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

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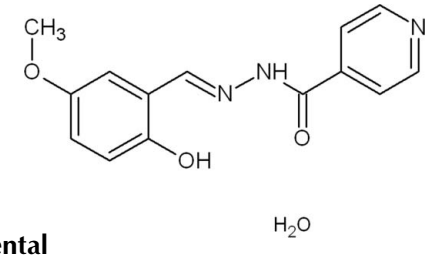
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.124; data-to-parameter ratio = 8.0.

The title compound, $C_{14}H_{13}N_3O_3\cdot H_2O$, adopts an *E* conformation with respect to the azomethine bond and crystallizes in the amide form. An intramolecular O—H···N hydrogen bond occurs. In the crystal, the lattice water molecule plays a major role in the supramolecular architecture by interconnecting adjacent molecules into a three-dimensional netwrok by means of O—H···O, O—H···N and N—H···O hydrogen-bonding interactions. The structure also features two non-classical C—H···O interactions.

Related literature

For properties of carbohydrazide and its derivatives, see: Mangalam & Kurup (2011). For molecular sensing of metals, see: Bakir & Brown (2002). For related structures and background references, see: Kargar *et al.* (2010); Shafiq *et al.* (2009); Sithambaresan & Kurup (2011). For the synthesis, see: Mangalam *et al.* (2009).



Experimental

Crystal data

$C_{14}H_{13}N_3O_3\cdot H_2O$
M_r = 289.29
Orthorhombic, $Pna2_1$
a = 12.6455 (16) Å
b = 12.7423 (16) Å
c = 8.9306 (9) Å
V = 1439.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.40 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.965, T_{max} = 0.976
10294 measured reflections
1668 independent reflections
1134 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.124
S = 1.00
1668 reflections
208 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2′···O1*S*^{i}	0.89 (1)	1.91 (1)	2.784 (4)	168 (4)
O1*S*—H1*A*···O3^{ii}	0.86 (1)	1.92 (2)	2.764 (4)	170 (4)
O1*S*—H1*B*···N3^{iii}	0.86 (1)	2.05 (2)	2.874 (5)	160 (4)
O2—H2*A*···N1	0.85 (1)	1.89 (3)	2.642 (4)	147 (4)
C11—H11···O1^{iv}	0.93	2.46	3.370 (5)	164
C14—H14*C*···O3^{v}	0.96	2.58	3.425 (5)	147

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); 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, 2012) and *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2628).

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supporting information

Acta Cryst. (2013). E**69**, o881 [doi:10.1107/S160053681301235X]

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

M. K. Prasanna, M. Sithambaresan, K. Pradeepkumar and M. R. Prathapachandra Kurup

S1. Comment

Derivatives of carbohydrazide and their metal complexes exhibit prominent biological activities and versatile binding properties. They also promote the formation of a chelate binding center (Mangalam & Kurup, 2011). Versatile applications in molecular sensing of metals have received substantial interest during the last decade (Bakir & Brown, 2002).

The compound crystallizes in orthorhombic P*na*2$_1$ space group. The molecule exists in the *E* configuration with respect to C7=N1 bond (Sithambaresan & Kurup, 2011) which is confirmed by the torsion angle of -177.6 (3)° of C6—C7—N1—N2 moiety (Fig. 1). The torsion angle of 7.2 (5)° corresponding to N1—N2—C8—O3 moiety supports the *cis* configuration of the O3 atom with respect to the hydrazine nitrogen atom N1 (Kargar *et al.*, 2010; Shafiq *et al.*, 2009). The C7=N1 [1.272 (4) Å] and C8=O3 [1.219 (3) Å] bond distances are very close to the formal C=N and C=O bond lengths [C=N; 1.28 Å and C═O; 1.21 Å] respectively confirming the azomethine bond formation and the existence of carbohydrazide in amido form in solid state.

Incorporation of water molecule in the crystal system of the title compound plays an important role in assembly of the molecules in the lattice through intermolecular hydrogen bonds and makes the crystal system entirely different from the reported one (Kargar *et al.*, 2010). Two classical hydrogen bonds are present in the molecular system (Fig. 2) between the both H atoms of the water molecule and O3 and N3 atoms of the neighbouring molecules with a D···A distances of 2.764 (4) and 2.874 (5) Å respectively. The phenolic oxygen O2 is involved in an intramolecular hydrogen bond with N1 to form a six membered ring. The hydrazinic nitrogen N2 is also involved in hydrogen bonding with oxygen of solvent water. Two non- classical C–H···O hydrogen bonds are also present in the molecule (Table 1). The packing diagram showing the molecular assembly of the title compound along *a* axis is shown in Fig. 3.

S2. Experimental

The title compound was prepared by adapting a reported procedure (Mangalam *et al.*, 2009). To a warm ethanolic solution of 2-hydroxy-5-methoxybenzaldehyde (0.152 g, 1 mmol), a methanolic solution of pyridine-4-carbohydrazide (0.137 g, 1 mmol) was added and the resulting solution was refluxed for 45 minutes after adding 3 drops of glacial acetic acid. On cooling the solution, yellow crystals separated out. Single crystals suitable for X-ray diffraction studies were obtained by slow evaporation of its solution in 1:1 mixture of ethanol and DMF.

S3. Refinement

All H atoms on C were placed in calculated positions, guided by difference maps, with C–H bond distances 0.93–0.96 Å. H atoms were assigned as U_{iso}(H)=1.2Ueq(carrier) or 1.5Ueq (methyl C). N2–H2′ and O2–H2A H atoms were located from difference maps and restrained using *DFIX* instructions. H atoms of the water molecule were also located from

difference maps and restrained using *DFIX* and *DANG* instructions. Omitted owing to bad disagreement was the reflection (1 1 0). In the absence of significant anomalous scattering effects Friedel pairs have been merged.

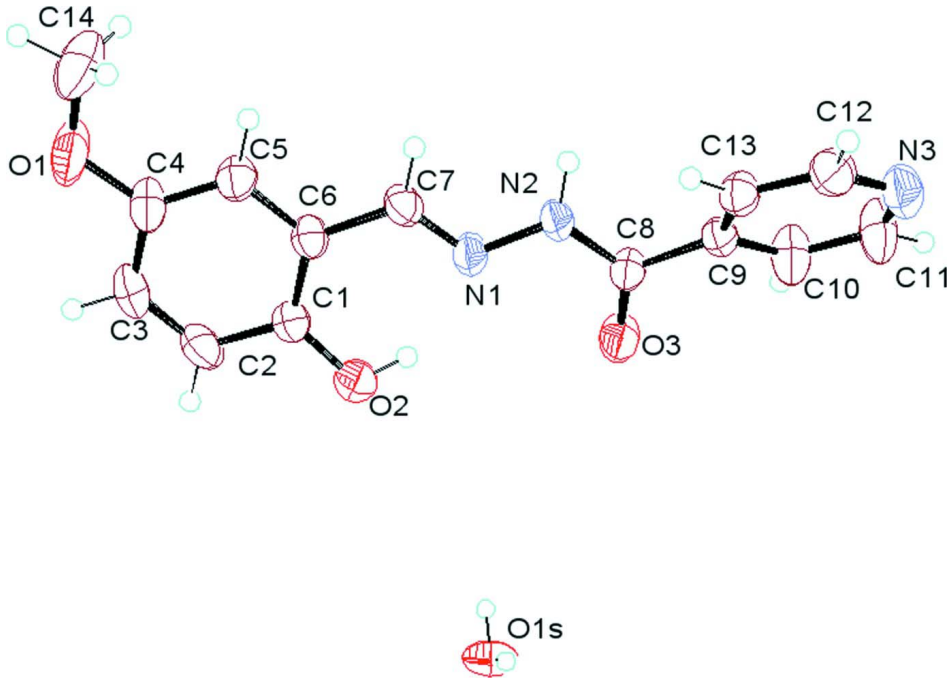

Figure 1

ORTEP view of the unique part of the compound, drawn with 50% probability displacement ellipsoids for the non-H atoms.

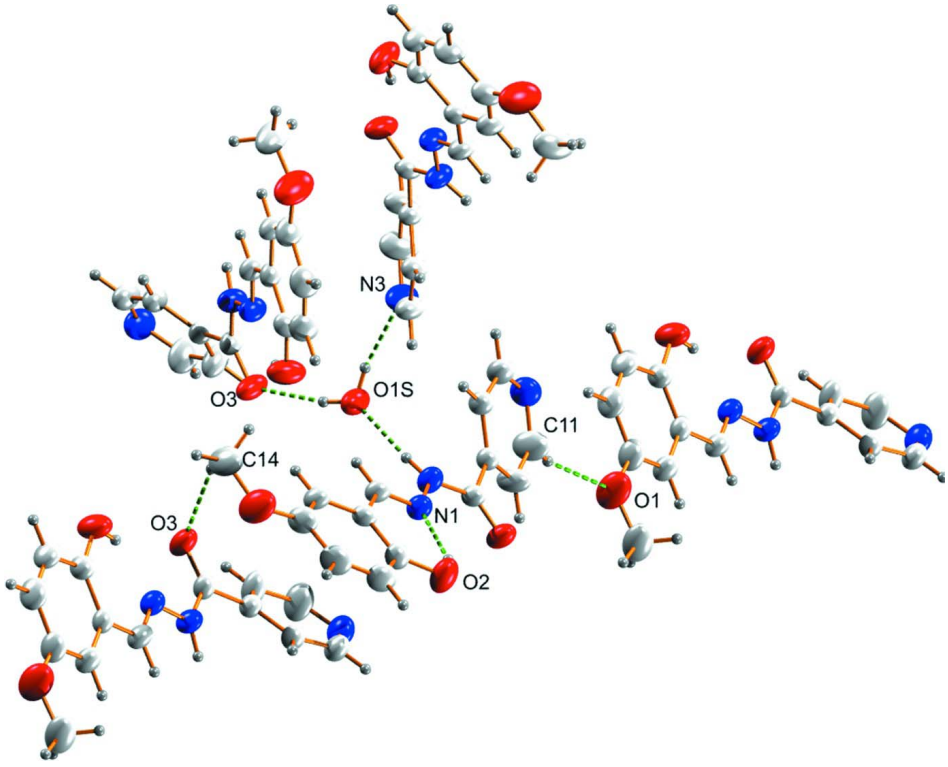

Figure 2

Graphical representation showing hydrogen bondings in the crystal structure of $C_{14}H_{13}N_3O_3.H_2O$.

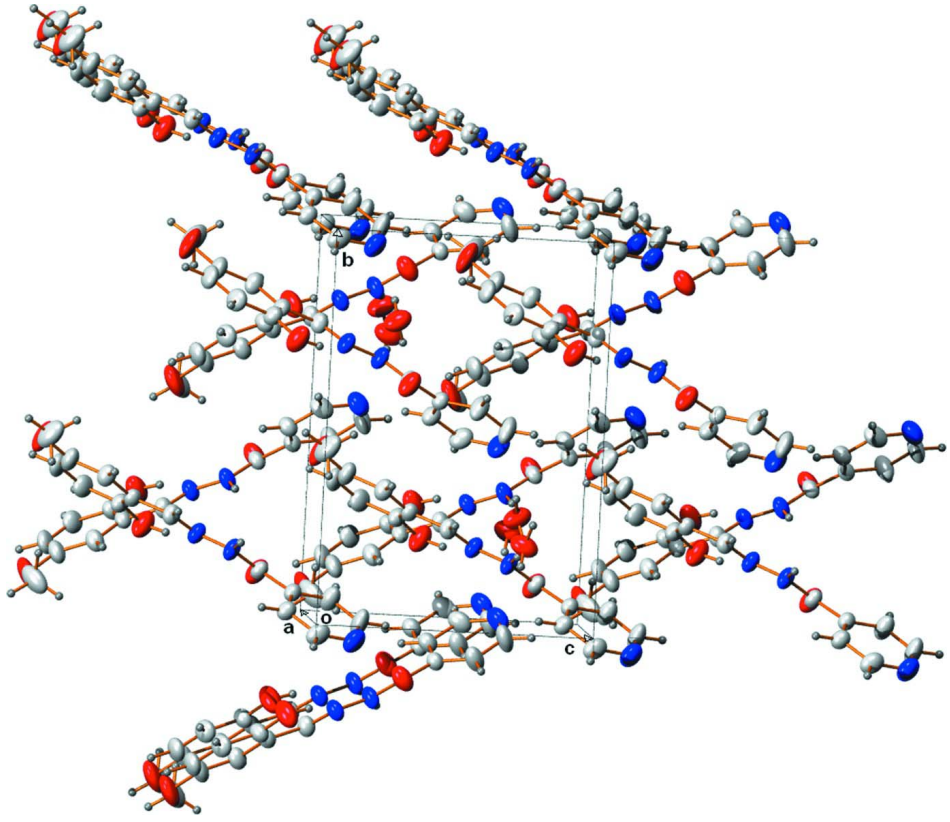

Figure 3

A view of the unit cell along *a* axis.

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Crystal data

$C_{14}H_{13}N_3O_3·H_2O$
M_r = 289.29
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
a = 12.6455 (16) Å
b = 12.7423 (16) Å
c = 8.9306 (9) Å
V = 1439.0 (3) Å^3
Z = 4
$F(000)$ = 608
D_x = 1.335 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1943 reflections
θ = 2.8–27.5°
μ = 0.10 mm^{-1}
T = 296 K
Block, yellow
0.40 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm^{-1}
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.965, T_{max} = 0.976
10294 measured reflections
1668 independent reflections
1134 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 27.0°, θ_{min} = 2.8°
h = −16→15
k = −14→16
l = −11→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.124$
$S = 1.00$
1668 reflections
208 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0701P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.012 (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	0.1808 (2)	0.4322 (3)	−0.0082 (3)	0.0751 (10)
O2	0.4338 (2)	0.2150 (3)	0.3839 (3)	0.0617 (9)
O3	0.37204 (18)	0.1124 (2)	0.7981 (3)	0.0518 (7)
O1S	1.0079 (2)	0.2238 (2)	0.7337 (4)	0.0590 (8)
N1	0.2710 (2)	0.2049 (2)	0.5685 (3)	0.0397 (7)
N2	0.2196 (2)	0.1700 (3)	0.6956 (3)	0.0408 (7)
N3	0.1091 (3)	−0.0404 (3)	1.1458 (4)	0.0575 (9)
C1	0.3661 (3)	0.2681 (3)	0.2933 (4)	0.0411 (8)
C2	0.4043 (3)	0.3044 (3)	0.1575 (4)	0.0507 (10)
H2	0.4747	0.2928	0.1326	0.061*
C3	0.3409 (3)	0.3566 (3)	0.0601 (4)	0.0533 (11)
H3	0.3679	0.3792	−0.0312	0.064*
C4	0.2361 (3)	0.3764 (3)	0.0963 (4)	0.0497 (10)
C5	0.1962 (3)	0.3413 (3)	0.2291 (4)	0.0428 (9)
H5	0.1257	0.3540	0.2528	0.051*
C6	0.2605 (3)	0.2865 (3)	0.3301 (3)	0.0353 (8)
C7	0.2147 (3)	0.2507 (3)	0.4707 (4)	0.0391 (8)
H7	0.1432	0.2615	0.4890	0.047*
C8	0.2760 (3)	0.1203 (3)	0.8009 (3)	0.0360 (8)
C9	0.2130 (2)	0.0700 (3)	0.9218 (3)	0.0345 (8)
C10	0.2574 (3)	0.0576 (3)	1.0612 (5)	0.0558 (11)
H10	0.3236	0.0856	1.0823	0.067*
C11	0.2026 (4)	0.0036 (4)	1.1683 (5)	0.0651 (13)

H11	0.2329	−0.0025	1.2628	0.078*
C12	0.0673 (3)	−0.0275 (3)	1.0122 (5)	0.0513 (10)
H12	0.0012	−0.0569	0.9941	0.062*
C13	0.1150 (3)	0.0265 (3)	0.8976 (4)	0.0404 (8)
H13	0.0817	0.0336	0.8053	0.049*
C14	0.0712 (4)	0.4431 (4)	0.0117 (5)	0.0759 (15)
H14A	0.0391	0.3750	0.0175	0.114*
H14B	0.0418	0.4810	−0.0714	0.114*
H14C	0.0576	0.4809	0.1027	0.114*
H2′	0.1551 (15)	0.191 (3)	0.720 (5)	0.054 (12)*
H1A	0.973 (3)	0.279 (2)	0.757 (6)	0.093 (19)*
H1B	0.962 (3)	0.175 (2)	0.722 (6)	0.081 (16)*
H2A	0.400 (3)	0.198 (3)	0.462 (3)	0.066 (14)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.069 (2)	0.106 (3)	0.0501 (17)	−0.0069 (18)	−0.0104 (16)	0.0408 (18)
O2	0.0470 (15)	0.080 (2)	0.0580 (18)	0.0194 (14)	0.0147 (16)	0.0220 (16)
O3	0.0316 (13)	0.0695 (19)	0.0542 (15)	−0.0047 (12)	−0.0016 (12)	0.0243 (13)
O1S	0.0376 (14)	0.0544 (18)	0.085 (2)	0.0050 (14)	−0.0006 (15)	−0.0197 (16)
N1	0.0355 (15)	0.0484 (18)	0.0351 (15)	−0.0004 (14)	0.0036 (14)	0.0125 (14)
N2	0.0352 (16)	0.0528 (19)	0.0343 (16)	0.0034 (15)	0.0074 (14)	0.0151 (13)
N3	0.056 (2)	0.063 (2)	0.054 (2)	−0.0059 (18)	0.0109 (17)	0.0184 (17)
C1	0.0422 (19)	0.042 (2)	0.0394 (18)	0.0026 (16)	0.0076 (16)	0.0070 (16)
C2	0.046 (2)	0.060 (3)	0.046 (2)	−0.0011 (19)	0.0176 (18)	0.0028 (18)
C3	0.063 (3)	0.063 (3)	0.0331 (19)	−0.006 (2)	0.0128 (19)	0.0101 (18)
C4	0.055 (3)	0.058 (3)	0.036 (2)	−0.0101 (19)	−0.0029 (19)	0.0129 (19)
C5	0.0341 (18)	0.055 (2)	0.040 (2)	−0.0037 (16)	−0.0040 (16)	0.0079 (18)
C6	0.0357 (18)	0.037 (2)	0.0327 (18)	−0.0067 (14)	0.0004 (15)	0.0028 (15)
C7	0.0307 (18)	0.051 (2)	0.0357 (19)	−0.0024 (16)	0.0034 (15)	0.0033 (16)
C8	0.0342 (18)	0.0392 (19)	0.0346 (18)	−0.0041 (15)	−0.0024 (16)	0.0083 (15)
C9	0.0324 (17)	0.0366 (19)	0.0346 (18)	−0.0009 (14)	0.0022 (15)	0.0044 (15)
C10	0.054 (3)	0.070 (3)	0.044 (2)	−0.022 (2)	−0.011 (2)	0.017 (2)
C11	0.072 (3)	0.086 (4)	0.036 (2)	−0.021 (3)	−0.0063 (19)	0.023 (2)
C12	0.0378 (19)	0.053 (3)	0.063 (3)	−0.0039 (17)	0.0056 (19)	0.014 (2)
C13	0.0373 (18)	0.043 (2)	0.0413 (19)	−0.0026 (15)	−0.0012 (16)	0.0073 (16)
C14	0.066 (3)	0.086 (4)	0.076 (3)	−0.016 (3)	−0.030 (3)	0.036 (3)

Geometric parameters (Å, º)

O1—C4	1.366 (4)	C3—H3	0.9300
O1—C14	1.405 (5)	C4—C5	1.364 (5)
O2—C1	1.358 (5)	C5—C6	1.402 (5)
O2—H2A	0.847 (10)	C5—H5	0.9300
O3—C8	1.218 (4)	C6—C7	1.456 (5)
O1S—H1A	0.856 (10)	C7—H7	0.9300
O1S—H1B	0.859 (10)	C8—C9	1.487 (4)

N1—C7	1.269 (4)	C9—C13	1.374 (5)
N1—N2	1.381 (4)	C9—C10	1.374 (5)
N2—C8	1.341 (4)	C10—C11	1.367 (6)
N2—H2′	0.885 (10)	C10—H10	0.9300
N3—C12	1.315 (5)	C11—H11	0.9300
N3—C11	1.325 (5)	C12—C13	1.373 (5)
C1—C2	1.384 (5)	C12—H12	0.9300
C1—C6	1.395 (5)	C13—H13	0.9300
C2—C3	1.357 (6)	C14—H14A	0.9600
C2—H2	0.9300	C14—H14B	0.9600
C3—C4	1.388 (6)	C14—H14C	0.9600

C4—O1—C14	118.0 (3)	N1—C7—H7	119.5
C1—O2—H2A	107 (3)	C6—C7—H7	119.5
H1A—O1S—H1B	106 (2)	O3—C8—N2	123.8 (3)
C7—N1—N2	116.7 (3)	O3—C8—C9	120.9 (3)
C8—N2—N1	118.5 (3)	N2—C8—C9	115.3 (3)
C8—N2—H2′	118 (3)	C13—C9—C10	117.7 (3)
N1—N2—H2′	122 (3)	C13—C9—C8	122.9 (3)
C12—N3—C11	116.3 (3)	C10—C9—C8	119.2 (3)
O2—C1—C2	117.9 (3)	C11—C10—C9	119.0 (4)
O2—C1—C6	123.1 (3)	C11—C10—H10	120.5
C2—C1—C6	118.9 (3)	C9—C10—H10	120.5
C3—C2—C1	121.3 (4)	N3—C11—C10	124.0 (4)
C3—C2—H2	119.3	N3—C11—H11	118.0
C1—C2—H2	119.3	C10—C11—H11	118.0
C2—C3—C4	120.2 (3)	N3—C12—C13	124.2 (4)
C2—C3—H3	119.9	N3—C12—H12	117.9
C4—C3—H3	119.9	C13—C12—H12	117.9
C5—C4—O1	125.1 (4)	C12—C13—C9	118.8 (3)
C5—C4—C3	119.8 (4)	C12—C13—H13	120.6
O1—C4—C3	115.1 (3)	C9—C13—H13	120.6
C4—C5—C6	120.5 (3)	O1—C14—H14A	109.5
C4—C5—H5	119.7	O1—C14—H14B	109.5
C6—C5—H5	119.7	H14A—C14—H14B	109.5
C1—C6—C5	119.2 (3)	O1—C14—H14C	109.5
C1—C6—C7	122.1 (3)	H14A—C14—H14C	109.5
C5—C6—C7	118.7 (3)	H14B—C14—H14C	109.5
N1—C7—C6	121.0 (3)		

C7—N1—N2—C8	179.3 (3)	C1—C6—C7—N1	3.1 (5)
O2—C1—C2—C3	179.0 (4)	C5—C6—C7—N1	−176.8 (3)
C6—C1—C2—C3	−0.4 (6)	N1—N2—C8—O3	7.1 (6)
C1—C2—C3—C4	1.1 (6)	N1—N2—C8—C9	−170.4 (3)
C14—O1—C4—C5	−8.9 (7)	O3—C8—C9—C13	−144.0 (4)
C14—O1—C4—C3	171.8 (4)	N2—C8—C9—C13	33.6 (5)
C2—C3—C4—C5	−1.3 (6)	O3—C8—C9—C10	30.2 (6)
C2—C3—C4—O1	178.1 (4)	N2—C8—C9—C10	−152.3 (4)

O1—C4—C5—C6	−178.6 (4)	C13—C9—C10—C11	−0.2 (6)
C3—C4—C5—C6	0.7 (6)	C8—C9—C10—C11	−174.6 (4)
O2—C1—C6—C5	−179.5 (4)	C12—N3—C11—C10	−1.9 (7)
C2—C1—C6—C5	−0.1 (5)	C9—C10—C11—N3	1.6 (7)
O2—C1—C6—C7	0.6 (5)	C11—N3—C12—C13	0.9 (6)
C2—C1—C6—C7	180.0 (3)	N3—C12—C13—C9	0.4 (6)
C4—C5—C6—C1	0.0 (5)	C10—C9—C13—C12	−0.7 (5)
C4—C5—C6—C7	179.9 (3)	C8—C9—C13—C12	173.5 (3)
N2—N1—C7—C6	−177.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2′···O1*S*^{i}	0.89 (1)	1.91 (1)	2.784 (4)	168 (4)
O1*S*—H1*A*···O3^{ii}	0.86 (1)	1.92 (2)	2.764 (4)	170 (4)
O1*S*—H1*B*···N3^{iii}	0.86 (1)	2.05 (2)	2.874 (5)	160 (4)
O2—H2*A*···N1	0.85 (1)	1.89 (3)	2.642 (4)	147 (4)
C11—H11···O1^{iv}	0.93	2.46	3.370 (5)	164
C14—H14*C*···O3^{v}	0.96	2.58	3.425 (5)	147

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