

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1-[(6-Chloro-3-pyridyl)methyl]-5-ethoxy-8-nitro-1,2,3,5,6,7-hexahydroimidazo-[1,2-a]pyridine

Zhongzhen Tian,^{a*} Dongmei Li^a and Zhong Li^{b*}

^aInstitute of Chemistry and Chemical Engineering, University of Jinan, 106 Jiwei Road, Jinan 250022, People's Republic of China, and ^bShanghai Key Laboratory of Chemical Biology, School of Pharmacy, East China University of Science and Technology, Shanghai 200237, People's Republic of China
Correspondence e-mail: chm_tianzz@ujn.edu.cn, lizhong@ecust.edu.cn

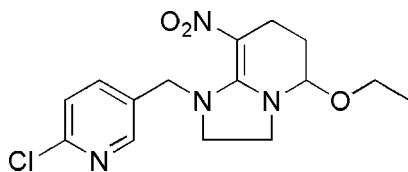
Received 26 July 2009; accepted 17 September 2009

Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.049; wR factor = 0.135; data-to-parameter ratio = 16.6.

In the title compound, $\text{C}_{15}\text{H}_{19}\text{ClN}_4\text{O}_3$, an active agrochemical possessing insecticidal activity, the dihedral angle between the mean planes passing through the pyridine ring and the five-membered ring is $87.3(2)^\circ$. The fused pyridine ring adopts a twisted sofa conformation. The molecular structure features close intramolecular $\text{C}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonding.

Related literature

For related literature, see: Kagabu *et al.* (2002); Moriya *et al.* (1992); Tian *et al.* (2007); Tokumitsu (1990).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{19}\text{ClN}_4\text{O}_3$
 $M_r = 338.79$
Monoclinic, $P2_1/c$

$a = 17.021(3)$ Å
 $b = 5.5737(8)$ Å
 $c = 18.334(3)$ Å

$\beta = 112.097(3)^\circ$
 $V = 1611.6(4)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation

$\mu = 0.26$ mm⁻¹
 $T = 290$ K
 $0.50 \times 0.24 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
 $T_{\min} = 0.922$, $T_{\max} = 0.969$
8970 measured reflections
3486 independent reflections
1870 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.082$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.135$
 $S = 0.82$
3486 reflections
210 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.32$ e Å⁻³
 $\Delta\rho_{\min} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C11}-\text{H11B}\cdots\text{O3}$	0.97	2.35	2.803(3)	108
$\text{C13}-\text{H13}\cdots\text{N1}$	0.93	2.54	2.891(3)	103

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

The authors thank the Opening Fund of Shanghai Key Laboratory of Chemical Biology (grant No. SKLCB-2008-08) and the Doctoral Foundation of the University of Jinan (grant No. XBS0823, B0542) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2230).

References

- Bruker (1997). *SADABS*, *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Kagabu, S., Nishiwaki, H., Sato, K., Hibi, M., Yamaoka, N. & Nakagawa, Y. (2002). *Pest. Manag. Sci.* **58**, 483–490.
Moriya, K., Shibuya, K., Hattori, Y., Tsuboi, S., Shiokawa, K. & Kagabu, S. (1992). *Biosci. Biotechnol. Biochem.* **56**, 364–365.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Tian, Z. Z., Shao, X. S., Li, Z., Qian, X. H. & Huang, Q. C. (2007). *J. Agric. Food. Chem.* **55**, 2288–2292.
Tokumitsu, T. (1990). *Bull. Chem. Soc. Jpn.*, **63**, 1921–1924.

supplementary materials

Acta Cryst. (2009). E65, o2517 [doi:10.1107/S1600536809037660]

1-[(6-Chloro-3-pyridyl)methyl]-5-ethoxy-8-nitro-1,2,3,5,6,7-hexahydroimidazo[1,2-*a*]pyridine

Z. Tian, D. Li and Z. Li

Comment

Since the debut of Imidacloprid in the 1990 decade (Moriya *et al.*, 1992), neonicotinoid insecticides have become rapidly an important chemical class of insecticides. Nitromethylene compounds (Kagabu *et al.*, 2002) exhibited remarkably higher biological activity but poor photostability compared with Imidacloprid. Our synthetic interest was introducing dicyclic ring into the lead structure to improve its photostability and synthesizing a series of new compounds, in which compound (I) exhibited good insecticidal activities against pea aphids and was slightly weaker than that of imidacloprid (Tian *et al.*, 2007). The dihedral angle between the mean planes passing through the pyridine ring and the five membered ring is 87.3 (2)°. The six membered N2/C3/C4/C5/C6/C7 ring adopts a twist sofa conformation. The title compound C₁₅H₁₉ClN₄O₃, is an active agrochemical possessing insecticidal activity. The dihedral angle between the mean planes passing through the pyridine ring and the five membered ring is 87.3 (2)°. The six membered N2/C3/C4/C5/C6/C7 ring adopts a twist sofa conformation. The molecular structure is stabilized by intramolecular C—H···N and C—H···O hydrogen bond, Table 1.

Experimental

The synthesis of the title compound was following the reported method by Tokumitsu, 1990. Single crystals suitable for X-ray analysis were obtained by slow evaporation of the solution of dichloromethane and petroleum ether of the title compound. m.p. 399.8–400.8 K.

Refinement

H atoms were positioned geometrically and included in the refinement in the riding-model approximation, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for pyridine H atoms, C—H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for the methylene H atoms, C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{C})$ for the methyl H atoms, C—H = 0.98 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ for the methenyl H atoms

Figures

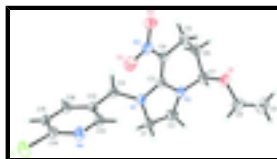


Fig. 1. The molecular structure of (a) with atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The H atoms are shown as circles of arbitrary size and intramolecular hydrogen bonds are indicated by dotted lines.

1-[(6-Chloro-3-pyridyl)methyl]-5-ethoxy-8-nitro-1,2,3,5,6,7-hexahydroimidazo[1,2-a]pyridine

Crystal data

$C_{15}H_{19}ClN_4O_3$	$F_{000} = 712$
$M_r = 338.79$	$D_x = 1.396 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ybc	Cell parameters from 1727 reflections
$a = 17.021 (3) \text{ \AA}$	$\theta = 4.8\text{--}47.4^\circ$
$b = 5.5737 (8) \text{ \AA}$	$\mu = 0.26 \text{ mm}^{-1}$
$c = 18.334 (3) \text{ \AA}$	$T = 290 \text{ K}$
$\beta = 112.097 (3)^\circ$	Prismatic, colourless
$V = 1611.6 (4) \text{ \AA}^3$	$0.50 \times 0.24 \times 0.12 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3486 independent reflections
Radiation source: fine-focus sealed tube	1870 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.082$
$T = 290 \text{ K}$	$\theta_{\text{max}} = 27.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.3^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -21 \rightarrow 21$
$T_{\text{min}} = 0.922$, $T_{\text{max}} = 0.969$	$k = -7 \rightarrow 7$
8970 measured reflections	$l = -23 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.069P)^2]$
$wR(F^2) = 0.135$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.82$	$(\Delta/\sigma)_{\text{max}} = 0.044$
3486 reflections	$\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$
210 parameters	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.020 (2)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.20916 (4)	0.34129 (13)	0.43476 (5)	0.0742 (3)
O1	0.58663 (11)	0.9036 (4)	0.35790 (10)	0.0669 (5)
O2	0.69588 (12)	0.4707 (4)	0.16844 (11)	0.0739 (6)
O3	0.81680 (12)	0.5033 (3)	0.26680 (11)	0.0653 (5)
N1	0.84352 (11)	0.9213 (3)	0.35853 (10)	0.0428 (5)
N2	0.71934 (11)	1.0384 (4)	0.35902 (11)	0.0484 (5)
N3	0.74299 (13)	0.5777 (4)	0.22900 (12)	0.0517 (5)
N4	1.05820 (12)	0.4680 (4)	0.42526 (12)	0.0542 (5)
C1	0.86309 (14)	1.0659 (5)	0.43064 (14)	0.0528 (6)
H1A	0.9076	1.1814	0.4361	0.063*
H1B	0.8806	0.9645	0.4770	0.063*
C2	0.77991 (15)	1.1909 (5)	0.41832 (15)	0.0594 (7)
H2A	0.7687	1.1946	0.4664	0.071*
H2B	0.7793	1.3533	0.3991	0.071*
C3	0.75815 (13)	0.9028 (4)	0.32102 (13)	0.0406 (5)
C4	0.71043 (14)	0.7723 (4)	0.25471 (13)	0.0451 (6)
C5	0.61813 (14)	0.8220 (5)	0.21354 (14)	0.0582 (7)
H5A	0.5857	0.6921	0.2236	0.070*
H5B	0.6045	0.8293	0.1572	0.070*
C6	0.59349 (15)	1.0563 (5)	0.24097 (15)	0.0602 (7)
H6A	0.5322	1.0689	0.2210	0.072*
H6B	0.6150	1.1890	0.2197	0.072*
C7	0.62807 (15)	1.0737 (5)	0.32935 (15)	0.0552 (7)
H7	0.6161	1.2340	0.3445	0.066*
C8	0.59553 (18)	0.9382 (6)	0.43754 (16)	0.0753 (9)
H8A	0.5732	1.0941	0.4433	0.090*
H8B	0.6551	0.9334	0.4715	0.090*
C9	0.5492 (2)	0.7483 (7)	0.46073 (19)	0.1023 (12)
H9A	0.4896	0.7620	0.4299	0.123*
H9B	0.5587	0.7652	0.5155	0.123*
H9C	0.5691	0.5940	0.4519	0.123*
C11	0.89956 (13)	0.9436 (4)	0.31525 (13)	0.0455 (6)
H11A	0.9131	1.1118	0.3130	0.055*

supplementary materials

H11B	0.8695	0.8891	0.2617	0.055*
C12	0.98050 (13)	0.8050 (4)	0.35017 (12)	0.0393 (5)
C13	0.98935 (14)	0.6091 (4)	0.39838 (13)	0.0490 (6)
H13	0.9443	0.5719	0.4134	0.059*
C14	1.12093 (14)	0.5302 (4)	0.40378 (13)	0.0454 (6)
C15	1.12235 (14)	0.7269 (4)	0.35956 (13)	0.0465 (6)
H15	1.1699	0.7651	0.3486	0.056*
C16	1.05008 (14)	0.8655 (4)	0.33212 (13)	0.0462 (6)
H16	1.0480	1.0000	0.3014	0.055*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0596 (4)	0.0681 (5)	0.0967 (6)	0.0181 (3)	0.0313 (4)	0.0041 (4)
O1	0.0668 (11)	0.0879 (15)	0.0610 (12)	-0.0114 (10)	0.0413 (10)	-0.0097 (10)
O2	0.0778 (12)	0.0823 (14)	0.0702 (13)	-0.0259 (11)	0.0374 (11)	-0.0376 (11)
O3	0.0691 (12)	0.0575 (12)	0.0737 (13)	0.0125 (9)	0.0320 (10)	-0.0075 (9)
N1	0.0411 (11)	0.0494 (12)	0.0425 (11)	-0.0023 (8)	0.0210 (9)	-0.0026 (9)
N2	0.0439 (11)	0.0575 (13)	0.0477 (12)	0.0013 (9)	0.0216 (9)	-0.0130 (10)
N3	0.0583 (13)	0.0558 (13)	0.0503 (13)	-0.0090 (11)	0.0311 (11)	-0.0095 (11)
N4	0.0553 (12)	0.0513 (13)	0.0624 (14)	0.0059 (10)	0.0293 (11)	0.0106 (10)
C1	0.0529 (14)	0.0594 (16)	0.0473 (14)	-0.0102 (12)	0.0201 (12)	-0.0093 (12)
C2	0.0641 (16)	0.0623 (18)	0.0556 (16)	-0.0076 (13)	0.0269 (13)	-0.0186 (13)
C3	0.0447 (13)	0.0413 (13)	0.0407 (13)	0.0016 (10)	0.0216 (11)	0.0027 (10)
C4	0.0475 (13)	0.0493 (15)	0.0436 (14)	-0.0033 (11)	0.0231 (11)	-0.0055 (11)
C5	0.0476 (14)	0.081 (2)	0.0484 (15)	-0.0038 (13)	0.0204 (12)	-0.0060 (13)
C6	0.0466 (14)	0.082 (2)	0.0545 (16)	0.0109 (13)	0.0218 (12)	0.0084 (14)
C7	0.0500 (14)	0.0604 (17)	0.0626 (17)	0.0079 (12)	0.0297 (13)	-0.0033 (13)
C8	0.0739 (19)	0.104 (3)	0.0543 (18)	0.0098 (17)	0.0314 (15)	0.0030 (17)
C9	0.111 (3)	0.143 (3)	0.071 (2)	-0.020 (2)	0.055 (2)	0.006 (2)
C11	0.0480 (13)	0.0474 (14)	0.0479 (14)	-0.0009 (11)	0.0257 (11)	0.0059 (11)
C12	0.0426 (12)	0.0410 (13)	0.0379 (12)	-0.0033 (10)	0.0193 (10)	-0.0017 (10)
C13	0.0483 (14)	0.0533 (16)	0.0545 (15)	-0.0001 (11)	0.0299 (12)	0.0080 (12)
C14	0.0433 (13)	0.0477 (15)	0.0453 (14)	0.0016 (11)	0.0167 (11)	-0.0066 (11)
C15	0.0435 (13)	0.0538 (15)	0.0494 (14)	-0.0068 (11)	0.0257 (11)	-0.0048 (12)
C16	0.0488 (14)	0.0493 (14)	0.0451 (14)	-0.0073 (11)	0.0230 (11)	0.0045 (11)

Geometric parameters (\AA , $^\circ$)

Cl—C14	1.745 (2)	C5—H5A	0.9700
O1—C7	1.396 (3)	C5—H5B	0.9700
O1—C8	1.423 (3)	C6—C7	1.505 (4)
O2—N3	1.250 (2)	C6—H6A	0.9700
O3—N3	1.255 (2)	C6—H6B	0.9700
N1—C3	1.358 (3)	C7—H7	0.9800
N1—C11	1.458 (3)	C8—C9	1.475 (4)
N1—C1	1.475 (3)	C8—H8A	0.9700
N2—C3	1.356 (3)	C8—H8B	0.9700
N2—C7	1.453 (3)	C9—H9A	0.9600

N2—C2	1.457 (3)	C9—H9B	0.9600
N3—C4	1.379 (3)	C9—H9C	0.9600
N4—C14	1.316 (3)	C11—C12	1.497 (3)
N4—C13	1.342 (3)	C11—H11A	0.9700
C1—C2	1.517 (3)	C11—H11B	0.9700
C1—H1A	0.9700	C12—C13	1.377 (3)
C1—H1B	0.9700	C12—C16	1.386 (3)
C2—H2A	0.9700	C13—H13	0.9300
C2—H2B	0.9700	C14—C15	1.369 (3)
C3—C4	1.387 (3)	C15—C16	1.378 (3)
C4—C5	1.491 (3)	C15—H15	0.9300
C5—C6	1.514 (4)	C16—H16	0.9300
C7—O1—C8	114.8 (2)	H6A—C6—H6B	108.0
C3—N1—C11	121.70 (18)	O1—C7—N2	112.8 (2)
C3—N1—C1	109.47 (18)	O1—C7—C6	108.2 (2)
C11—N1—C1	117.89 (18)	N2—C7—C6	108.9 (2)
C3—N2—C7	122.79 (19)	O1—C7—H7	108.9
C3—N2—C2	111.33 (18)	N2—C7—H7	108.9
C7—N2—C2	123.86 (19)	C6—C7—H7	108.9
O2—N3—O3	120.5 (2)	O1—C8—C9	109.7 (3)
O2—N3—C4	118.2 (2)	O1—C8—H8A	109.7
O3—N3—C4	121.2 (2)	C9—C8—H8A	109.7
C14—N4—C13	115.5 (2)	O1—C8—H8B	109.7
N1—C1—C2	103.53 (17)	C9—C8—H8B	109.7
N1—C1—H1A	111.1	H8A—C8—H8B	108.2
C2—C1—H1A	111.1	C8—C9—H9A	109.5
N1—C1—H1B	111.1	C8—C9—H9B	109.5
C2—C1—H1B	111.1	H9A—C9—H9B	109.5
H1A—C1—H1B	109.0	C8—C9—H9C	109.5
N2—C2—C1	101.66 (19)	H9A—C9—H9C	109.5
N2—C2—H2A	111.4	H9B—C9—H9C	109.5
C1—C2—H2A	111.4	N1—C11—C12	114.11 (18)
N2—C2—H2B	111.4	N1—C11—H11A	108.7
C1—C2—H2B	111.4	C12—C11—H11A	108.7
H2A—C2—H2B	109.3	N1—C11—H11B	108.7
N2—C3—N1	109.43 (19)	C12—C11—H11B	108.7
N2—C3—C4	120.32 (19)	H11A—C11—H11B	107.6
N1—C3—C4	130.3 (2)	C13—C12—C16	116.7 (2)
N3—C4—C3	122.3 (2)	C13—C12—C11	123.00 (19)
N3—C4—C5	117.1 (2)	C16—C12—C11	120.3 (2)
C3—C4—C5	120.3 (2)	N4—C13—C12	124.8 (2)
C4—C5—C6	111.3 (2)	N4—C13—H13	117.6
C4—C5—H5A	109.4	C12—C13—H13	117.6
C6—C5—H5A	109.4	N4—C14—C15	125.8 (2)
C4—C5—H5B	109.4	N4—C14—C1	116.08 (18)
C6—C5—H5B	109.4	C15—C14—C1	118.11 (18)
H5A—C5—H5B	108.0	C14—C15—C16	117.0 (2)
C5—C6—C7	111.6 (2)	C14—C15—H15	121.5
C5—C6—H6A	109.3	C16—C15—H15	121.5

supplementary materials

C7—C6—H6A	109.3	C15—C16—C12	120.1 (2)
C5—C6—H6B	109.3	C15—C16—H16	119.9
C7—C6—H6B	109.3	C12—C16—H16	119.9
C3—N1—C1—C2	-16.3 (3)	C8—O1—C7—N2	75.1 (3)
C11—N1—C1—C2	128.5 (2)	C8—O1—C7—C6	-164.3 (2)
C3—N2—C2—C1	-19.3 (3)	C3—N2—C7—O1	91.2 (3)
C7—N2—C2—C1	176.5 (2)	C2—N2—C7—O1	-106.4 (3)
N1—C1—C2—N2	20.5 (2)	C3—N2—C7—C6	-28.9 (3)
C7—N2—C3—N1	174.3 (2)	C2—N2—C7—C6	133.5 (2)
C2—N2—C3—N1	9.9 (3)	C5—C6—C7—O1	-67.8 (3)
C7—N2—C3—C4	-6.0 (3)	C5—C6—C7—N2	55.2 (3)
C2—N2—C3—C4	-170.4 (2)	C7—O1—C8—C9	180.0 (2)
C11—N1—C3—N2	-138.6 (2)	C3—N1—C11—C12	-140.6 (2)
C1—N1—C3—N2	4.7 (3)	C1—N1—C11—C12	79.0 (2)
C11—N1—C3—C4	41.7 (4)	N1—C11—C12—C13	23.2 (3)
C1—N1—C3—C4	-175.0 (2)	N1—C11—C12—C16	-159.4 (2)
O2—N3—C4—C3	-179.6 (2)	C14—N4—C13—C12	1.3 (3)
O3—N3—C4—C3	3.1 (3)	C16—C12—C13—N4	-3.6 (3)
O2—N3—C4—C5	7.1 (3)	C11—C12—C13—N4	173.9 (2)
O3—N3—C4—C5	-170.2 (2)	C13—N4—C14—C15	2.3 (3)
N2—C3—C4—N3	-158.8 (2)	C13—N4—C14—C1	-177.37 (17)
N1—C3—C4—N3	20.8 (4)	N4—C14—C15—C16	-3.2 (3)
N2—C3—C4—C5	14.3 (3)	C1—C14—C15—C16	176.44 (17)
N1—C3—C4—C5	-166.1 (2)	C14—C15—C16—C12	0.6 (3)
N3—C4—C5—C6	-173.1 (2)	C13—C12—C16—C15	2.4 (3)
C3—C4—C5—C6	13.5 (3)	C11—C12—C16—C15	-175.1 (2)
C4—C5—C6—C7	-48.2 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C11—H11B \cdots O3	0.97	2.35	2.803 (3)	108
C13—H13 \cdots N1	0.93	2.54	2.891 (3)	103

Fig. 1

