
N1—H2N1	0.916 (19)	C9—C10	1.4844 (18)
N1—H1N1	0.91 (2)	C10—C15	1.395 (2)
N2—C16	1.3144 (17)	C10—C11	1.398 (2)
N2—C7	1.3589 (17)	C11—C12	1.387 (2)
N3—C18	1.1513 (18)	C11—H11A	0.9500
C1—C2	1.401 (2)	C12—C13	1.388 (3)
C1—C6	1.4032 (18)	C12—H12A	0.9500
C1—C7	1.4718 (18)	C13—C14	1.383 (3)
C2—C3	1.3815 (19)	C13—H13A	0.9500
C2—H2A	0.9500	C14—C15	1.390 (2)
C3—C4	1.4052 (19)	C14—H14A	0.9500
C3—H3A	0.9500	C15—H15A	0.9500
C4—C5	1.401 (2)	C16—C17	1.4094 (19)
C5—C6	1.3811 (19)	C17—C18	1.4317 (19)

C5—H5A	0.9500	C19—H19A	0.9800
C6—H6A	0.9500	C19—H19B	0.9800
C7—C8	1.3968 (19)	C19—H19C	0.9800
C16—O1—C19	116.38 (10)	C15—C10—C11	119.30 (13)
C4—N1—H2N1	116.6 (11)	C15—C10—C9	119.85 (13)
C4—N1—H1N1	117.2 (12)	C11—C10—C9	120.84 (14)
H2N1—N1—H1N1	116.0 (17)	C12—C11—C10	120.01 (15)
C16—N2—C7	118.28 (12)	C12—C11—H11A	120.0
C2—C1—C6	117.41 (12)	C10—C11—H11A	120.0
C2—C1—C7	122.29 (12)	C11—C12—C13	120.37 (16)
C6—C1—C7	120.29 (12)	C11—C12—H12A	119.8
C3—C2—C1	121.80 (13)	C13—C12—H12A	119.8
C3—C2—H2A	119.1	C14—C13—C12	119.87 (15)
C1—C2—H2A	119.1	C14—C13—H13A	120.1
C2—C3—C4	120.24 (13)	C12—C13—H13A	120.1
C2—C3—H3A	119.9	C13—C14—C15	120.24 (16)
C4—C3—H3A	119.9	C13—C14—H14A	119.9
N1—C4—C5	120.41 (13)	C15—C14—H14A	119.9
N1—C4—C3	121.11 (13)	C14—C15—C10	120.19 (16)
C5—C4—C3	118.45 (12)	C14—C15—H15A	119.9
C6—C5—C4	120.69 (13)	C10—C15—H15A	119.9
C6—C5—H5A	119.7	N2—C16—O1	119.59 (12)
C4—C5—H5A	119.7	N2—C16—C17	124.49 (13)
C5—C6—C1	121.41 (13)	O1—C16—C17	115.92 (12)
C5—C6—H6A	119.3	C9—C17—C16	117.80 (12)
C1—C6—H6A	119.3	C9—C17—C18	123.51 (12)
N2—C7—C8	121.10 (12)	C16—C17—C18	118.60 (13)
N2—C7—C1	115.91 (12)	N3—C18—C17	177.54 (15)
C8—C7—C1	122.99 (12)	O1—C19—H19A	109.5
C9—C8—C7	120.85 (12)	O1—C19—H19B	109.5
C9—C8—H8A	119.6	H19A—C19—H19B	109.5
C7—C8—H8A	119.6	O1—C19—H19C	109.5
C8—C9—C17	117.39 (12)	H19A—C19—H19C	109.5
C8—C9—C10	120.36 (12)	H19B—C19—H19C	109.5
C17—C9—C10	122.24 (12)		
C6—C1—C2—C3	0.6 (2)	C8—C9—C10—C11	-135.09 (16)
C7—C1—C2—C3	-178.29 (15)	C17—C9—C10—C11	43.4 (2)
C1—C2—C3—C4	-0.5 (2)	C15—C10—C11—C12	0.2 (2)
C2—C3—C4—N1	-178.14 (15)	C9—C10—C11—C12	178.71 (14)
C2—C3—C4—C5	-0.2 (2)	C10—C11—C12—C13	1.1 (2)
N1—C4—C5—C6	178.73 (16)	C11—C12—C13—C14	-1.0 (3)
C3—C4—C5—C6	0.7 (2)	C12—C13—C14—C15	-0.3 (3)
C4—C5—C6—C1	-0.7 (2)	C13—C14—C15—C10	1.6 (3)
C2—C1—C6—C5	0.0 (2)	C11—C10—C15—C14	-1.5 (2)
C7—C1—C6—C5	178.90 (15)	C9—C10—C15—C14	179.94 (14)
C16—N2—C7—C8	2.8 (2)	C7—N2—C16—O1	179.46 (13)
C16—N2—C7—C1	-177.88 (13)	C7—N2—C16—C17	-0.5 (2)

C2—C1—C7—N2	169.00 (15)	C19—O1—C16—N2	-1.2 (2)
C6—C1—C7—N2	-9.9 (2)	C19—O1—C16—C17	178.69 (14)
C2—C1—C7—C8	-11.7 (2)	C8—C9—C17—C16	2.7 (2)
C6—C1—C7—C8	169.48 (15)	C10—C9—C17—C16	-175.87 (14)
N2—C7—C8—C9	-2.3 (2)	C8—C9—C17—C18	-173.75 (14)
C1—C7—C8—C9	178.41 (14)	C10—C9—C17—C18	7.7 (2)
C7—C8—C9—C17	-0.5 (2)	N2—C16—C17—C9	-2.3 (2)
C7—C8—C9—C10	178.05 (14)	O1—C16—C17—C9	177.76 (14)
C8—C9—C10—C15	43.4 (2)	N2—C16—C17—C18	174.30 (15)
C17—C9—C10—C15	-138.05 (15)	O1—C16—C17—C18	-5.6 (2)

Hydrogen-bond geometry (Å, °)

Cg2 and *Cg3* are the centroids of the C1–C6 and C10–C15 rings, respectively.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H2M1...N3 ⁱ	0.915 (19)	2.338 (19)	3.2416 (18)	169.5 (19)
N1—H1M1...N3 ⁱⁱ	0.91 (2)	2.28 (2)	3.1773 (19)	168 (2)
C11—H11A... <i>Cg3</i> ⁱⁱⁱ	0.95	2.87	3.7667 (17)	158
C19—H19C... <i>Cg2</i> ^{iv}	0.98	2.69	3.5156 (17)	142

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