organic compounds

Acta Crystallographica Section E

Structure Reports Online

ISSN 1600-5368

(*E*)-3-Chloro-*N*-[(2-ethoxynaphthalen-1-yl)methylidene]aniline

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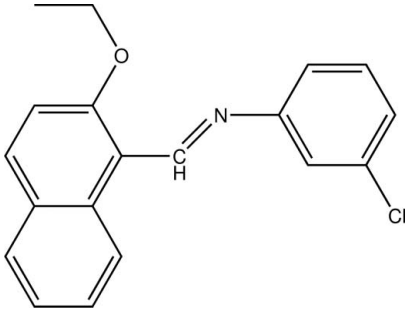
Received 4 July 2012; accepted 14 July 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.058; wR factor = 0.180; data-to-parameter ratio = 13.5.

In the title compound, $C_{19}H_{16}ClNO$, the dihedral angle between the naphthalene ring system and the chlorobenzene ring is 61.90 (10)° and the C—N—C—C torsion angle is 174.6 (2)°. The molecular structure is stabilized by an intramolecular C—H···N hydrogen bond. The crystal structure features π–π stacking interactions [centroid–centroid distances = 3.7325 (17) and 3.8150 (17) Å].

Related literature

For applications of Schiff bases in the pharmaceutical industry, medicine, industry and technology, see: Güler (1998). For their biological properties, see: Lozier *et al.* (1975); Calligaris *et al.* (1972); Williams (1972). For hydrogen-bonding motifs, see: Bernstein *et al.* (1995). For related structures, see: Zhang (2009); Pavlović *et al.* (2002); Özdemir *et al.* (2003); Inaç *et al.* (2012); Ağar *et al.* (2010).



Experimental

Crystal data

$C_{19}H_{16}ClNO$ M_r = 309.78

Triclinic, $P\overline{1}$
a = 8.0084 (14) Å
b = 8.7315 (19) Å
c = 11.7043 (8) Å
α = 76.253 (13)°
β = 79.794 (10)°
γ = 84.337 (17)°
V = 781.0 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 296 K
0.3 × 0.25 × 0.15 mm

Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: multi-scan (*X-AREA* and *X-RED32*; Stoe & Cie, 2001)
T_{min} = 0.793, T_{max} = 1.000
5144 measured reflections
3057 independent reflections
2098 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.180
S = 1.05
3057 reflections
227 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···N1	0.96 (3)	2.24 (3)	2.915 (3)	127 (2)

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences, Giresun University, Turkey, for the use of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2419).

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supporting information

Acta Cryst. (2012). E**68**, o2518 [https://doi.org/10.1107/S1600536812032114]

(*E*)-3-Chloro-*N*-[(2-ethoxynaphthalen-1-yl)methylidene]aniline

Hilal Vesek, Canan Kazak, Ayşen Alaman Ağar, Mustafa Macit and Mustafa Serkan Soylu

S1. Comment

Studies with the Schiff bases, started in 1869 to the present and continued intensively. This chemistry is a multi-site and at the same time, lubricants in the pharmaceutical industry, medicine, industry and technology, a wide finds areas (Güler, 1998). Schiff bases are important in diverse fields of chemistry and biochemistry owing to their biological activites (Calligaris *et al.*, 1972; Lozier *et al.*, 1975). Most Schiff bases have antibacterial, anticancer, antinflammatory and antioxic properties (Williams, 1972).As an extension of the study on the structural characterization of Schiff base compounds, the crystal structure of the title compound is reported here. The molecular structure of the title compound are shown in Fig. 1. Bond lengths and angles are normal and comparable with other related compounds (Özdemir *et al.*,2003; (Zhang, 2009; Inaç *et al.*, 2012; Ağar *et al.*, 2010 & Zhang, 2009). The dihedral angle between the naphthalene ring and the chlorobenzene ring is 61.90 (10)°. The molecular structure is stabilized by one intramolecular C—H···N hydrogen bond interaction with S(6) is motif (Bernstein *et al.*, 1995), Table 1. The crystal structure is stabilized by π-π stacking interactions (Cg1–Cg1^{i} = 3.7325 (17) and Cg2–Cg2^{ii} = 3.8150 (17)Å, Cg1 = C5/C6/C7/C8/C9/C10; Cg2 = C12/C13/C14/C15/C16/C17; symmetry codes: (i) -x,-y,-z; (ii) 1-x,-y, 1-z).

S2. Experimental

(*E*)-3-chloro-*N*-((2-ethoxynaphthalen-1-yl)methylene)aniline was prepared by reflux of a mixture of a solution containing 2-ethoxy-1-naphthaldehyde (20,0 mg, 0,1 mmol) in ethanol (20 ml) and a solution containing 3-chloroaniline (12,8 mg, 0,1 mmol) in ethanol (20 ml).The reaction mixture was stirred for 5 h under reflux.Single crystals of the title compound for X-ray analysis were obtained by slow evaporation of an ethanol solution (Yield 64%; m.p. 345 - 347 K).

S3. Refinement

All other H atoms were placed in calculated positions and constrained to ride on their parents atoms, with C—H=0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C).

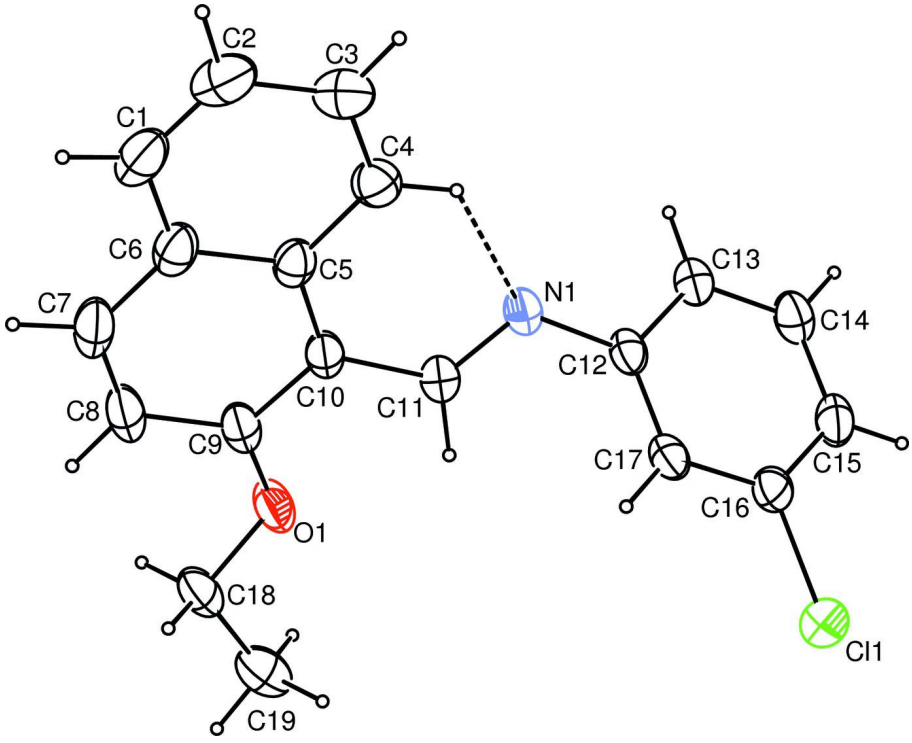

Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme. C—H···N hydrogen bond interaction is shown as dashed lines.

(*E*)-3-Chloro-*N*-[(2-ethoxynaphthalen-1-yl)methylidene]aniline

Crystal data

$C_{19}H_{16}ClNO$
$M_r = 309.78$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.0084\ (14)$ Å
$b = 8.7315\ (19)$ Å
$c = 11.7043\ (8)$ Å
$\alpha = 76.253\ (13)°$
$\beta = 79.794\ (10)°$
$\gamma = 84.337\ (17)°$
$V = 781.0\ (2)$ Å^3
$Z = 2$
$F(000) = 324$
$D_x = 1.317$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1666 reflections
$\theta = 3.3–28.7°$
$\mu = 0.25$ mm^{-1}
$T = 296$ K
Prism, yellow
0.3 × 0.25 × 0.15 mm

Data collection

Stoe IPDS II two-circle diffractometer
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 16.0454 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*X-AREA* and *X-RED32*; Stoe & Cie, 2001)
$T_{min} = 0.793$, $T_{max} = 1.000$
5144 measured reflections
3057 independent reflections
2098 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 26.0°$, $\theta_{min} = 3.3°$
$h = -9\rightarrow9$
$k = -10\rightarrow6$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.180$
$S = 1.05$
3057 reflections
227 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
$w = 1/[\sigma^2(F_o^2) + (0.0836P)^2 + 0.0386P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ 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}
C1	0.1125 (3)	−0.4097 (4)	0.1075 (3)	0.0711 (9)
C2	0.1030 (4)	−0.4953 (4)	0.2214 (3)	0.0742 (9)
C3	0.1347 (4)	−0.4241 (4)	0.3093 (3)	0.0672 (8)
C4	0.1766 (3)	−0.2695 (3)	0.2822 (2)	0.0556 (6)
C5	0.1905 (3)	−0.1770 (3)	0.1640 (2)	0.0479 (6)
C6	0.1568 (3)	−0.2514 (3)	0.0751 (2)	0.0568 (7)
C7	0.1717 (3)	−0.1636 (4)	−0.0440 (2)	0.0647 (8)
C8	0.2206 (3)	−0.0141 (4)	−0.0766 (2)	0.0622 (7)
C9	0.2572 (3)	0.0618 (3)	0.01000 (19)	0.0516 (6)
C10	0.2407 (3)	−0.0173 (3)	0.12978 (18)	0.0463 (6)
C11	0.2871 (3)	0.0684 (3)	0.21183 (19)	0.0463 (5)
C12	0.3167 (3)	0.1180 (3)	0.39163 (17)	0.0443 (5)
C13	0.2129 (3)	0.1546 (3)	0.49135 (19)	0.0519 (6)
H13	0.1021	0.1226	0.5121	0.062*
C14	0.2746 (3)	0.2383 (3)	0.5593 (2)	0.0587 (7)
H14	0.2037	0.2650	0.6246	0.070*
C15	0.4401 (3)	0.2833 (3)	0.5319 (2)	0.0570 (6)
H15	0.4814	0.3395	0.5781	0.068*
C16	0.5424 (3)	0.2431 (3)	0.43502 (19)	0.0514 (6)
C17	0.4833 (3)	0.1615 (3)	0.36474 (18)	0.0478 (6)
H17	0.5549	0.1355	0.2995	0.057*
C18	0.3509 (3)	0.2904 (3)	−0.13867 (19)	0.0616 (7)
H18A	0.2530	0.3109	−0.1796	0.074*
H18B	0.4349	0.2246	−0.1785	0.074*

C19	0.4234 (4)	0.4418 (4)	−0.1407 (2)	0.0731 (8)
H19A	0.4575	0.4964	−0.2218	0.110*
H19B	0.5203	0.4202	−0.1002	0.110*
H19C	0.3391	0.5062	−0.1015	0.110*
Cl1	0.75193 (9)	0.29581 (10)	0.40024 (6)	0.0792 (3)
O1	0.3019 (2)	0.2125 (2)	−0.01705 (13)	0.0651 (5)
N1	0.2496 (3)	0.0308 (2)	0.32487 (15)	0.0513 (5)
H1	0.100 (4)	−0.449 (4)	0.045 (3)	0.100 (11)*
H2	0.076 (4)	−0.609 (5)	0.246 (3)	0.106 (11)*
H3	0.125 (5)	−0.485 (5)	0.387 (3)	0.128 (14)*
H4	0.197 (3)	−0.222 (3)	0.344 (2)	0.072 (8)*
H7	0.154 (4)	−0.209 (4)	−0.107 (2)	0.085 (9)*
H8	0.232 (3)	0.048 (3)	−0.159 (2)	0.054 (6)*
H11	0.352 (3)	0.164 (3)	0.1718 (19)	0.048 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0488 (15)	0.087 (2)	0.092 (2)	−0.0112 (14)	−0.0097 (14)	−0.048 (2)
C2	0.0591 (17)	0.066 (2)	0.101 (3)	−0.0156 (14)	0.0025 (15)	−0.0316 (19)
C3	0.0612 (17)	0.0616 (19)	0.0737 (19)	−0.0087 (13)	0.0030 (13)	−0.0132 (16)
C4	0.0558 (15)	0.0559 (17)	0.0557 (15)	−0.0067 (11)	−0.0038 (11)	−0.0158 (13)
C5	0.0385 (12)	0.0591 (16)	0.0510 (13)	0.0016 (10)	−0.0099 (9)	−0.0217 (12)
C6	0.0416 (13)	0.0746 (19)	0.0641 (16)	0.0000 (11)	−0.0107 (10)	−0.0346 (14)
C7	0.0607 (16)	0.088 (2)	0.0599 (16)	0.0032 (14)	−0.0191 (12)	−0.0404 (16)
C8	0.0665 (16)	0.086 (2)	0.0394 (14)	0.0064 (14)	−0.0172 (11)	−0.0224 (14)
C9	0.0552 (14)	0.0638 (17)	0.0378 (12)	0.0032 (11)	−0.0113 (9)	−0.0151 (11)
C10	0.0454 (12)	0.0582 (15)	0.0385 (12)	0.0012 (10)	−0.0105 (9)	−0.0164 (10)
C11	0.0505 (13)	0.0500 (14)	0.0408 (12)	−0.0008 (10)	−0.0113 (9)	−0.0126 (11)
C12	0.0597 (14)	0.0403 (13)	0.0329 (11)	−0.0023 (10)	−0.0128 (9)	−0.0046 (9)
C13	0.0580 (15)	0.0598 (16)	0.0400 (12)	−0.0040 (11)	−0.0113 (10)	−0.0123 (11)
C14	0.0674 (17)	0.0709 (18)	0.0413 (13)	0.0027 (13)	−0.0109 (11)	−0.0205 (12)
C15	0.0750 (17)	0.0586 (16)	0.0436 (13)	−0.0063 (12)	−0.0201 (11)	−0.0151 (12)
C16	0.0622 (15)	0.0508 (15)	0.0407 (12)	−0.0116 (11)	−0.0159 (10)	−0.0005 (11)
C17	0.0593 (14)	0.0496 (14)	0.0325 (11)	−0.0040 (10)	−0.0071 (9)	−0.0050 (10)
C18	0.0633 (16)	0.080 (2)	0.0346 (12)	0.0044 (13)	−0.0065 (10)	−0.0043 (12)
C19	0.0744 (19)	0.077 (2)	0.0536 (16)	0.0060 (15)	−0.0002 (13)	0.0011 (14)
Cl1	0.0712 (5)	0.1066 (7)	0.0619 (5)	−0.0328 (4)	−0.0157 (3)	−0.0082 (4)
O1	0.0954 (14)	0.0659 (13)	0.0335 (9)	−0.0121 (10)	−0.0121 (8)	−0.0060 (8)
N1	0.0615 (12)	0.0582 (13)	0.0373 (10)	−0.0089 (9)	−0.0095 (8)	−0.0136 (9)

Geometric parameters (Å, º)

C1—C2	1.358 (5)	C11—H11	1.00 (2)
C1—C6	1.407 (4)	C12—C17	1.385 (3)
C1—H1	0.90 (3)	C12—C13	1.391 (3)
C2—C3	1.392 (4)	C12—N1	1.411 (3)
C2—H2	1.00 (4)	C13—C14	1.377 (3)

C3—C4	1.372 (4)	C13—H13	0.9300
C3—H3	0.93 (4)	C14—C15	1.381 (4)
C4—C5	1.418 (3)	C14—H14	0.9300
C4—H4	0.96 (3)	C15—C16	1.372 (3)
C5—C6	1.425 (3)	C15—H15	0.9300
C5—C10	1.434 (3)	C16—C17	1.375 (3)
C6—C7	1.413 (4)	C16—Cl1	1.737 (2)
C7—C8	1.347 (4)	C17—H17	0.9300
C7—H7	0.95 (3)	C18—O1	1.427 (3)
C8—C9	1.420 (3)	C18—C19	1.488 (4)
C8—H8	0.98 (2)	C18—H18A	0.9700
C9—O1	1.347 (3)	C18—H18B	0.9700
C9—C10	1.397 (3)	C19—H19A	0.9600
C10—C11	1.464 (3)	C19—H19B	0.9600
C11—N1	1.273 (3)	C19—H19C	0.9600

C2—C1—C6	121.8 (3)	C17—C12—C13	119.2 (2)
C2—C1—H1	124 (2)	C17—C12—N1	122.46 (19)
C6—C1—H1	114 (2)	C13—C12—N1	118.3 (2)
C1—C2—C3	119.3 (3)	C14—C13—C12	119.9 (2)
C1—C2—H2	123.2 (19)	C14—C13—H13	120.0
C3—C2—H2	117.6 (19)	C12—C13—H13	120.0
C4—C3—C2	121.0 (3)	C13—C14—C15	120.9 (2)
C4—C3—H3	122 (2)	C13—C14—H14	119.5
C2—C3—H3	118 (2)	C15—C14—H14	119.5
C3—C4—C5	121.4 (3)	C16—C15—C14	118.6 (2)
C3—C4—H4	120.0 (16)	C16—C15—H15	120.7
C5—C4—H4	118.6 (16)	C14—C15—H15	120.7
C4—C5—C6	116.9 (2)	C15—C16—C17	121.7 (2)
C4—C5—C10	123.8 (2)	C15—C16—Cl1	119.33 (18)
C6—C5—C10	119.2 (2)	C17—C16—Cl1	119.01 (18)
C1—C6—C7	121.9 (2)	C16—C17—C12	119.7 (2)
C1—C6—C5	119.5 (3)	C16—C17—H17	120.2
C7—C6—C5	118.5 (3)	C12—C17—H17	120.2
C8—C7—C6	122.3 (2)	O1—C18—C19	107.9 (2)
C8—C7—H7	116.0 (18)	O1—C18—H18A	110.1
C6—C7—H7	121.6 (18)	C19—C18—H18A	110.1
C7—C8—C9	120.2 (3)	O1—C18—H18B	110.1
C7—C8—H8	123.2 (14)	C19—C18—H18B	110.1
C9—C8—H8	116.6 (14)	H18A—C18—H18B	108.4
O1—C9—C10	117.03 (19)	C18—C19—H19A	109.5
O1—C9—C8	122.7 (2)	C18—C19—H19B	109.5
C10—C9—C8	120.2 (3)	H19A—C19—H19B	109.5
C9—C10—C5	119.4 (2)	C18—C19—H19C	109.5
C9—C10—C11	116.3 (2)	H19A—C19—H19C	109.5
C5—C10—C11	124.1 (2)	H19B—C19—H19C	109.5
N1—C11—C10	125.3 (2)	C9—O1—C18	119.71 (19)
N1—C11—H11	120.4 (12)	C11—N1—C12	118.1 (2)

C10—C11—H11	114.3 (12)		
C6—C1—C2—C3	1.2 (4)	C6—C5—C10—C9	−0.6 (3)
C1—C2—C3—C4	−0.5 (4)	C4—C5—C10—C11	1.4 (3)
C2—C3—C4—C5	−0.6 (4)	C6—C5—C10—C11	−176.68 (19)
C3—C4—C5—C6	0.8 (3)	C9—C10—C11—N1	165.2 (2)
C3—C4—C5—C10	−177.3 (2)	C5—C10—C11—N1	−18.7 (4)
C2—C1—C6—C7	178.1 (2)	C17—C12—C13—C14	2.4 (3)
C2—C1—C6—C5	−0.9 (4)	N1—C12—C13—C14	179.4 (2)
C4—C5—C6—C1	−0.1 (3)	C12—C13—C14—C15	−1.8 (4)
C10—C5—C6—C1	178.1 (2)	C13—C14—C15—C16	0.2 (4)
C4—C5—C6—C7	−179.1 (2)	C14—C15—C16—C17	0.7 (4)
C10—C5—C6—C7	−0.9 (3)	C14—C15—C16—Cl1	−179.04 (19)
C1—C6—C7—C8	−177.3 (2)	C15—C16—C17—C12	0.0 (4)
C5—C6—C7—C8	1.7 (4)	Cl1—C16—C17—C12	179.73 (17)
C6—C7—C8—C9	−0.9 (4)	C13—C12—C17—C16	−1.5 (3)
C7—C8—C9—O1	−178.1 (2)	N1—C12—C17—C16	−178.4 (2)
C7—C8—C9—C10	−0.8 (4)	C10—C9—O1—C18	168.6 (2)
O1—C9—C10—C5	178.94 (19)	C8—C9—O1—C18	−14.0 (3)
C8—C9—C10—C5	1.5 (3)	C19—C18—O1—C9	−169.7 (2)
O1—C9—C10—C11	−4.7 (3)	C10—C11—N1—C12	174.6 (2)
C8—C9—C10—C11	177.9 (2)	C17—C12—N1—C11	−42.5 (3)
C4—C5—C10—C9	177.4 (2)	C13—C12—N1—C11	140.6 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···N1	0.96 (3)	2.24 (3)	2.915 (3)	127 (2)