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N-(2-Pyridylmethyl)phthalimide

Olga Garduño-Beltrán, Perla Román-Bravo, Felipe Medrano* and Hugo Tlahuext

Centro de Investigaciones Químicas, Universidad Autónoma del Estado de Morelos. Av. Universidad 1001 Col., Chamilpa, CP 62209, Cuernavaca Mor., Mexico
Correspondence e-mail: fmedrano@uaem.mx

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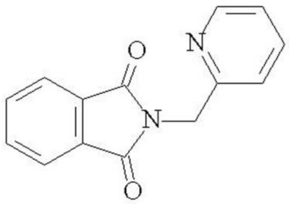
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.063; wR factor = 0.155; data-to-parameter ratio = 12.2.

In the title compound, $C_{14}H_{10}N_2O_2$, the phtalimide and 2-pyridylmethyl units are almost perpendicular, with an interplanar angle of 85.74 (2)°. In the crystal, molecules are linked by weak C—H···O interactions, forming chains running along the b axis. The packing is further stabilized by offset π–π interactions between adjacent pyridine rings, with a centroid–centroid distance of 3.855 (2) Å.

Related literature

For general backround to phthalimides, see: Ing & Manske (1926); Gibson & Bradshaw (1968); Ishii & Sakaguchi (2004). For their applications in photochemical synthesis and catalytic and chiral reactions, see: Yoon & Mariano (2001); Huang *et al.* (2006); Rodríguez *et al.* 2006. For their biological activity, see: Miyachi *et al.* (1997); Vázquez *et al.* (2005). For phthalimide derivatives, see: Vamecq *et al.* (2000). For analysis of hydrogen-bonding patterns, see: Hunter (1994); Desiraju (1991); Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{14}H_{10}N_2O_2$
M_r = 238.24
Monoclinic, $P2_1/c$
a = 11.7734 (18) Å
b = 14.239 (2) Å
c = 7.0698 (11) Å
β = 106.373 (3)°
V = 1137.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.45 × 0.28 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.958, $T_{\max}$ = 0.982
7150 measured reflections
1994 independent reflections
1567 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.155
S = 1.20
1994 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.18 e Å^{-3}
$\Delta\rho_{\min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2$^{\rm i}$	0.93	2.53	3.452 (3)	171
C6—H6···O1$^{\rm ii}$	0.93	2.53	3.452 (3)	171
C14—H14···O1$^{\rm iii}$	0.93	2.65	3.373 (3)	135
C11—H11···O2$^{\rm iv}$	0.93	2.57	3.401 (3)	148

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus*-NT (Bruker, 2001); data reduction: *SAINT-Plus*-NT; program(s) used to solve structure: *SHELXTL-NT* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2266).

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S1. Comment

Phthalimides are indispensable in protection and deprotection of primary amines (Ing & Manske, 1926; Gibson & Bradshaw, 1968; Ishii & Sakaguchi, 2004). Phthalimide derivatives are useful in photochemical synthesis (Yoon & Mariano, 2001) and catalytic reactions (Huang *et al.*, 2006; Rodríguez *et al.*, 2006). Some of the phthalimide derivatives have applications as drugs (Vamecq *et al.*, 2000). Thus, they have been used as novel biological modifiers for tumor necrosis (Miyachi *et al.*, 1997). Their fluorescence properties are highly environment sensitive (Vázquez *et al.*, 2005) and find application as biological probes. In our ongoing research on phthalimides as intermediates in supramolecular host design, we have synthesized the title compound, (I).

In (I), all bond lengths and angles show normal values. The phtalimide and 2-pyridylmethyl moieties are almost pependicular with an interplanar angle of 85.74° (Fig.1).

In the crystal, molecules are linked by weak C—H···O interactions (Table 1) (Desiraju, 1991; Hunter, 1994), forming chains running along the *b* axis.

In the hydrogen-bonding pattern, two graph sets (Bernstein *et al.*, 1995) can be distinguished: $R_2^2(10)$, involving atoms (···H6/C6—C8/O2···H3/C3—C1/O1)and $R_2^2(16)$, involving atoms $(\cdots\text{H14/C14/N2/C10/C9/N1/C1/O1}\cdots)_2$. Both patterns $R_2^2(10)$ and $R_2^2(16)$ are linked through weak C—H···O···H—C three center interactions, generating a motif belonging to the unitary graph set $R_6^4(30)$ (Fig. 2).

The packing is further stabilized by aromatic *π*-*π* interactions, with distances between the centroids of the pyridine rings [$Cg1$, $Cg1^{\prime i}$ (symmetry code: (i) 1 - *x*, -*y*, -*z*)] of 3.855 Å (Fig. 2).

S2. Experimental

A solution of 2-aminomethyl-pyridine (1 g, 9.25 mmol) in dimethylformamide(DMF) (5 ml) was added dropwise to (1.36 g, 9.18 mmol) of phthalic anhydride dissolved in 10 ml of DMF and refluxed for 6 h. The resulting solution was concentrated under reduced pressure to a viscous yellow liquid. Addition of water (25 ml) gave a colorless solid which was recovered by filtration and dried under vacuum. The product was recrystallized from ethanol to give suitable crystals for X-ray diffraction analysis (m.p. 399 K)

S3. Refinement

Non-hydrogen atoms were refined anisotropically. Aromatic and methylene H atoms were positioned geometrically and constrained using the riding-model approximation [$C—H_{aryl}$ = 0.93 Å, $U_{iso}(H_{aryl}) = 1.2\, U_{eq}(C_{aryl})$; $C—H_{methylene}$ = 0.97 Å, $U_{iso}(H_{methylene}) = 1.2\, U_{eq}(C_{methylene})$], but the coordinates were refined freely.

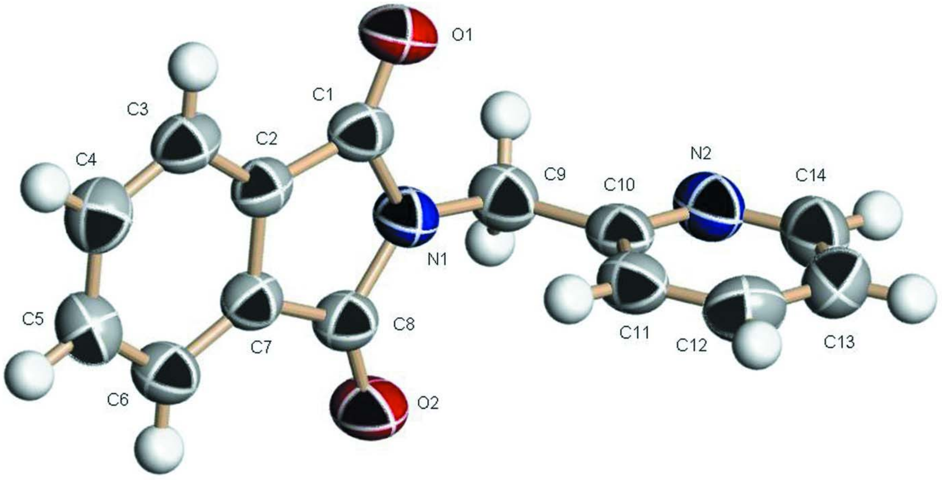

Figure 1

The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radius.

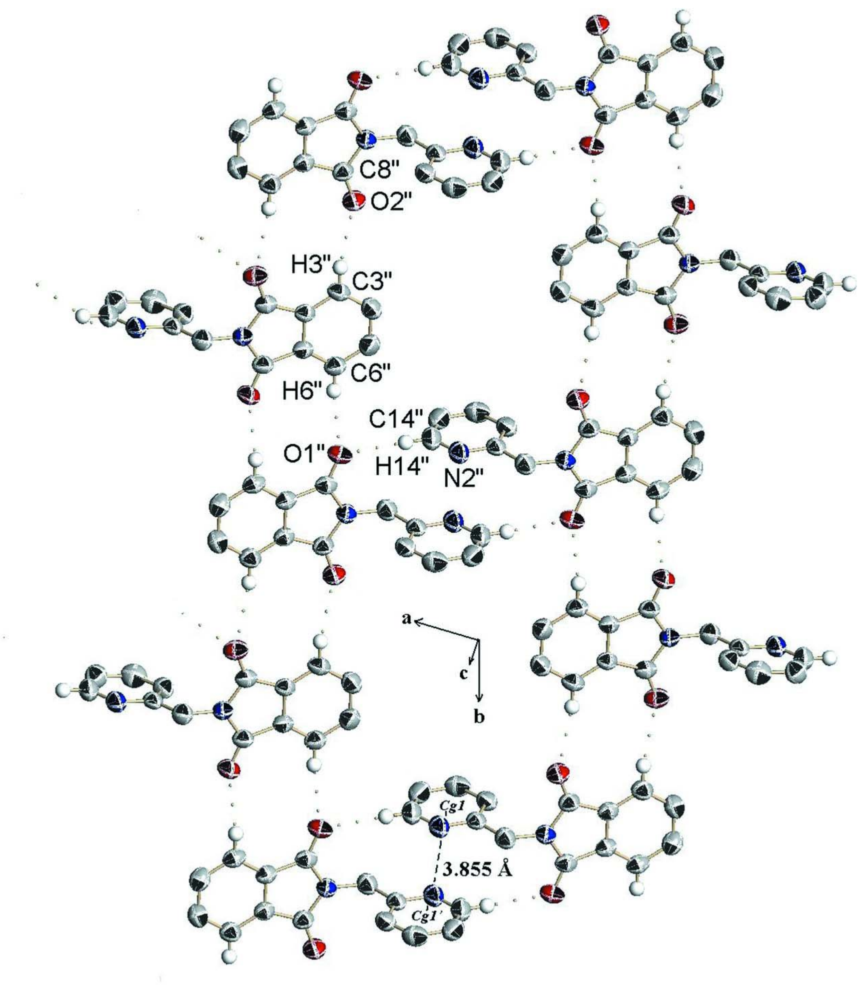

Figure 2

A view of the hydrogen bonds (dotted lines) in (I), showing the C3—H3···O2, C6—H6···O1, C14—H14···O1 interactions and the $R_2^2(10)$, $R_2^2(16)$, $R_6^4(30)$ motifs. Dashed line indicates the vector between pyridyl centroids (*Cg*1, *Cg*1′).

N-(2-Pyridylmethyl)phthalimide

Crystal data

$C_{14}H_{10}N_2O_2$
$M_r = 238.24$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.7734$ (18) Å
$b = 14.239$ (2) Å
$c = 7.0698$ (11) Å
$\beta = 106.373$ (3)°
$V = 1137.1$ (3) Å^3
$Z = 4$

$F(000) = 496$
$D_x = 1.392$ Mg m^{-3}
Melting point: 399 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2665 reflections
$\theta = 2.3$–26.8°
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Prism, colourless
0.45 × 0.28 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.958$, $T_{\max} = 0.982$

7150 measured reflections
1994 independent reflections
1567 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.028$
$\theta_{\max} = 25.0°$, $\theta_{\min} = 1.8°$
$h = -13 \rightarrow 13$
$k = -16 \rightarrow 16$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.155$
$S = 1.20$
1994 reflections
163 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
$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 0.1417P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.29$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8978 (2)	0.03798 (15)	0.1337 (3)	0.0493 (6)
C2	1.01324 (19)	0.07017 (14)	0.2618 (3)	0.0456 (5)
C3	1.1103 (2)	0.01983 (16)	0.3657 (3)	0.0533 (6)
H3	1.1100	−0.0455	0.3665	0.064*
C4	1.2086 (2)	0.07039 (18)	0.4690 (3)	0.0613 (7)
H4	1.2760	0.0384	0.5399	0.074*
C5	1.2088 (2)	0.16764 (17)	0.4691 (3)	0.0612 (6)
H5	1.2761	0.1997	0.5405	0.073*
C6	1.1106 (2)	0.21791 (16)	0.3648 (3)	0.0557 (6)
H6	1.1105	0.2832	0.3646	0.067*
C7	1.01340 (18)	0.16754 (14)	0.2616 (3)	0.0466 (5)
C8	0.8971 (2)	0.19976 (15)	0.1347 (3)	0.0515 (6)
C9	0.7148 (2)	0.11883 (15)	−0.0729 (3)	0.0576 (6)
H9A	0.7048	0.0621	−0.1517	0.069*
H9B	0.7075	0.1718	−0.1617	0.069*
C10	0.61635 (19)	0.12393 (13)	0.0243 (3)	0.0484 (6)

C11	0.6362 (2)	0.13358 (14)	0.2231 (3)	0.0573 (6)
H11	0.7128	0.1380	0.3066	0.069*
C12	0.5388 (3)	0.13668 (17)	0.2973 (4)	0.0705 (7)
H12	0.5489	0.1437	0.4319	0.085*
C13	0.4280 (2)	0.12929 (16)	0.1695 (5)	0.0708 (7)
H13	0.3614	0.1303	0.2156	0.085*
C14	0.4168 (2)	0.12042 (16)	−0.0258 (4)	0.0672 (7)
H14	0.3410	0.1159	−0.1118	0.081*
N1	0.83334 (16)	0.11904 (11)	0.0626 (3)	0.0530 (5)
N2	0.50806 (18)	0.11779 (12)	−0.1016 (3)	0.0610 (6)
O1	0.86171 (15)	−0.04110 (11)	0.0924 (2)	0.0652 (5)
O2	0.85977 (15)	0.27886 (11)	0.0976 (2)	0.0681 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0604 (15)	0.0411 (13)	0.0521 (13)	−0.0013 (10)	0.0249 (11)	0.0003 (10)
C2	0.0532 (13)	0.0419 (12)	0.0483 (12)	0.0033 (10)	0.0251 (10)	0.0040 (9)
C3	0.0655 (16)	0.0427 (12)	0.0571 (13)	0.0090 (11)	0.0260 (12)	0.0072 (10)
C4	0.0564 (15)	0.0678 (17)	0.0592 (14)	0.0082 (12)	0.0154 (12)	0.0116 (12)
C5	0.0554 (15)	0.0658 (17)	0.0603 (14)	−0.0079 (12)	0.0126 (12)	0.0027 (12)
C6	0.0610 (15)	0.0447 (13)	0.0630 (14)	−0.0036 (11)	0.0201 (12)	0.0014 (11)
C7	0.0528 (13)	0.0407 (12)	0.0507 (12)	0.0014 (9)	0.0217 (10)	0.0034 (9)
C8	0.0566 (14)	0.0404 (13)	0.0608 (14)	0.0018 (10)	0.0218 (11)	0.0040 (10)
C9	0.0572 (14)	0.0559 (15)	0.0555 (13)	−0.0027 (11)	0.0088 (11)	0.0002 (10)
C10	0.0528 (13)	0.0335 (12)	0.0540 (12)	0.0012 (9)	0.0069 (10)	0.0016 (9)
C11	0.0575 (14)	0.0506 (14)	0.0571 (13)	−0.0010 (11)	0.0052 (11)	−0.0051 (10)
C12	0.088 (2)	0.0634 (17)	0.0610 (15)	0.0016 (14)	0.0220 (15)	−0.0102 (12)
C13	0.0612 (16)	0.0625 (17)	0.091 (2)	0.0054 (12)	0.0250 (15)	−0.0024 (14)
C14	0.0513 (15)	0.0626 (17)	0.0794 (18)	−0.0002 (11)	0.0050 (13)	0.0013 (13)
N1	0.0516 (11)	0.0409 (11)	0.0647 (12)	−0.0015 (8)	0.0135 (9)	0.0013 (8)
N2	0.0555 (12)	0.0563 (13)	0.0627 (12)	−0.0001 (9)	0.0029 (10)	0.0025 (9)
O1	0.0795 (12)	0.0428 (10)	0.0732 (11)	−0.0070 (8)	0.0214 (9)	−0.0059 (8)
O2	0.0689 (11)	0.0409 (10)	0.0873 (12)	0.0063 (8)	0.0100 (9)	0.0071 (8)

Geometric parameters (Å, º)

C1—O1	1.210 (3)	C8—N1	1.389 (3)
C1—N1	1.395 (3)	C9—N1	1.453 (3)
C1—C2	1.477 (3)	C9—C10	1.506 (3)
C2—C3	1.374 (3)	C9—H9A	0.9700
C2—C7	1.386 (3)	C9—H9B	0.9700
C3—C4	1.383 (3)	C10—N2	1.336 (3)
C3—H3	0.9300	C10—C11	1.366 (3)
C4—C5	1.385 (4)	C11—C12	1.391 (3)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.382 (3)	C12—C13	1.365 (4)
C5—H5	0.9300	C12—H12	0.9300

C6—C7	1.373 (3)	C13—C14	1.356 (4)
C6—H6	0.9300	C13—H13	0.9300
C7—C8	1.483 (3)	C14—N2	1.329 (3)
C8—O2	1.210 (2)	C14—H14	0.9300

O1—C1—N1	124.4 (2)	N1—C9—H9A	108.6
O1—C1—C2	129.5 (2)	C10—C9—H9A	108.6
N1—C1—C2	106.10 (18)	N1—C9—H9B	108.6
C3—C2—C7	121.4 (2)	C10—C9—H9B	108.6
C3—C2—C1	130.5 (2)	H9A—C9—H9B	107.5
C7—C2—C1	108.13 (18)	N2—C10—C11	123.1 (2)
C2—C3—C4	117.2 (2)	N2—C10—C9	113.95 (19)
C2—C3—H3	121.4	C11—C10—C9	122.9 (2)
C4—C3—H3	121.4	C10—C11—C12	118.1 (2)
C3—C4—C5	121.5 (2)	C10—C11—H11	120.9
C3—C4—H4	119.3	C12—C11—H11	120.9
C5—C4—H4	119.3	C13—C12—C11	118.9 (3)
C6—C5—C4	121.1 (2)	C13—C12—H12	120.5
C6—C5—H5	119.4	C11—C12—H12	120.5
C4—C5—H5	119.4	C14—C13—C12	118.8 (2)
C7—C6—C5	117.3 (2)	C14—C13—H13	120.6
C7—C6—H6	121.3	C12—C13—H13	120.6
C5—C6—H6	121.3	N2—C14—C13	123.8 (2)
C6—C7—C2	121.5 (2)	N2—C14—H14	118.1
C6—C7—C8	130.5 (2)	C13—C14—H14	118.1
C2—C7—C8	107.97 (19)	C8—N1—C1	111.69 (19)
O2—C8—N1	124.4 (2)	C8—N1—C9	124.25 (18)
O2—C8—C7	129.5 (2)	C1—N1—C9	124.06 (18)
N1—C8—C7	106.11 (18)	C14—N2—C10	117.2 (2)
N1—C9—C10	114.79 (19)		

O1—C1—C2—C3	0.9 (4)	N1—C9—C10—C11	3.7 (3)
N1—C1—C2—C3	−178.73 (19)	N2—C10—C11—C12	0.3 (3)
O1—C1—C2—C7	179.4 (2)	C9—C10—C11—C12	−179.42 (19)
N1—C1—C2—C7	−0.2 (2)	C10—C11—C12—C13	0.5 (3)
C7—C2—C3—C4	−0.5 (3)	C11—C12—C13—C14	−0.9 (4)
C1—C2—C3—C4	177.91 (19)	C12—C13—C14—N2	0.5 (4)
C2—C3—C4—C5	0.5 (3)	O2—C8—N1—C1	−178.6 (2)
C3—C4—C5—C6	−0.3 (3)	C7—C8—N1—C1	0.7 (2)
C4—C5—C6—C7	0.0 (3)	O2—C8—N1—C9	2.3 (3)
C5—C6—C7—C2	0.1 (3)	C7—C8—N1—C9	−178.38 (18)
C5—C6—C7—C8	−178.8 (2)	O1—C1—N1—C8	−180.0 (2)
C3—C2—C7—C6	0.2 (3)	C2—C1—N1—C8	−0.3 (2)
C1—C2—C7—C6	−178.53 (18)	O1—C1—N1—C9	−0.9 (3)
C3—C2—C7—C8	179.31 (18)	C2—C1—N1—C9	178.74 (18)
C1—C2—C7—C8	0.6 (2)	C10—C9—N1—C8	−87.1 (2)
C6—C7—C8—O2	−2.5 (4)	C10—C9—N1—C1	93.9 (2)
C2—C7—C8—O2	178.4 (2)	C13—C14—N2—C10	0.3 (3)

C6—C7—C8—N1	178.2 (2)	C11—C10—N2—C14	−0.7 (3)
C2—C7—C8—N1	−0.8 (2)	C9—C10—N2—C14	179.06 (18)
N1—C9—C10—N2	−176.06 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O2^{i}	0.93	2.53	3.452 (3)	171
C6—H6···O1^{ii}	0.93	2.53	3.452 (3)	171
C14—H14···O1^{iii}	0.93	2.65	3.373 (3)	135
C11—H11···O2^{iv}	0.93	2.57	3.401 (3)	148

Symmetry codes: (i) −*x*+2, *y*−1/2, −*z*+1/2; (ii) −*x*+2, *y*+1/2, −*z*+1/2; (iii) −*x*+1, −*y*, −*z*; (iv) *x*, −*y*+1/2, *z*+1/2.