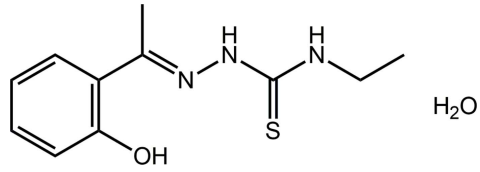
Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

OPEN ACCESS

ISSN 2056-9890




# Crystal structure of 2′-hydroxyacetophenone 4-methylthiosemicarbazide

**Junita Jamsari,[a] Nur Fatihah Abas,[a] Thahira Begum S. A. Ravoof[a]* and Edward R. T. Tiekink[b]**

[a]Department of Chemistry, Universiti Putra Malaysia, 43400 Serdang, Malaysia, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia. *Correspondence e-mail: thahira@upm.edu.my

Received 9 March 2015; accepted 11 March 2015

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

In the organic molecule of the title hydrate, $C_{11}H_{15}N_3OS\cdot H_2O$, {systematic name: 3-ethyl-1-{(*E*)-[1-(2-hydroxyphenyl)ethylidene]amino}thiourea monohydrate}, a dihedral angle of 5.39 (2)° is formed between the hydroxybenzene ring and the non-H atoms comprising the side chain (r.m.s. deviation = 0.0625 Å), with the major deviation from planarity noted for the terminal ethyl group [the C—N—C—C torsion angle = −172.17 (13)°]. The N—H H atoms are *syn* and an intramolecular hydroxy–imine O—H···N hydrogen bond is noted. In the crystal, the N-bonded H atoms form hydrogen bonds to symmetry-related water molecules, and the latter form donor interactions with the hydroxy O atom and with a hydroxybenzene ring, forming a O—H···$\pi$ interaction. The hydrogen bonding leads to supramolecular tubes aligned along the *b* axis. The tubes are connected into layers *via* C—H···O interactions, and these stack along the *c* axis with no directional interactions between them.

**Keywords:** crystal structure; thiosemicarbazide; hydrogen bonding; O—H···$\pi$ interactions.

**CCDC reference**: 1053189

## 1. Related literature

For background to thiosemicarbazones and their coordination chemistry, see: Mazlan *et al.* (2014). The conformational flexibility in these molecules is reflected in the structure of the 4-methyl derivative where one molecule comprising the asymmetric unit is approximately planar and the other exhibits a clear twist between the hydroxybenzene and side chain, and in the structure of the 6-methoxy derivative where these residues are almost normal to each other, see: Anderson *et al.* (2012, 2014). For synthesis and methodology, see: Omar *et al.* (2014).

## 2. Experimental

### 2.1. Crystal data

$C_{11}H_{15}N_3OS\cdot H_2O$
$M_r$ = 255.33
Triclinic, $P\overline{1}$
$a$ = 6.7947 (5) Å
$b$ = 8.5169 (8) Å
$c$ = 11.1199 (9) Å
$\alpha$ = 84.948 (7)°
$\beta$ = 81.825 (6)°
$\gamma$ = 84.084 (7)°
$V$ = 631.81 (9) Å$^3$
$Z$ = 2
Cu $K\alpha$ radiation
$\mu$ = 2.25 mm$^{-1}$
$T$ = 100 K
0.30 × 0.20 × 0.10 mm

### 2.2. Data collection

Oxford Diffraction Xcaliber Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min}$ = 0.923, $T_{max}$ = 1.000
8119 measured reflections
2408 independent reflections
2187 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.095
$S$ = 1.03
2408 reflections
171 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

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

*Cg*1 is the centroid of the C3–C8 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1*O*···N2 | 0.84 (1) | 1.76 (1) | 2.5292 (16) | 150 (2) |
| N1—H1*N*···O1*W*$^{i}$ | 0.86 (2) | 2.09 (2) | 2.8918 (17) | 156 (2) |
| N3—H3*N*···O1*W*$^{i}$ | 0.87 (2) | 2.16 (2) | 2.9625 (18) | 154 (2) |
| O1*W*—H1*W*···O1 | 0.84 (2) | 1.96 (2) | 2.7894 (16) | 174 (2) |
| O1*W*—H2*W*···*Cg*1$^{ii}$ | 0.83 (1) | 2.86 (1) | 3.4165 (13) | 127 (1) |
| C5—H5···O1$^{iii}$ | 0.95 | 2.56 | 3.3702 (18) | 143 |

Symmetry codes: (i) $x, y+1, z$; (ii) $-x, -y+1, -z$; (iii) $-x+1, -y+1, -z$.

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2015); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

## Acknowledgements

Support for this project came from Universiti Putra Malaysia (UPM) under their Research University Grant Scheme

(RUGS No. 9419400), Malaysian Fundamental Research Grant Scheme (FRGS No. 5524425) and the ScienceFund (Science Fund No. 5450726). We also thank Siti Khadijah Densabali for collecting the X-ray data. JJ wishes to acknowledge the Malaysian Government for sponsorship under the SGRA Scheme.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7380).

## References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Anderson, B. J., Hall, J. R. & Jasinski, J. P. (2014). *Acta Cryst.* E**70**, o735.
Anderson, B. J., Kennedy, C. J. & Jasinski, J. P. (2012). *Acta Cryst.* E**68**, o2982.
Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Mazlan, N. A., Ravoof, T. B. S., Tiekink, E. R. T., Tahir, M. I. M., Veerakumarasivam, A. & Crouse, K. A. (2014). *Transition Met. Chem.* **39**, 633–639.
Omar, S. A., Ravoof, T. B., Tahir, M. I. M. & Crouse, K. A. (2014). *Transition Met. Chem.* **39**, 119–126.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

# supporting information

*Acta Cryst.* (2015). E**71**, o244–o245 [doi:10.1107/S2056989015004958]

## Crystal structure of 2′-hydroxyacetophenone 4-methylthiosemicarbazide

**Junita Jamsari, Nur Fatihah Abas, Thahira Begum S. A. Ravoof and Edward R. T. Tiekink**

### S1. Experimental

4-Methyl-3-thiosemicarbazide (0.02 mol) was dissolved in hot ethanol (95%; 40 ml). A solution of 0.02 mol of 2′-hydroxyacetophenone was added drop-wise into the first solution. The mixture was heated and stirred to reduce the volume to half of its initial volume. Then, it was allowed to stand at room temperature until a white crystalline precipitate formed. The precipitate was then collected and recrystallized from ethanol and dried over silica gel. Colourless crystals were obtained from the ethanolic solution. Yield: 92%. *M*.pt: 116 °C. Anal. Found (Calc): C: 56.1 (55.7); H: 5.9 (6.4); N: 18.5 (17.7).

### S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H = 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation with $U_{iso}$(H) = 1.2–1.5$U_{eq}$(C). The O—H H atoms were refined with O—H = 0.84±0.01 Å, and with $U_{iso}$(H) = 1.5$U_{eq}$(O). The N—H H atoms were refined similarly with N—H = 0.88±0.01 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(N).

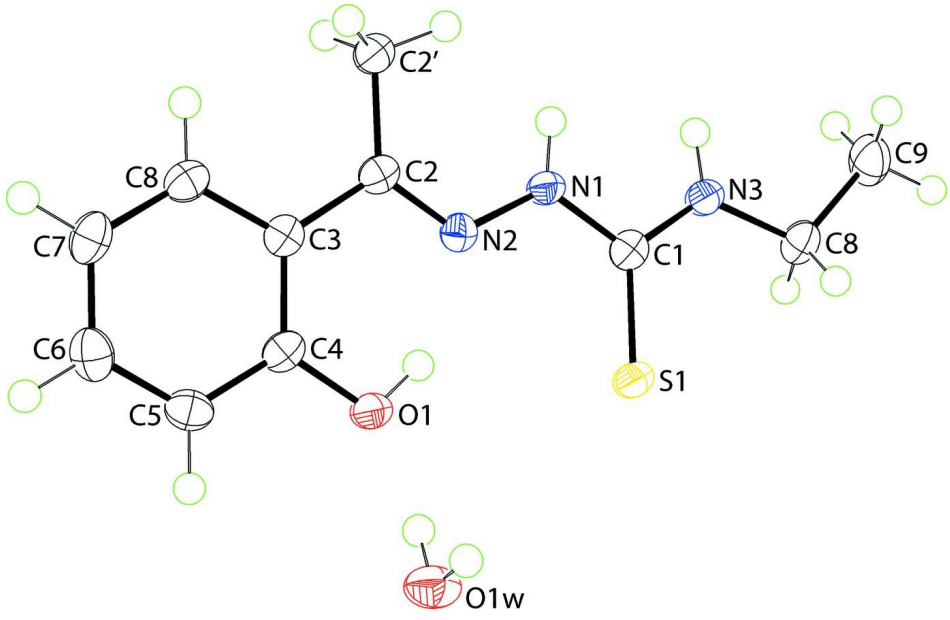



**Figure 1**

The molecular structure of the title compound showing the atom-labelling scheme and displacement ellipsoids at the 70% probability level.

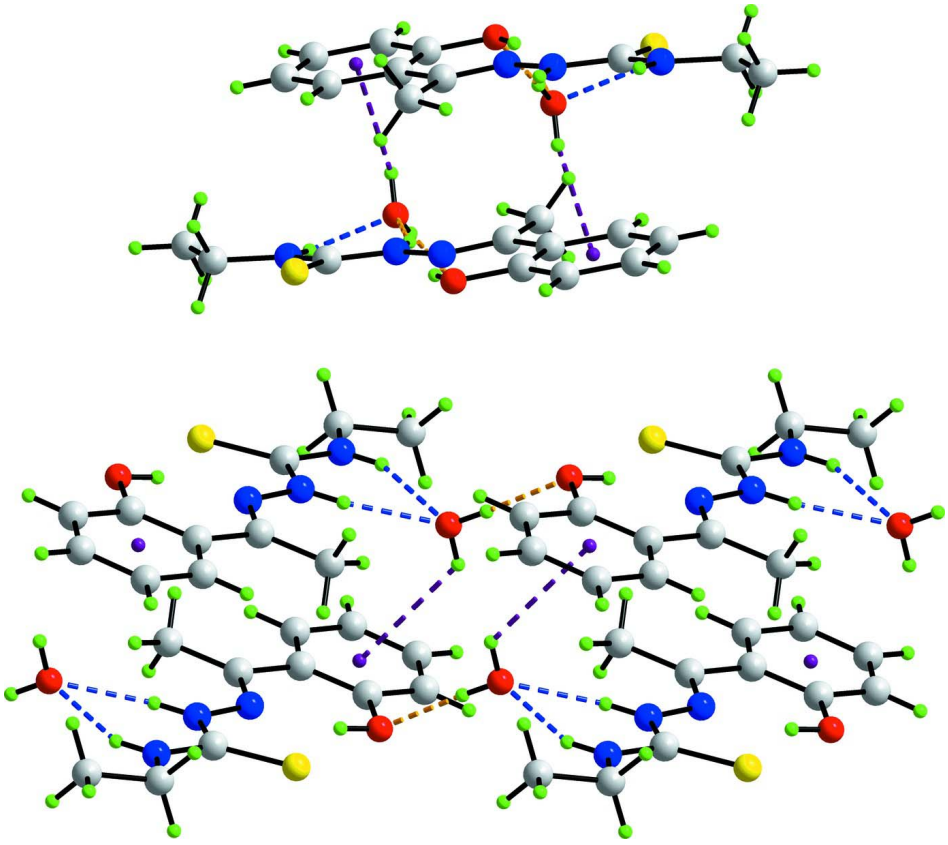


**Figure 2**

Two views of the supramolecular tube along the *b* axis sustained by O—H···O, N—H···O and O—H···$\pi$ hydrogen bonding, shown as orange, blue and purple dashed lines, respectively.

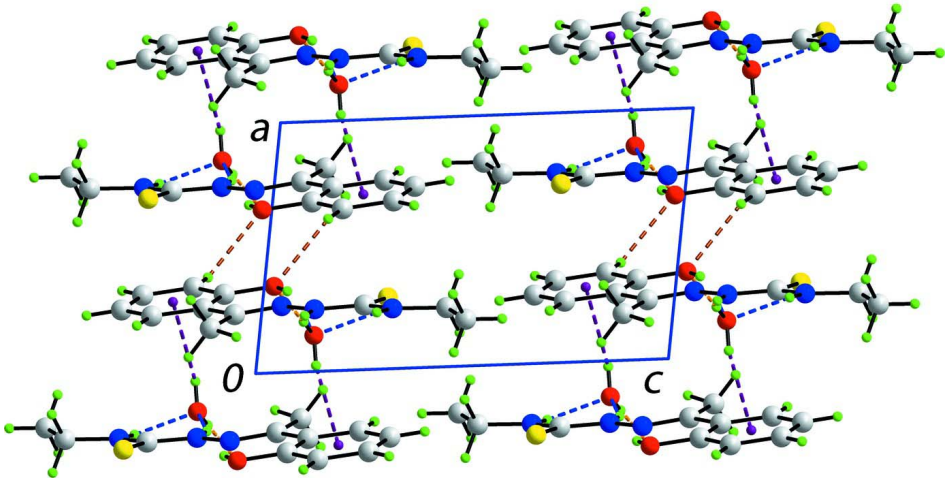



**Figure 3**

A view of the unit-cell contents in projection down the *b* axis. The O—H···O, N—H···O, O—H···$\pi$ and C—H···O interactions are shown as orange, blue, purple and brown dashed lines, respectively.

**3-Ethyl-1-[(*E*)-[1-(2-hydroxyphenyl)ethylidene]amino]thiourea monohydrate**

*Crystal data*

$C_{11}H_{15}N_3OS·H_2O$
$M_r = 255.33$
Triclinic, $P\overline{1}$
$a = 6.7947$ (5) Å
$b = 8.5169$ (8) Å
$c = 11.1199$ (9) Å
$\alpha = 84.948$ (7)°
$\beta = 81.825$ (6)°
$\gamma = 84.084$ (7)°
$V = 631.81$ (9) Å$^3$
$Z = 2$
$F(000) = 272$
$D_x = 1.342$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å
Cell parameters from 4230 reflections
$\theta = 4.0$–$71.4°$
$\mu = 2.25$ mm$^{-1}$
$T = 100$ K
Prism, pale-yellow
0.30 × 0.20 × 0.10 mm

*Data collection*

Oxford Diffraction Xcaliber Eos Gemini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.1952 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.923$, $T_{max} = 1.000$
8119 measured reflections
2408 independent reflections
2187 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 71.5°$, $\theta_{min} = 4.0°$
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 9$
$l = -13 \rightarrow 13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.095$
$S = 1.03$
2408 reflections
171 parameters
6 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.1686P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å$^{-3}$
$\Delta\rho_{min} = -0.25$ 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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.28553 (5) | 0.84923 (4) | 0.30332 (3) | 0.01932 (14) |
| O1 | 0.34603 (16) | 0.67711 (12) | 0.02373 (9) | 0.0193 (2) |
| H1O | 0.325 (3) | 0.7637 (15) | 0.0568 (16) | 0.029* |
| N1 | 0.24861 (18) | 1.08372 (15) | 0.12735 (11) | 0.0163 (3) |
| H1N | 0.224 (3) | 1.1825 (17) | 0.1053 (16) | 0.020* |
| N2 | 0.26593 (17) | 0.97046 (14) | 0.04679 (11) | 0.0150 (3) |
| N3 | 0.24119 (18) | 1.16243 (16) | 0.31656 (11) | 0.0174 (3) |
| H3N | 0.227 (3) | 1.2558 (18) | 0.2795 (15) | 0.021* |
| C1 | 0.2583 (2) | 1.03944 (18) | 0.24810 (13) | 0.0160 (3) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.2391 (2) | 1.00570 (18) | −0.06558 (13) | 0.0153 (3) |
| C2′ | 0.1872 (2) | 1.16980 (18) | −0.12094 (13) | 0.0192 (3) |
| H2′1 | 0.1497 | 1.2423 | −0.0561 | 0.029* |
| H2′2 | 0.0750 | 1.1686 | −0.1672 | 0.029* |
| H2′3 | 0.3030 | 1.2053 | −0.1755 | 0.029* |
| C3 | 0.2674 (2) | 0.86995 (18) | −0.14260 (13) | 0.0154 (3) |
| C4 | 0.3216 (2) | 0.71390 (18) | −0.09556 (13) | 0.0164 (3) |
| C5 | 0.3532 (2) | 0.58929 (18) | −0.17128 (14) | 0.0193 (3) |
| H5 | 0.3914 | 0.4854 | −0.1391 | 0.023* |
| C6 | 0.3291 (2) | 0.61601 (19) | −0.29349 (14) | 0.0214 (3) |
| H6 | 0.3503 | 0.5303 | −0.3445 | 0.026* |
| C7 | 0.2739 (2) | 0.76788 (19) | −0.34155 (13) | 0.0206 (3) |
| H7 | 0.2562 | 0.7863 | −0.4250 | 0.025* |
| C8 | 0.2451 (2) | 0.89188 (19) | −0.26665 (13) | 0.0179 (3) |
| H8 | 0.2089 | 0.9955 | −0.3004 | 0.021* |
| C9 | 0.2364 (2) | 1.14844 (19) | 0.44845 (13) | 0.0202 (3) |
| H9A | 0.3678 | 1.1022 | 0.4697 | 0.024* |
| H9B | 0.1344 | 1.0773 | 0.4859 | 0.024* |
| C10 | 0.1872 (3) | 1.3101 (2) | 0.49712 (14) | 0.0271 (4) |
| H10A | 0.2892 | 1.3797 | 0.4605 | 0.041* |
| H10B | 0.1840 | 1.3003 | 0.5858 | 0.041* |
| H10C | 0.0563 | 1.3549 | 0.4766 | 0.041* |
| O1W | 0.14391 (17) | 0.42112 (13) | 0.13237 (11) | 0.0243 (3) |
| H1W | 0.200 (3) | 0.5018 (17) | 0.1042 (17) | 0.036* |
| H2W | 0.0232 (16) | 0.452 (2) | 0.1447 (19) | 0.036* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0267 (2) | 0.0159 (2) | 0.01519 (19) | −0.00163 (15) | −0.00399 (14) | 0.00149 (14) |
| O1 | 0.0279 (6) | 0.0139 (5) | 0.0164 (5) | −0.0010 (4) | −0.0056 (4) | 0.0005 (4) |
| N1 | 0.0221 (6) | 0.0121 (6) | 0.0147 (6) | −0.0017 (5) | −0.0036 (5) | 0.0003 (5) |
| N2 | 0.0142 (6) | 0.0156 (6) | 0.0151 (6) | −0.0024 (5) | −0.0014 (4) | −0.0012 (5) |
| N3 | 0.0215 (6) | 0.0155 (7) | 0.0151 (6) | −0.0020 (5) | −0.0033 (5) | 0.0005 (5) |
| C1 | 0.0126 (6) | 0.0191 (8) | 0.0166 (7) | −0.0030 (6) | −0.0022 (5) | −0.0002 (6) |
| C2 | 0.0126 (6) | 0.0168 (8) | 0.0165 (7) | −0.0037 (5) | −0.0014 (5) | 0.0014 (6) |
| C2′ | 0.0239 (7) | 0.0174 (8) | 0.0164 (7) | −0.0017 (6) | −0.0036 (6) | −0.0003 (6) |
| C3 | 0.0120 (6) | 0.0179 (8) | 0.0164 (7) | −0.0034 (5) | −0.0016 (5) | −0.0007 (6) |
| C4 | 0.0146 (6) | 0.0187 (8) | 0.0162 (7) | −0.0045 (6) | −0.0028 (5) | 0.0017 (6) |
| C5 | 0.0191 (7) | 0.0152 (8) | 0.0239 (7) | −0.0037 (6) | −0.0032 (6) | −0.0006 (6) |
| C6 | 0.0202 (7) | 0.0235 (9) | 0.0218 (7) | −0.0070 (6) | −0.0013 (6) | −0.0066 (6) |
| C7 | 0.0198 (7) | 0.0276 (9) | 0.0156 (7) | −0.0063 (6) | −0.0036 (5) | −0.0014 (6) |
| C8 | 0.0162 (7) | 0.0194 (8) | 0.0179 (7) | −0.0027 (6) | −0.0027 (5) | 0.0021 (6) |
| C9 | 0.0232 (7) | 0.0228 (8) | 0.0151 (7) | −0.0049 (6) | −0.0028 (5) | −0.0006 (6) |
| C10 | 0.0361 (9) | 0.0257 (9) | 0.0204 (8) | −0.0072 (7) | −0.0004 (6) | −0.0072 (6) |
| O1W | 0.0227 (6) | 0.0173 (6) | 0.0314 (6) | −0.0025 (5) | −0.0014 (5) | 0.0029 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C1 | 1.6825 (16) | C4—C5 | 1.393 (2) |
| O1—C4 | 1.3653 (17) | C5—C6 | 1.388 (2) |
| O1—H1O | 0.843 (9) | C5—H5 | 0.9500 |
| N1—N2 | 1.3586 (17) | C6—C7 | 1.391 (2) |
| N1—C1 | 1.3713 (18) | C6—H6 | 0.9500 |
| N1—H1N | 0.862 (14) | C7—C8 | 1.383 (2) |
| N2—C2 | 1.2931 (18) | C7—H7 | 0.9500 |
| N3—C1 | 1.3344 (19) | C8—H8 | 0.9500 |
| N3—C9 | 1.4569 (18) | C9—C10 | 1.511 (2) |
| N3—H3N | 0.865 (14) | C9—H9A | 0.9900 |
| C2—C3 | 1.480 (2) | C9—H9B | 0.9900 |
| C2—C2′ | 1.505 (2) | C10—H10A | 0.9800 |
| C2′—H2′1 | 0.9800 | C10—H10B | 0.9800 |
| C2′—H2′2 | 0.9800 | C10—H10C | 0.9800 |
| C2′—H2′3 | 0.9800 | O1W—H1W | 0.834 (9) |
| C3—C8 | 1.403 (2) | O1W—H2W | 0.831 (9) |
| C3—C4 | 1.417 (2) | | |
| | | | |
| C4—O1—H1O | 105.5 (13) | C6—C5—C4 | 120.42 (14) |
| N2—N1—C1 | 119.33 (12) | C6—C5—H5 | 119.8 |
| N2—N1—H1N | 121.6 (12) | C4—C5—H5 | 119.8 |
| C1—N1—H1N | 119.0 (12) | C5—C6—C7 | 120.19 (14) |
| C2—N2—N1 | 121.39 (13) | C5—C6—H6 | 119.9 |
| C1—N3—C9 | 124.21 (13) | C7—C6—H6 | 119.9 |
| C1—N3—H3N | 116.9 (12) | C8—C7—C6 | 119.35 (13) |
| C9—N3—H3N | 118.8 (12) | C8—C7—H7 | 120.3 |
| N3—C1—N1 | 112.99 (13) | C6—C7—H7 | 120.3 |
| N3—C1—S1 | 123.95 (11) | C7—C8—C3 | 122.27 (14) |
| N1—C1—S1 | 123.06 (11) | C7—C8—H8 | 118.9 |
| N2—C2—C3 | 115.00 (13) | C3—C8—H8 | 118.9 |
| N2—C2—C2′ | 125.29 (13) | N3—C9—C10 | 109.63 (13) |
| C3—C2—C2′ | 119.70 (12) | N3—C9—H9A | 109.7 |
| C2—C2′—H2′1 | 109.5 | C10—C9—H9A | 109.7 |
| C2—C2′—H2′2 | 109.5 | N3—C9—H9B | 109.7 |
| H2′1—C2′—H2′2 | 109.5 | C10—C9—H9B | 109.7 |
| C2—C2′—H2′3 | 109.5 | H9A—C9—H9B | 108.2 |
| H2′1—C2′—H2′3 | 109.5 | C9—C10—H10A | 109.5 |
| H2′2—C2′—H2′3 | 109.5 | C9—C10—H10B | 109.5 |
| C8—C3—C4 | 117.28 (13) | H10A—C10—H10B | 109.5 |
| C8—C3—C2 | 120.87 (13) | C9—C10—H10C | 109.5 |
| C4—C3—C2 | 121.84 (13) | H10A—C10—H10C | 109.5 |
| O1—C4—C5 | 116.68 (13) | H10B—C10—H10C | 109.5 |
| O1—C4—C3 | 122.84 (13) | H1W—O1W—H2W | 105 (2) |
| C5—C4—C3 | 120.48 (13) | | |
| | | | |
| C1—N1—N2—C2 | 173.45 (12) | C2—C3—C4—O1 | 1.8 (2) |

| | | | |
|---|---|---|---|
| C9—N3—C1—N1 | 176.76 (12) | C8—C3—C4—C5 | 0.8 (2) |
| C9—N3—C1—S1 | −2.4 (2) | C2—C3—C4—C5 | −177.99 (12) |
| N2—N1—C1—N3 | 179.36 (12) | O1—C4—C5—C6 | 179.21 (12) |
| N2—N1—C1—S1 | −1.51 (19) | C3—C4—C5—C6 | −1.0 (2) |
| N1—N2—C2—C3 | 178.75 (11) | C4—C5—C6—C7 | 0.3 (2) |
| N1—N2—C2—C2′ | 0.0 (2) | C5—C6—C7—C8 | 0.6 (2) |
| N2—C2—C3—C8 | −179.27 (12) | C6—C7—C8—C3 | −0.7 (2) |
| C2′—C2—C3—C8 | −0.4 (2) | C4—C3—C8—C7 | 0.1 (2) |
| N2—C2—C3—C4 | −0.5 (2) | C2—C3—C8—C7 | 178.85 (13) |
| C2′—C2—C3—C4 | 178.29 (12) | C1—N3—C9—C10 | −172.17 (13) |
| C8—C3—C4—O1 | −179.39 (12) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C3–C8 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*O*···N2 | 0.84 (1) | 1.76 (1) | 2.5292 (16) | 150 (2) |
| N1—H1*N*···O1*W*$^{i}$ | 0.86 (2) | 2.09 (2) | 2.8918 (17) | 156 (2) |
| N3—H3*N*···O1*W*$^{i}$ | 0.87 (2) | 2.16 (2) | 2.9625 (18) | 154 (2) |
| O1*W*—H1*W*···O1 | 0.84 (2) | 1.96 (2) | 2.7894 (16) | 174 (2) |
| O1*W*—H2*W*···*Cg*1$^{ii}$ | 0.83 (1) | 2.86 (1) | 3.4165 (13) | 127 (1) |
| C5—H5···O1$^{iii}$ | 0.95 | 2.56 | 3.3702 (18) | 143 |

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