Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-[(*E*)-2-Hydroxy-5-methoxybenzylidene]pyridine-4-carbohydrazide

Hadi Kargar,[a] Reza Kia,[b] Mehmet Akkurt[c]* and Orhan Büyükgüngör[d]

[a]Department of Chemistry, School of Science, Payame Noor University, Ardakan, Yazd, Iran, [b]Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran, [c]Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, and [d]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey
Correspondence e-mail: akkurt@erciyes.edu.tr

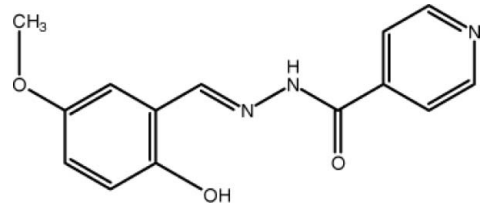
Received 24 October 2010; accepted 24 October 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.046; wR factor = 0.114; data-to-parameter ratio = 8.1.

In the title compound, $C_{14}H_{13}N_3O_3$, the dihedral angle between the pyridine and benzene rings is 15.17 (18)°. The torsion angle of the –C=N–N–C– system between two aromatic rings is −167.1 (3)°. Intramolecular O—H···N hydrogen bonding generates S(6) rings. In the crystal structure, neighbouring molecules are linked together along the c axis by weak intermolecular C—H···O and N—H···O hydrogen bonds, generating $R_1^2(6)$ ring motifs.

Related literature

For the tuberculostatic activity of isoniazid (isonicotinylhydrazine) derivatives, see: Janin (2007); Maccari *et al.* (2005). For the synthesis of the isoniazid derivative, see: Lourenco *et al.* (2008). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{14}H_{13}N_3O_3$
M_r = 271.27
Monoclinic, *Cc*
a = 6.1114 (6) Å
b = 29.489 (3) Å
c = 7.4820 (7) Å
β = 96.696 (8)°
V = 1339.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.67 × 0.34 × 0.12 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.962, T_{max} = 0.988
4353 measured reflections
1542 independent reflections
1166 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.114
S = 1.11
1542 reflections
191 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.96 (4)	1.80 (4)	2.628 (4)	142 (4)
N2—H2···O3^{i}	0.88 (4)	2.03 (4)	2.872 (4)	161 (4)
C8—H8···O3^{i}	0.93	2.43	3.188 (4)	139

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS 2 diffractometer (purchased under grant F.279 of the University Research Fund). HK thanks Payame Noor University for the financial support of this work. RK thanks the Science and Research Branch of Islamic Azad University of Tehran.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5051).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Janin, Y. L. (2007). *Bioorg. Med. Chem.* **15**, 2479–2513.
Lourenco, M. C. S., Ferreira, M. L., de Souza, M. V. N., Peralta, M. A., Vasconcelos, T. R. A. & Henriques, M. G. M. O. (2008). *Eur. J. Med. Chem.* **43**, 1344–1347.
Maccari, R., Ottana, R. & Vigorita, M. G. (2005). *Bioorg. Med. Chem. Lett.* **15**, 2509–2513.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stoe & Cie (2002). *X-AREA* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.

supporting information

Acta Cryst. (2010). E**66**, o2982 [https://doi.org/10.1107/S1600536810043382]

N′-[(*E*)-2-Hydroxy-5-methoxybenzylidene]pyridine-4-carbohydrazide

Hadi Kargar, Reza Kia, Mehmet Akkurt and Orhan Büyükgüngör

S1. Comment

In the search for new biologically active compounds, isoniazid (isonicotinylhydrazine) derivatives have been found to possess potential tuberculostatic activity (Janin, 2007; Maccari *et al.*, 2005). Here, we present the crystal structure of the title compound, (I).

In the title compound (I), (Fig. 1), the dihedral angle between the pyridine (C10–C14) and benzene (C1–C6) rings is 15.17 (18)°. The C8–N1–N2–C9 torsion angle is -167.1 (3) °.

Intramolecular O1—H1···N1 hydrogen bonding generates *S*(6) rings (Bernstein *et al.*, 1995) (Table 1, Fig. 2). In the crystal structure, neighbouring molecules are linked together by weak intermolecular C—H···O and N—H···O hydrogen bonds (Table 1, Fig. 2), generating $R_1^2(6)$ ring motifs (Bernstein *et al.*, 1995), and linking the molecules along the *c* axis.

S2. Experimental

The isoniazid derivative was prepared following procedure reported by Lourenco *et al.*, (2008). 5-methoxysalicyl-aldehyde (1.0 mmol) was added to isoniazid (1.0 mmol) in ethanol. After stirring for 3 h at reflux condition, the resulting mixture was concentrated at room temperature. The residue was purified by washing with cold ethanol and diethyl ether to give the pure derivative. Colourless single crystals suitable for X-ray analysis were obtained by re-crystallization from methanol.

S3. Refinement

In the absence of significant anomalous dispersion effects, Freidel pairs were merged. The calculation of the Flack (1983) parameter was suppressed by the MERG 4 command in *SHELXL*97 (Sheldrick, 2008), as the lack of anomalous scatterers did not allow the determination of the absolute configuration from the X-ray measurements. The H atoms of the O—H and N—H groups were found from a difference Fourier map and refined freely [O1—H1 = 0.96 (4) and N2—H2 = 0.88 (4) Å]. The remaining H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and U_{iso}(H) = 1.5U_{eq}(C) for methyl H and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H.

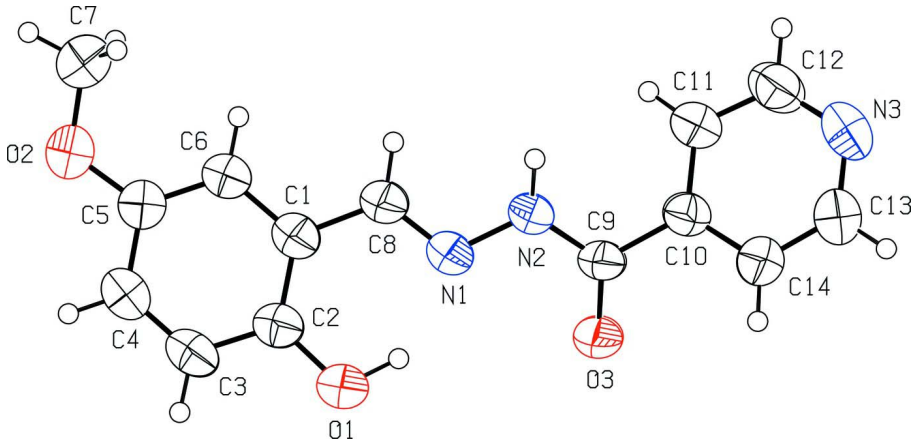


Figure 1

The title molecule, with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

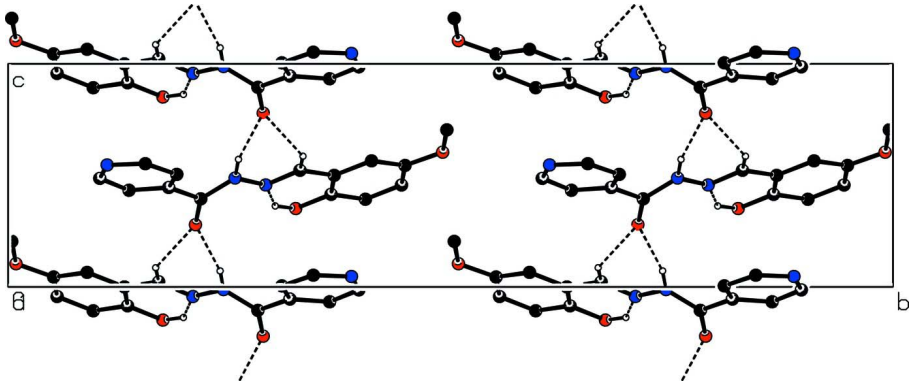


Figure 2

The packing and hydrogen bonding interactions of (I), down *a* axis, showing $R_1^2(6)$ ring motifs. All H atoms not involved in hydrogen bonding are omitted for clarity.

N′-[(*E*)-2-Hydroxy-5-methoxybenzylidene]pyridine-4-carbohydrazide

Crystal data

$C_{14}H_{13}N_3O_3$
$M_r = 271.27$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 6.1114\ (6)$ Å
$b = 29.489\ (3)$ Å
$c = 7.4820\ (7)$ Å
$\beta = 96.696\ (8)°$
$V = 1339.2\ (2)$ Å^3
$Z = 4$

$F(000) = 568$
$D_x = 1.345$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7613 reflections
$\theta = 2.8–28.0°$
$\mu = 0.10$ mm^{-1}
$T = 296$ K
Prism, colourless
0.67 × 0.34 × 0.12 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.962, T_{max} = 0.988
4353 measured reflections
1542 independent reflections
1166 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 27.5°, θ_{min} = 2.8°
h = −7→7
k = −38→35
l = −9→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.114
S = 1.11
1542 reflections
191 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0090 (19)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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}
O1	−0.1045 (4)	0.82503 (10)	0.3515 (4)	0.0727 (9)
O2	0.2101 (5)	0.99107 (9)	0.6041 (5)	0.0844 (10)
O3	0.2501 (4)	0.71171 (8)	0.2791 (4)	0.0743 (9)
N1	0.2870 (4)	0.79115 (10)	0.4570 (4)	0.0619 (9)
N2	0.4398 (4)	0.75656 (9)	0.4882 (4)	0.0622 (9)
N3	0.8707 (5)	0.61195 (13)	0.5468 (5)	0.0794 (11)
C1	0.1994 (5)	0.86852 (12)	0.5002 (4)	0.0572 (10)
C2	−0.0172 (5)	0.86497 (12)	0.4151 (5)	0.0599 (11)
C3	−0.1453 (5)	0.90380 (14)	0.3930 (6)	0.0753 (15)
C4	−0.0645 (6)	0.94459 (14)	0.4568 (6)	0.0766 (13)
C5	0.1486 (5)	0.94855 (12)	0.5445 (5)	0.0646 (11)
C6	0.2792 (5)	0.91072 (12)	0.5652 (5)	0.0611 (11)
C7	0.4191 (7)	0.99583 (16)	0.7042 (7)	0.0830 (14)
C8	0.3464 (5)	0.82985 (12)	0.5228 (5)	0.0591 (11)

C9	0.4075 (4)	0.71774 (11)	0.3949 (4)	0.0574 (10)
C10	0.5728 (5)	0.68156 (11)	0.4456 (4)	0.0564 (10)
C11	0.7920 (5)	0.69069 (13)	0.5046 (5)	0.0672 (11)
C12	0.9319 (6)	0.65507 (17)	0.5525 (6)	0.0778 (15)
C13	0.6605 (6)	0.60362 (13)	0.4866 (6)	0.0739 (14)
C14	0.5073 (5)	0.63664 (12)	0.4332 (5)	0.0655 (11)
H1	0.007 (7)	0.8019 (15)	0.363 (6)	0.080 (12)*
H2	0.552 (7)	0.7604 (14)	0.572 (6)	0.079 (11)*
H3	−0.28770	0.90210	0.33400	0.0900*
H4	−0.15340	0.97020	0.44150	0.0920*
H6	0.42200	0.91300	0.62290	0.0730*
H7A	0.53150	0.98860	0.62920	0.1250*
H7B	0.43020	0.97560	0.80540	0.1250*
H7C	0.43790	1.02650	0.74600	0.1250*
H8	0.48570	0.83320	0.58600	0.0710*
H11	0.84350	0.72040	0.51180	0.0810*
H12	1.07860	0.66170	0.59120	0.0940*
H13	0.61430	0.57360	0.48040	0.0880*
H14	0.36330	0.62890	0.38980	0.0790*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0555 (12)	0.0673 (16)	0.0905 (19)	0.0003 (11)	−0.0119 (12)	−0.0055 (13)
O2	0.0782 (15)	0.0598 (16)	0.111 (2)	0.0057 (12)	−0.0066 (15)	−0.0122 (16)
O3	0.0669 (13)	0.0602 (14)	0.0864 (19)	0.0021 (11)	−0.0310 (12)	−0.0050 (13)
N1	0.0523 (12)	0.0570 (17)	0.0721 (19)	0.0056 (12)	−0.0115 (12)	0.0015 (14)
N2	0.0541 (12)	0.0544 (16)	0.0716 (18)	0.0064 (12)	−0.0195 (12)	−0.0042 (14)
N3	0.0687 (18)	0.079 (2)	0.090 (2)	0.0237 (16)	0.0069 (15)	0.0059 (19)
C1	0.0511 (15)	0.061 (2)	0.0581 (19)	0.0045 (13)	0.0008 (13)	0.0026 (15)
C2	0.0478 (14)	0.065 (2)	0.066 (2)	−0.0007 (14)	0.0023 (13)	0.0000 (17)
C3	0.0481 (17)	0.078 (3)	0.097 (3)	0.0108 (16)	−0.0031 (18)	0.003 (2)
C4	0.0616 (18)	0.069 (2)	0.096 (3)	0.0148 (17)	−0.0043 (18)	−0.002 (2)
C5	0.0606 (17)	0.058 (2)	0.074 (2)	0.0017 (15)	0.0028 (15)	−0.0040 (18)
C6	0.0495 (15)	0.062 (2)	0.070 (2)	0.0014 (13)	−0.0011 (14)	−0.0002 (16)
C7	0.081 (2)	0.072 (2)	0.093 (3)	−0.0038 (19)	−0.003 (2)	−0.011 (2)
C8	0.0519 (14)	0.059 (2)	0.063 (2)	0.0013 (13)	−0.0081 (13)	0.0011 (16)
C9	0.0458 (13)	0.0562 (19)	0.066 (2)	−0.0026 (12)	−0.0107 (13)	0.0011 (16)
C10	0.0504 (14)	0.0602 (19)	0.0565 (18)	0.0030 (13)	−0.0027 (13)	−0.0032 (16)
C11	0.0520 (15)	0.070 (2)	0.077 (2)	0.0048 (15)	−0.0028 (15)	−0.0028 (19)
C12	0.0548 (16)	0.090 (3)	0.087 (3)	0.0123 (18)	0.0011 (17)	−0.001 (2)
C13	0.074 (2)	0.061 (2)	0.086 (3)	0.0101 (17)	0.007 (2)	−0.0042 (19)
C14	0.0616 (17)	0.058 (2)	0.076 (2)	0.0017 (14)	0.0039 (16)	−0.0093 (18)

Geometric parameters (Å, º)

O1—C2	1.356 (5)	C5—C6	1.370 (5)
O2—C5	1.369 (5)	C9—C10	1.488 (4)

O2—C7	1.410 (6)	C10—C11	1.387 (4)
O3—C9	1.230 (4)	C10—C14	1.384 (5)
O1—H1	0.96 (4)	C11—C12	1.375 (6)
N1—N2	1.384 (4)	C13—C14	1.377 (5)
N1—C8	1.279 (5)	C3—H3	0.9300
N2—C9	1.343 (4)	C4—H4	0.9300
N3—C13	1.334 (5)	C6—H6	0.9300
N3—C12	1.325 (6)	C7—H7A	0.9600
N2—H2	0.88 (4)	C7—H7B	0.9600
C1—C6	1.403 (5)	C7—H7C	0.9600
C1—C2	1.404 (4)	C8—H8	0.9300
C1—C8	1.449 (5)	C11—H11	0.9300
C2—C3	1.386 (5)	C12—H12	0.9300
C3—C4	1.365 (6)	C13—H13	0.9300
C4—C5	1.393 (5)	C14—H14	0.9300

O1···N1	2.628 (4)	C7···H6	2.5200
O1···C10^{i}	3.347 (4)	C8···H1	2.42 (4)
O2···C7^{ii}	3.409 (6)	C11···H2	2.61 (4)
O3···N2^{i}	2.872 (4)	C12···H3^{viii}	3.0600
O3···C12^{iii}	3.418 (5)	C14···H12^{iii}	3.0900
O3···N1	2.691 (4)	H1···N1	1.80 (4)
O3···C8^{i}	3.188 (4)	H1···C8	2.42 (4)
O1···H12^{iv}	2.6100	H2···C11	2.61 (4)
O2···H13^{v}	2.6500	H2···H8	2.1900
O2···H7B^{ii}	2.9100	H2···H11	2.2300
O3···H14	2.6400	H2···O3^{vi}	2.03 (4)
O3···H2^{i}	2.03 (4)	H3···N3^{iv}	2.8500
O3···H8^{i}	2.4300	H3···C12^{iv}	3.0600
N1···O1	2.628 (4)	H4···H7A^{iii}	2.5700
N1···O3	2.691 (4)	H6···C7	2.5200
N1···C11^{i}	3.431 (5)	H6···H7A	2.3300
N2···O3^{vi}	2.872 (4)	H6···H7B	2.2900
N1···H1	1.80 (4)	H6···H8	2.4100
N2···H11	2.6700	H7A···C6	2.7800
N3···H7C^{vii}	2.9300	H7A···H4^{xi}	2.5700
N3···H3^{viii}	2.8500	H7A···H6	2.3300
C1···C14^{ix}	3.576 (5)	H7B···C6	2.7100
C5···C7^{ii}	3.590 (6)	H7B···H6	2.2900
C6···C13^{ix}	3.344 (6)	H7B···O2^{x}	2.9100
C7···O2^{x}	3.409 (6)	H7C···C5^{x}	3.0900
C7···C5^{x}	3.590 (6)	H7C···N3^{v}	2.9300
C8···O3^{vi}	3.188 (4)	H8···H2	2.1900
C10···O1^{vi}	3.347 (4)	H8···H6	2.4100
C11···N1^{vi}	3.431 (5)	H8···O3^{vi}	2.4300
C12···O3^{xi}	3.418 (5)	H11···N2	2.6700
C13···C6^{xii}	3.344 (6)	H11···H2	2.2300
C14···C1^{xii}	3.576 (5)	H12···C14^{xi}	3.0900

C5···H7C^{ii}	3.0900	H12···O1^{viii}	2.6100
C6···H7A	2.7800	H13···O2^{vii}	2.6500
C6···H7B	2.7100	H14···O3	2.6400

C5—O2—C7	117.5 (3)	C10—C11—C12	118.9 (3)
C2—O1—H1	110 (3)	N3—C12—C11	124.1 (4)
N2—N1—C8	115.9 (3)	N3—C13—C14	124.3 (4)
N1—N2—C9	119.0 (3)	C10—C14—C13	118.4 (3)
C12—N3—C13	116.4 (4)	C2—C3—H3	120.00
C9—N2—H2	122 (3)	C4—C3—H3	120.00
N1—N2—H2	119 (3)	C3—C4—H4	119.00
C2—C1—C6	119.6 (3)	C5—C4—H4	119.00
C2—C1—C8	122.2 (3)	C1—C6—H6	120.00
C6—C1—C8	118.2 (3)	C5—C6—H6	120.00
O1—C2—C3	118.8 (3)	O2—C7—H7A	109.00
O1—C2—C1	122.4 (3)	O2—C7—H7B	109.00
C1—C2—C3	118.8 (3)	O2—C7—H7C	109.00
C2—C3—C4	120.7 (3)	H7A—C7—H7B	109.00
C3—C4—C5	121.3 (4)	H7A—C7—H7C	109.00
C4—C5—C6	119.0 (3)	H7B—C7—H7C	110.00
O2—C5—C4	115.9 (3)	N1—C8—H8	120.00
O2—C5—C6	125.1 (3)	C1—C8—H8	120.00
C1—C6—C5	120.6 (3)	C10—C11—H11	121.00
N1—C8—C1	120.9 (3)	C12—C11—H11	121.00
O3—C9—N2	123.0 (3)	N3—C12—H12	118.00
O3—C9—C10	121.9 (3)	C11—C12—H12	118.00
N2—C9—C10	115.1 (2)	N3—C13—H13	118.00
C11—C10—C14	117.9 (3)	C14—C13—H13	118.00
C9—C10—C11	122.9 (3)	C10—C14—H14	121.00
C9—C10—C14	119.1 (3)	C13—C14—H14	121.00

C7—O2—C5—C6	−4.1 (6)	O1—C2—C3—C4	179.3 (4)
C7—O2—C5—C4	175.8 (4)	C2—C3—C4—C5	0.5 (6)
N2—N1—C8—C1	−179.4 (3)	C3—C4—C5—O2	−179.3 (4)
C8—N1—N2—C9	−167.1 (3)	C3—C4—C5—C6	0.6 (6)
N1—N2—C9—C10	−176.4 (3)	O2—C5—C6—C1	179.5 (3)
N1—N2—C9—O3	1.7 (5)	C4—C5—C6—C1	−0.4 (5)
C13—N3—C12—C11	1.5 (6)	O3—C9—C10—C14	−30.5 (4)
C12—N3—C13—C14	−0.7 (6)	O3—C9—C10—C11	149.2 (3)
C8—C1—C6—C5	178.8 (3)	N2—C9—C10—C14	147.6 (3)
C6—C1—C2—C3	1.8 (5)	N2—C9—C10—C11	−32.7 (4)
C2—C1—C6—C5	−0.8 (5)	C14—C10—C11—C12	−1.8 (5)
C8—C1—C2—O1	1.3 (5)	C9—C10—C11—C12	178.5 (3)
C8—C1—C2—C3	−177.8 (3)	C9—C10—C14—C13	−177.8 (3)
C6—C1—C2—O1	−179.2 (3)	C11—C10—C14—C13	2.5 (5)
C2—C1—C8—N1	3.7 (5)	C10—C11—C12—N3	−0.3 (6)

C6—C1—C8—N1	−175.9 (3)	N3—C13—C14—C10	−1.4 (6)
C1—C2—C3—C4	−1.6 (6)		

Symmetry codes: (i) *x*−1/2, −*y*+3/2, *z*−1/2; (ii) *x*, −*y*+2, *z*−1/2; (iii) *x*−1, *y*, *z*; (iv) *x*−3/2, −*y*+3/2, *z*−1/2; (v) *x*−1/2, *y*+1/2, *z*; (vi) *x*+1/2, −*y*+3/2, *z*+1/2; (vii) *x*+1/2, *y*−1/2, *z*; (viii) *x*+3/2, −*y*+3/2, *z*+1/2; (ix) *x*−1/2, −*y*+3/2, *z*+1/2; (x) *x*, −*y*+2, *z*+1/2; (xi) *x*+1, *y*, *z*; (xii) *x*+1/2, −*y*+3/2, *z*−1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.96 (4)	1.80 (4)	2.628 (4)	142 (4)
N2—H2···O3^{vi}	0.88 (4)	2.03 (4)	2.872 (4)	161 (4)
C8—H8···O3^{vi}	0.93	2.43	3.188 (4)	139

Symmetry code: (vi) *x*+1/2, −*y*+3/2, *z*+1/2.