Acta Cryst E STRUCTURE REPORTS

ISSN 1600-5368

Received 14 November 2014
Accepted 25 November 2014

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

Keywords: crystal structure; hydroxyimino; acetohydrazide; pyridylethylidene; hydrogen bonding; π–π stacking interactions

CCDC reference: 1035993
Supporting information: this article has supporting information at journals.iucr.org/e

Crystal structure of 2-hydroxyimino-2-(pyridin-2-yl)-*N*′-[1-(pyridin-2-yl)ethylidene]acetohydrazide

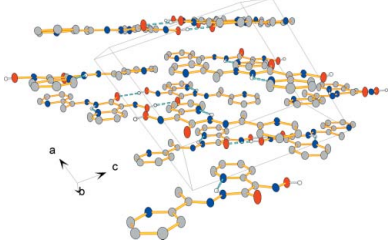
Maxym O. Plutenko,[a]* Rostislav D. Lampeka,[a] Matti Haukka[b] and Ebbe Nordlander[c]

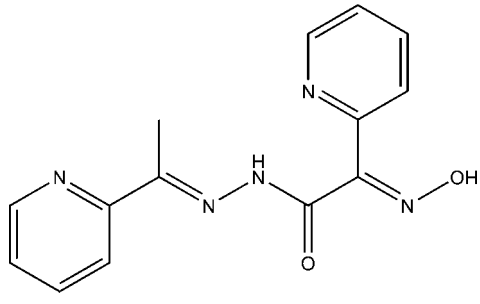
[a]Department of Chemistry, National Taras Shevchenko University, Volodymyrska Street 64, 01601 Kyiv, Ukraine, [b]Department of Chemistry, University of Jyvaskyla, PO Box 35, FI-40014 Jyvaskyla, Finland, and [c]Inorganic Chemistry, Center for Chemistry and Chemical Engineering, Lund University, Box 124, SE-221 00 Lund, Sweden. *Correspondence e-mail: plutenkom@gmail.com

The molecule of the title compound, $C_{14}H_{13}N_5O_2$, is approximately planar (r.m.s deviation for all non-H atoms = 0.093 Å), with the planes of the two pyridine rings inclined to one another by 5.51 (7)°. The oxime group is *syn* to the amide group, probably due to the formation of an intramolecular N—H···N hydrogen bond that forms an *S*(6) ring motif. In the crystal, molecules are linked by pairs of bifurcated O—H···(O,N) hydrogen bonds, forming inversion dimers. The latter are linked *via* C—H···O and C—H···N hydrogen bonds, forming sheets lying parallel to (502). The sheets are linked *via* π–π stacking interactions [inter-centroid distance = 3.7588 (9) Å], involving the pyridine rings of inversion-related molecules, forming a three-dimensional structure.

1. Chemical context

Polynuclear oxime-containing ligands have attracted considerable interest because of their ability to act as efficient bridging ligands and for their tendency to form polynuclear metal complexes (Penkova *et al.*, 2010; Pavlishchuk *et al.*, 2010, 2011). The presence of additional non-oxime donor functions (*e.g.* hydrazide, azomethine, pyridine) in the ligand molecule favours the formation of metal complexes with strong magnetic exchange interactions between the metal ions (Pavlishchuk *et al.*, 2011), and complexes which efficiently stabilize unusual high oxidation states of 3*d* metal ions (Kanderal *et al.*, 2005; Fritsky *et al.*, 2006). As a part of our research study, we present the structure of the title compound, which contains several donor functions of a different nature; oxime, hydrazide, and two different pyridine groups.





2. Structural commentary

The molecular structure of the title compound is illustrated in Fig. 1. The molecule is approximately planar (r.m.s deviation

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···N1	0.89 (2)	1.84 (2)	2.6126 (17)	144 (2)
O1—H1···O2^{i}	0.93 (2)	1.98 (2)	2.8327 (14)	151 (2)
O1—H1···N2^{i}	0.93 (2)	2.13 (2)	2.8489 (16)	133 (2)
C2—H2···O2^{ii}	0.95	2.54	3.1985 (15)	127
C3—H3*A*···O1^{iii}	0.95	2.56	3.4755 (15)	163
C13—H13···N5^{iv}	0.95	2.46	3.3811 (19)	163

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

for all non-H atoms = 0.093 Å) with the maximum deviations from the mean plane being 0.255 (1) Å for atom N1, and 0.198 (1) Å for atom O1. The two pyridine rings (N1/C1–C5) and N5/C10–C14) are inclined to one another by 5.51 (7)°. The N2—O1 [1.3691 (14) Å] and C6—N2 [1.2866 (17) Å] bond lengths of the oxime group have typical values (Fritsky *et al.*, 1998). The pyridine N atom, N1, is situated in an *anti* position with respect to the azomethine group, in accordance with the structures of earlier synthesized ligands of this type (Plutenko *et al.*, 2011, 2013).

The N4—N3, N3—C7 and C7—O2 bond lengths of the hydrazide group are 1.3776 (16), 1.3471 (18) and 1.2269 (17) Å, respectively, typical for protonated moieties of this type (Plutenko *et al.*, 2011, 2013). The oxime group is situated in a *syn* position with respect to the amide group, in contrast to earlier synthesized ligands of this type (Plutenko *et al.*, 2012, 2013). Such a disposition of these moieties is atypical for amide derivatives of 2-hydroxyiminopropanoic acid (Onindo *et al.*, 1995; Sliva *et al.*, 1997; Duda *et al.*, 1997). It can be explained by the presence of an intramolecular N3—H3···N1 hydrogen bond in which the azomethine N atom, N3, acts as donor and the pyridine N atom, N1, acts as an acceptor (Fig. 1 and Table 1).

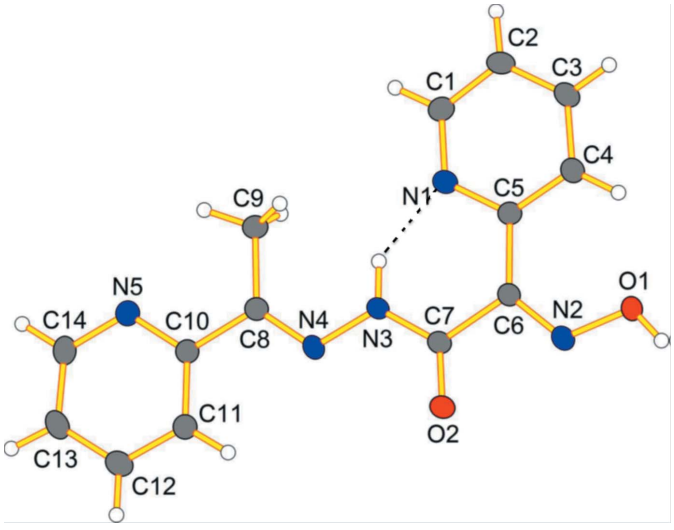


Figure 1
A view of the molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular N—H···N hydrogen bond is shown as a dashed line (see Table 1 for details).

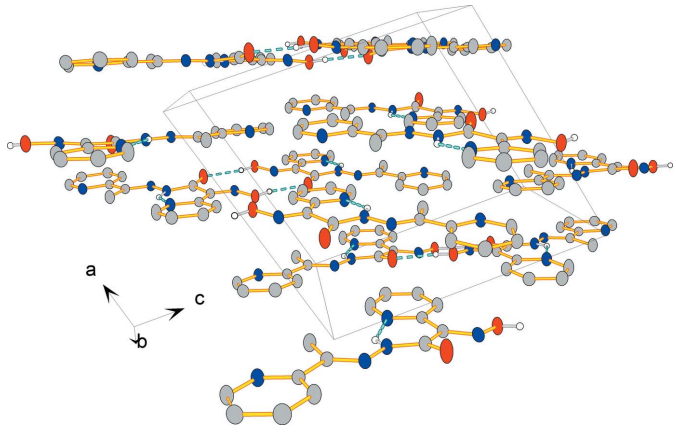


Figure 2
Crystal packing of the title compound viewed along the *b* axis. Hydrogen bonds are indicated by dashed lines (see Table 1 for details). H atoms not involved in hydrogen bonds have been omitted for clarity.

3. Supramolecular features

In the crystal, molecules are linked by pairs of bifurcated O—H···(O,N) hydrogen bonds forming inversion dimers (Fig. 2 and Table 1). The dimers are linked *via* C—H···O and C—H···N hydrogen bonds, forming sheets lying parallel to plane (502). The sheets are linked *via* π–π stacking interactions, forming a three-dimensional structure [$Cg1\cdots Cg2^{i}$ = 3.7588 (9) Å; *Cg*1 and *Cg*2 are the centroids of pyridine rings N1/C1–C5 and N5/C10–C14, respectively; symmetry code: (i) $-x+1, -y+2, -z+1$].

4. Database survey

The crystal structures of two very similar compounds have been reported, *viz.* 2-hydroxyimino-*N*′-(1-(pyridin-2-yl)ethylidene)propanohydrazide (Moroz *et al.*, 2009) and two polymorphs of 2-(3,5-dimethyl-1*H*-pyrazol-1-yl)-2-(hydroxyimino)-*N*′-(1-(pyridin-2-yl) ethylidene)acetohydrazide (Plutenko *et al.*, 2012, 2013).

5. Synthesis and crystallization

A solution of 2-hydroxyimino-2-(pyridin-2-yl)acetohydrazide (0.36 g, 2 mmol), prepared according to a published procedure (Zyl *et al.*, 1961; Kolar *et al.*, 1991), in methanol (20 ml) was treated with 2-acetylpyridine (0.242 g, 2 mmol) and the mixture was heated under reflux for 3 h. After cooling, the solvent was evaporated under vacuum and the resulting product was recrystallized from methanol, giving colourless block-like crystals of the title compound (yield 0.52 g; 92%).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The N—H and O—H hydrogen atoms were located in difference Fourier maps and freely refined. The C-bound H atoms were positioned geometrically

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{13}N_5O_2$
M_r	283.29
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	123
a, b, c (Å)	11.4319 (9), 9.3598 (4), 12.4297 (9)
β (°)	105.016 (3)
V (Å^3)	1284.57 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.27 × 0.15 × 0.14
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 1996)
T_{min}, T_{max}	0.973, 0.986
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7900, 2850, 2226
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.115, 1.05
No. of reflections	2850
No. of parameters	196
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.22

Computer programs: *APEX2* and *SAINT* (Bruker, 2010), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *DIAMOND* (Brandenburg, 2008) and *PLATON* (Spek, 2009).

and constrained to ride on their parent atoms, with C—H = 0.95–0.98 Å, and with $U_{iso} = 1.5U_{eq}$(C) for methyl H atoms and = $1.2U_{eq}$(C) for other H atoms.

Acknowledgements

Financial support from the State Fund for Fundamental Researches of Ukraine (grant No. F40.3/041) and the Swedish Institute (Visby Program) is gratefully acknowledged.

References

Brandenburg, K. (2008). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2010). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Duda, A. M., Karaczyn, A., Kozłowski, H., Fritsky, I. O., Głowiak, T., Prisyazhnaya, E. V., Sliva, T. Yu. & Świątek-Kozłowska, J. (1997). *J. Chem. Soc. Dalton Trans.* pp. 3853–3859.
Fritsky, I. O., Kozłowski, H., Kanderal, O. M. M., Świątek-Kozłowska, J., Gumienna-Kontecka, E. & Meyer, F. (2006). *Chem. Commun.* pp. 4125–4127.
Fritsky, I. O., Kozłowski, H., Sadler, P. J., Yefetova, O. P., Świątek-Kozłowska, J., Kalibabchuk, V. A. & Głowiak, T. (1998). *J. Chem. Soc. Dalton Trans.* pp. 3269–3274.
Kanderal, O. M., Kozłowski, H., Dobosz, A., Świątek-Kozłowska, J., Meyer, F. & Fritsky, I. O. (2005). *Dalton Trans.* pp. 1428–1437.
Kolar, P., Petrič, A., Tišler, M. & Felluga, F. (1991). *J. Heterocycl. Chem.* **28**, 1715–1720.
Moroz, Y. S., Konovalova, I. S., Iskenderov, T. S., Pavlova, S. V. & Shishkin, O. V. (2009). *Acta Cryst.* E**65**, o2242.
Onindo, C. O., Sliva, T. Yu., Kowalik-Jankowska, T., Fritsky, I. O., Buglyo, P., Pettit, L. D., Kozłowski, H. & Kiss, T. (1995). *J. Chem. Soc. Dalton Trans.* pp. 3911–3915.
Pavlishchuk, A. V., Kolotilov, S. V., Zeller, M., Shvets, O. V., Fritsky, I. O., Lofland, S. E., Addison, A. W. & Hunter, A. D. (2011). *Eur. J. Inorg. Chem.* **31**, 4826–4836.
Pavlishchuk, A. V., Kolotilov, S. V., Zeller, M., Thompson, L. K., Fritsky, I. O., Addison, A. W. & Hunter, A. D. (2010). *Eur. J. Inorg. Chem.* **30**, 4851–4858.
Penkova, L. V., Demeshko, S., Pavlenko, V. A., Dechert, S., Meyer, F. & Fritsky, I. O. (2010). *Inorg. Chim. Acta*, **363**, 3036–3040.
Plutenko, M. O., Lampeka, R. D., Haukka, M. & Nordlander, E. (2012). *Acta Cryst.* E**68**, o3381.
Plutenko, M. O., Lampeka, R. D., Haukka, M. & Nordlander, E. (2013). *Acta Cryst.* E**69**, o765–o766.
Plutenko, M. O., Lampeka, R. D., Moroz, Y. S., Haukka, M. & Pavlova, S. V. (2011). *Acta Cryst.* E**67**, o3282–o3283.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sliva, T. Yu., Kowalik-Jankowska, T., Amirkhanov, V. M., Głowiak, T., Onindo, C. O., Fritskii, I. O. & Kozłowski, H. (1997). *J. Inorg. Biochem.* **65**, 287–294.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Zyl, G. V., Devries, D. L., Decker, R. H. & Niles, E. T. (1961). *J. Org. Chem.* **26**, 3373–3375.

supporting information

Acta Cryst. (2014). E**70**, 584-586 [doi:10.1107/S1600536814025793]

Crystal structure of 2-hydroxyimino-2-(pyridin-2-yl)-*N*′-[1-(pyridin-2-yl)ethylidene]acetohydrazide

Maxym O. Plutenko, Rostislav D. Lampeka, Matti Haukka and Ebbe Nordlander

Computing details

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); data reduction: *SAINT* (Bruker, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

2-Hydroxyimino-2-(pyridin-2-yl)-*N*′-[1-(pyridin-2-yl)ethylidene]acetohydrazide

Crystal data

$C_{14}H_{13}N_5O_2$
M_r = 283.29
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 11.4319 (9) Å
b = 9.3598 (4) Å
c = 12.4297 (9) Å
β = 105.016 (3)°
V = 1284.57 (15) Å^3
Z = 4
$F(000)$ = 592
D_x = 1.465 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 12859 reflections
θ = 1.0–27.5°
μ = 0.10 mm^{-1}
T = 123 K
Block, colourless
0.27 × 0.15 × 0.14 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Horizontally mounted graphite crystal monochromator
Detector resolution: 16 pixels mm^{-1}
φ scans and ω scans with κ offset
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.973, T_{max} = 0.986
7900 measured reflections
2850 independent reflections
2226 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.6°, θ_{min} = 3.6°
h = −14→7
k = −11→12
l = −13→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.115
S = 1.05
2850 reflections
196 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

$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.5602P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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}
O1	0.53771 (10)	0.81661 (11)	0.01882 (9)	0.0275 (3)
H1	0.547 (2)	0.873 (3)	−0.0406 (19)	0.061 (7)*
O2	0.41325 (12)	1.10609 (11)	0.18548 (9)	0.0365 (3)
N1	0.42020 (13)	0.68309 (13)	0.29508 (10)	0.0269 (3)
N2	0.49655 (12)	0.91005 (12)	0.08547 (10)	0.0227 (3)
N3	0.39671 (12)	0.95674 (13)	0.32531 (10)	0.0217 (3)
H3	0.3983 (18)	0.865 (2)	0.3433 (16)	0.045 (6)*
N4	0.36523 (11)	1.06522 (12)	0.38730 (9)	0.0211 (3)
N5	0.27415 (12)	1.10442 (13)	0.63724 (10)	0.0249 (3)
C1	0.40835 (17)	0.54907 (16)	0.32784 (14)	0.0332 (4)
H1A	0.3841	0.5347	0.3946	0.040*
C2	0.42966 (11)	0.43023 (11)	0.26956 (9)	0.0279 (3)
H2	0.4195	0.3363	0.2946	0.033*
C3	0.46609 (11)	0.45322 (11)	0.17415 (9)	0.0261 (3)
H3A	0.4818	0.3742	0.1320	0.031*
C4	0.48006 (15)	0.59117 (15)	0.13888 (12)	0.0258 (3)
H4	0.5061	0.6074	0.0732	0.031*
C5	0.45529 (13)	0.70606 (14)	0.20141 (11)	0.0196 (3)
C6	0.46209 (13)	0.85875 (14)	0.16827 (11)	0.0198 (3)
C7	0.42130 (14)	0.98666 (14)	0.22744 (12)	0.0225 (3)
C8	0.33284 (13)	1.02516 (14)	0.47426 (11)	0.0206 (3)
C9	0.32455 (16)	0.87266 (15)	0.50997 (13)	0.0282 (4)
H9A	0.2782	0.8166	0.4466	0.042*
H9B	0.2838	0.8694	0.5702	0.042*
H9C	0.4062	0.8327	0.5363	0.042*
C10	0.30190 (13)	1.14279 (14)	0.54298 (11)	0.0200 (3)
C11	0.30120 (14)	1.28513 (15)	0.50943 (12)	0.0253 (3)
H11	0.3217	1.3094	0.4424	0.030*
C12	0.27019 (15)	1.39034 (16)	0.57523 (13)	0.0281 (3)
H12	0.2690	1.4879	0.5539	0.034*
C13	0.24098 (14)	1.35182 (16)	0.67237 (12)	0.0257 (3)
H13	0.2188	1.4216	0.7190	0.031*

C14	0.24502 (15)	1.20881 (16)	0.69948 (12)	0.0275 (3)
H14	0.2259	1.1824	0.7667	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0449 (7)	0.0188 (5)	0.0253 (6)	0.0028 (4)	0.0206 (5)	−0.0006 (4)
O2	0.0691 (9)	0.0166 (5)	0.0338 (6)	0.0044 (5)	0.0315 (6)	0.0034 (4)
N1	0.0415 (8)	0.0172 (6)	0.0263 (6)	0.0000 (5)	0.0165 (6)	−0.0005 (5)
N2	0.0321 (7)	0.0180 (6)	0.0197 (6)	0.0003 (5)	0.0100 (5)	−0.0028 (4)
N3	0.0323 (7)	0.0147 (6)	0.0213 (6)	0.0013 (5)	0.0128 (5)	−0.0003 (4)
N4	0.0278 (7)	0.0173 (6)	0.0203 (6)	0.0010 (5)	0.0102 (5)	−0.0027 (4)
N5	0.0344 (7)	0.0215 (6)	0.0219 (6)	−0.0003 (5)	0.0126 (6)	−0.0005 (5)
C1	0.0550 (11)	0.0207 (7)	0.0314 (8)	−0.0003 (7)	0.0247 (8)	0.0026 (6)
C2	0.0387 (9)	0.0165 (7)	0.0310 (8)	−0.0002 (6)	0.0136 (7)	0.0024 (6)
C3	0.0354 (9)	0.0177 (7)	0.0276 (8)	0.0000 (6)	0.0124 (7)	−0.0035 (5)
C4	0.0372 (9)	0.0196 (7)	0.0242 (7)	−0.0003 (6)	0.0143 (7)	−0.0020 (5)
C5	0.0218 (7)	0.0174 (7)	0.0199 (6)	−0.0007 (5)	0.0062 (5)	−0.0001 (5)
C6	0.0251 (7)	0.0165 (7)	0.0192 (7)	−0.0003 (5)	0.0080 (6)	−0.0008 (5)
C7	0.0315 (8)	0.0164 (7)	0.0218 (7)	−0.0015 (5)	0.0107 (6)	−0.0018 (5)
C8	0.0241 (7)	0.0177 (7)	0.0211 (7)	0.0001 (5)	0.0079 (6)	0.0000 (5)
C9	0.0432 (10)	0.0188 (7)	0.0275 (8)	−0.0003 (6)	0.0177 (7)	0.0015 (5)
C10	0.0229 (7)	0.0188 (7)	0.0190 (7)	−0.0008 (5)	0.0066 (6)	−0.0008 (5)
C11	0.0357 (9)	0.0201 (7)	0.0236 (7)	0.0008 (6)	0.0138 (7)	0.0002 (5)
C12	0.0365 (9)	0.0197 (7)	0.0297 (8)	0.0017 (6)	0.0117 (7)	−0.0011 (6)
C13	0.0289 (8)	0.0237 (7)	0.0257 (7)	0.0024 (6)	0.0090 (6)	−0.0063 (6)
C14	0.0360 (9)	0.0277 (8)	0.0223 (7)	0.0000 (6)	0.0141 (7)	−0.0028 (6)

Geometric parameters (Å, º)

O1—N2	1.3691 (14)	C4—C5	1.3981 (19)
O1—H1	0.93 (2)	C4—H4	0.9500
O2—C7	1.2269 (17)	C5—C6	1.4950 (18)
N1—C1	1.3365 (19)	C6—C7	1.5392 (18)
N1—C5	1.3435 (18)	C8—C10	1.4911 (18)
N2—C6	1.2866 (17)	C8—C9	1.5051 (19)
N3—C7	1.3471 (18)	C9—H9A	0.9800
N3—N4	1.3776 (16)	C9—H9B	0.9800
N3—H3	0.89 (2)	C9—H9C	0.9800
N4—C8	1.2858 (18)	C10—C11	1.3954 (19)
N5—C10	1.3398 (18)	C11—C12	1.3837 (19)
N5—C14	1.3407 (18)	C11—H11	0.9500
C1—C2	1.3831 (18)	C12—C13	1.382 (2)
C1—H1A	0.9500	C12—H12	0.9500
C2—C3	1.3719	C13—C14	1.378 (2)
C2—H2	0.9500	C13—H13	0.9500
C3—C4	1.3861 (17)	C14—H14	0.9500
C3—H3A	0.9500		

N2—O1—H1	104.1 (14)	O2—C7—C6	120.28 (12)
C1—N1—C5	119.39 (12)	N3—C7—C6	115.45 (11)
C6—N2—O1	118.04 (11)	N4—C8—C10	115.40 (12)
C7—N3—N4	119.85 (12)	N4—C8—C9	125.33 (12)
C7—N3—H3	115.7 (13)	C10—C8—C9	119.27 (12)
N4—N3—H3	124.4 (13)	C8—C9—H9A	109.5
C8—N4—N3	115.41 (12)	C8—C9—H9B	109.5
C10—N5—C14	117.37 (12)	H9A—C9—H9B	109.5
N1—C1—C2	123.35 (13)	C8—C9—H9C	109.5
N1—C1—H1A	118.3	H9A—C9—H9C	109.5
C2—C1—H1A	118.3	H9B—C9—H9C	109.5
C3—C2—C1	117.44 (8)	N5—C10—C11	122.20 (12)
C3—C2—H2	121.3	N5—C10—C8	116.62 (12)
C1—C2—H2	121.3	C11—C10—C8	121.17 (12)
C2—C3—C4	120.34 (7)	C12—C11—C10	119.04 (13)
C2—C3—H3A	119.8	C12—C11—H11	120.5
C4—C3—H3A	119.8	C10—C11—H11	120.5
C3—C4—C5	118.95 (12)	C13—C12—C11	119.20 (14)
C3—C4—H4	120.5	C13—C12—H12	120.4
C5—C4—H4	120.5	C11—C12—H12	120.4
N1—C5—C4	120.51 (12)	C14—C13—C12	117.83 (13)
N1—C5—C6	116.12 (12)	C14—C13—H13	121.1
C4—C5—C6	123.34 (12)	C12—C13—H13	121.1
N2—C6—C5	128.74 (12)	N5—C14—C13	124.36 (14)
N2—C6—C7	106.58 (11)	N5—C14—H14	117.8
C5—C6—C7	124.62 (11)	C13—C14—H14	117.8
O2—C7—N3	124.27 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···N1	0.89 (2)	1.84 (2)	2.6126 (17)	144 (2)
O1—H1···O2^{i}	0.93 (2)	1.98 (2)	2.8327 (14)	151 (2)
O1—H1···N2^{i}	0.93 (2)	2.13 (2)	2.8489 (16)	133 (2)
C2—H2···O2^{ii}	0.95	2.54	3.1985 (15)	127
C3—H3*A*···O1^{iii}	0.95	2.56	3.4755 (15)	163
C13—H13···N5^{iv}	0.95	2.46	3.3811 (19)	163

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