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1,5-Bis[(*E*)-1-(2-hydroxyphenyl)ethylidene]thiocarbonohydrazide monohydrate

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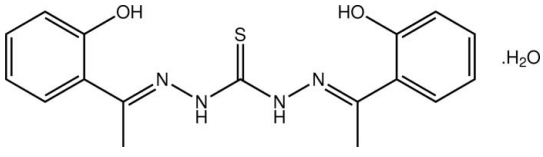
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.102; data-to-parameter ratio = 16.1.

In the title compound, $C_{17}H_{18}N_4O_2S\cdot H_2O$, the thiourea derivative is almost planar, with an r.m.s. deviation for the non-H atoms of 0.057 Å. The hydroxyl groups lie to the same side of the molecule as the thione S atom, a conformation that allows the formation of intramolecular O—H···S and O—H···N hydrogen bonds. In the crystal structure, the thiourea and water molecules self-assemble into a two-dimensional array by a combination of O_{water}—H···$O_{hydroxyl}$, N—H···O_{water} and O_{water}—H···S hydrogen bonds and C—H···π interactions.

Related literature

For background and recent studies of the biological activity of organotin compounds, see: Gielen & Tiekink (2005); Affan *et al.* (2009). For the structure of the ketone analogue of the title compound, see: Zukerman-Schpector *et al.* (2009).



Experimental

Crystal data

$C_{17}H_{18}N_4O_2S\cdot H_2O$
M_r = 360.43
Monoclinic, $P2_1/n$
a = 15.8654 (3) Å
b = 7.3938 (1) Å
c = 16.3697 (3) Å
β = 115.922 (1)°
V = 1727.06 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 100 K
0.44 × 0.13 × 0.07 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.905, T_{max} = 1
15464 measured reflections
3968 independent reflections
3136 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.102
S = 1.03
3968 reflections
246 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

*Cg*1 is the centroid of the C4–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···N2	0.83 (2)	1.79 (2)	2.5191 (17)	147 (2)
O1—H1*O*···S1	0.83 (2)	2.86 (2)	3.5126 (13)	138 (2)
O2—H2*O*···N4	0.82 (2)	1.81 (2)	2.542 (2)	148 (2)
O2—H2*O*···S1	0.82 (2)	2.96 (2)	3.6220 (15)	139 (2)
O3—H3*O*···O1	0.84 (2)	1.91 (2)	2.7525 (18)	174 (2)
O3—H4*O*···S1^{i}	0.82 (2)	2.76 (2)	3.5089 (14)	154 (2)
N1—H1*N*···O3^{ii}	0.87 (2)	2.04 (2)	2.8169 (19)	150 (2)
N3—H3*N*···O3^{ii}	0.88 (2)	2.04 (2)	2.854 (2)	154 (2)
C11—H11*C*···*Cg*1^{iii}	0.98	2.61	3.4497 (17)	144

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5327).

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supplementary materials

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1,5-Bis[(*E*)-1-(2-hydroxyphenyl)ethylidene]thiocarbonohydrazide monohydrate

M. A. Affan, D. N. A. Chee, F. B. Ahmad and E. R. T. Tiekink

Comment

The molecule in the title hydrate, (I), was synthesised as part of an on-going study into biological studies of organotin compounds (Gielen & Tiekink, 2005; Affan *et al.*, 2009). The thiourea derivative in (I) is effectively planar with the maximum deviation of any of the torsion angles from 0 or 180° being 4.6 (2)° for N4—C10—C12—C13 and -174.62 (15)° for C11—C10—C12—C13. The r.m.s. deviation for all non-hydrogen atoms in the thiourea molecule = 0.057 Å. The conformation about each of the C1═N2 [1.290 (2) Å] and C10═N4 [1.2956 (19) Å] double bonds is *E*. Finally, the hydroxyl groups are orientated to the same side of the molecule as the thione-S atom. The described molecular conformation is stabilised by intramolecular $O_{hydroxyl}$—H···N_{imine} and $O_{hydroxyl}$—H···S_{thione} hydrogen bonds, Table 1. Allowing for substitution of the thione by a ketone group, the described molecular conformation for the thiourea molecule in (I) resembles that in the recently reported ketone derivative (Zukerman-Schpector *et al.*, 2009).

In addition to the intramolecular hydrogen bonds, the crystal structure features O_{water}—H···$O_{hydroxyl}$, N—H···O_{water} and O_{water}—H···S hydrogen bonds, Table 1. The N—H atoms of one molecule connect to a water molecule which in turn forms a hydrogen bond with a hydroxyl-O1 atom of a second thiourea derivative. These interactions give rise to a supramolecular chain with base vector [101]. However, this does not take into account a second donor hydrogen bond involving the water molecule. This forms a hydrogen bond with a thione-S atom of a third thiourea derivative, Fig. 2. The latter interactions link chains into a 2-D array with additional stabilisation afforded by C—H···π, Table 1, and π···π interactions. The latter occur between the benzene rings: ring centroid(C4–C9)···ring centroid$(C12–C17)^{i}$ distance = 3.7821 (10) Å, with a dihedral angle between the least-squares plane through the rings of 2.25 (7)°; symmetry operation i: 1 - x, -y, 1 - z.

Experimental

A mixture of thiocarbohydrazone (0.53 g, 0.005 mol) and 2-hydroxyacetophenone (1.36 g, 0.01 mol) in absolute ethanol was heated under reflux for 4–5 h in the presence of 1–2 drops of glacial acetic acid. The reaction mixture was allowed to cool to room temperature for 1 h. The light-yellow precipitate was filtered off and washed several times using absolute ethanol, and was purified by recrystallization from hot absolute ethanol and dried under vacuum over P_2O_5. Colourless prisms of (I) were obtained by slow evaporation of acetone solution at room temperature. Yield: 1.66 g, 88.0%. m.p. = 494–496 K. IR (KBr): ν_{OH} (3561–3391), ν_{NH} 3230, $\nu_{C=N}$ 1619, $\nu_{N—N}$ 963, $\nu_{C=S}$ 857 cm^{-1}.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95–0.98 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) set to 1.2–1.5U_{eq}(C). The O- and N-bound H-atoms were located in a difference Fourier map and were refined with O–H and N–H restraints of 0.84 (10) Å and 0.88 (10) Å, respectively, and with U_{iso}(H) = 1.2U_{eq}(N) and 1.5U_{eq}(O).

Figures

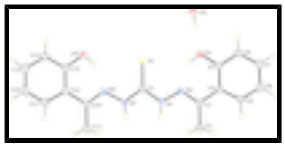

Fig. 1. Molecular structure of (I) showing displacement ellipsoids at the 50% probability level.

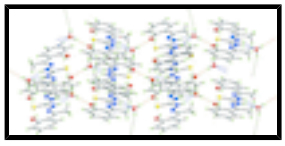

Fig. 2. Supramolecular 2-D array in (I) mediated by O—H···O (orange dashed lines), N—H···O (blue dashed lines) and O—H···S (green dashed lines) hydrogen bonds. Colour code: S, yellow; O, red; N, blue; C, grey; H, green.

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Crystal data

$C_{17}H_{18}N_4O_2S·H_2O$	$F(000) = 760$
$M_r = 360.43$	$D_x = 1.386$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 4324 reflections
$a = 15.8654$ (3) Å	$\theta = 2.9$–$27.4°$
$b = 7.3938$ (1) Å	$\mu = 0.21$ mm^{-1}
$c = 16.3697$ (3) Å	$T = 100$ K
$\beta = 115.922$ (1)°	Prism, colourless
$V = 1727.06$ (5) Å^3	0.44 × 0.13 × 0.07 mm
$Z = 4$	

Data collection

Bruker SMART APEXII CCD diffractometer	3968 independent reflections
Radiation source: sealed tube	3136 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.033$
φ and ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 1.5°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -20 \rightarrow 20$
$T_{min} = 0.905$, $T_{max} = 1$	$k = -9 \rightarrow 8$
15464 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.038$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.102$	H atoms treated by a mixture of independent and constrained refinement

S = 1.03	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.7503P]$ where $P = (F_o^2 + 2F_c^2)/3$
3968 reflections	$(\Delta/\sigma)_{max} = 0.001$
246 parameters	$\Delta\rho_{max} = 0.35$ e Å^{-3}
7 restraints	$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
S1	0.65089 (3)	0.17338 (6)	0.56929 (3)	0.02002 (12)
O1	0.65341 (7)	0.31213 (16)	0.77557 (8)	0.0213 (3)
H1O	0.6224 (14)	0.300 (3)	0.7201 (15)	0.032*
O2	0.70052 (8)	−0.01110 (17)	0.38996 (7)	0.0225 (3)
H2O	0.6629 (14)	0.041 (3)	0.4040 (14)	0.034*
O3	0.82009 (8)	0.13214 (18)	0.86971 (9)	0.0240 (3)
H3O	0.7673 (15)	0.180 (3)	0.8392 (15)	0.036*
H4O	0.8143 (14)	0.022 (3)	0.8646 (15)	0.036*
N1	0.47863 (9)	0.29267 (19)	0.53363 (9)	0.0179 (3)
H1N	0.4205 (13)	0.313 (2)	0.4972 (12)	0.022*
N2	0.51214 (9)	0.33207 (18)	0.62387 (8)	0.0166 (3)
N3	0.49527 (9)	0.19563 (19)	0.41174 (9)	0.0179 (3)
H3N	0.4365 (13)	0.229 (3)	0.3827 (13)	0.021*
N4	0.54462 (9)	0.12100 (18)	0.36967 (9)	0.0172 (3)
C1	0.53819 (10)	0.2217 (2)	0.50290 (11)	0.0170 (3)
C2	0.45776 (10)	0.4008 (2)	0.65560 (10)	0.0158 (3)
C3	0.35589 (10)	0.4419 (2)	0.59818 (11)	0.0203 (3)
H3A	0.3499	0.5603	0.5693	0.030*
H3B	0.3227	0.4433	0.6365	0.030*
H3C	0.3287	0.3488	0.5513	0.030*
C4	0.50342 (10)	0.4407 (2)	0.75353 (10)	0.0163 (3)
C5	0.59838 (11)	0.3942 (2)	0.80910 (11)	0.0175 (3)
C6	0.63916 (11)	0.4332 (2)	0.90125 (11)	0.0206 (3)
H6	0.7024	0.3997	0.9379	0.025*
C7	0.58878 (11)	0.5202 (2)	0.94020 (11)	0.0225 (4)
H7	0.6175	0.5468	1.0033	0.027*
C8	0.49609 (11)	0.5689 (2)	0.88708 (11)	0.0223 (4)

H8	0.4613	0.6295	0.9136	0.027*
C9	0.45484 (11)	0.5287 (2)	0.79543 (11)	0.0191 (3)
H9	0.3913	0.5619	0.7598	0.023*
C10	0.50214 (11)	0.0843 (2)	0.28371 (10)	0.0172 (3)
C11	0.39945 (11)	0.1186 (2)	0.22693 (11)	0.0235 (4)
H11A	0.3647	0.0869	0.2618	0.035*
H11B	0.3771	0.0445	0.1718	0.035*
H11C	0.3896	0.2468	0.2101	0.035*
C12	0.56124 (11)	0.0036 (2)	0.24484 (10)	0.0178 (3)
C13	0.65610 (11)	−0.0429 (2)	0.29941 (11)	0.0187 (3)
C14	0.70852 (11)	−0.1286 (2)	0.26121 (11)	0.0227 (4)
H14	0.7713	−0.1634	0.2990	0.027*
C15	0.67062 (12)	−0.1635 (2)	0.16938 (12)	0.0242 (4)
H15	0.7073	−0.2212	0.1440	0.029*
C16	0.57851 (12)	−0.1140 (2)	0.11390 (11)	0.0247 (4)
H16	0.5523	−0.1360	0.0504	0.030*
C17	0.52543 (12)	−0.0331 (2)	0.15140 (11)	0.0217 (4)
H17	0.4624	−0.0010	0.1128	0.026*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01439 (18)	0.0259 (2)	0.01724 (19)	0.00368 (15)	0.00456 (14)	0.00086 (17)
O1	0.0168 (5)	0.0242 (6)	0.0187 (6)	0.0036 (5)	0.0039 (5)	−0.0026 (5)
O2	0.0162 (5)	0.0326 (7)	0.0167 (6)	0.0010 (5)	0.0054 (5)	−0.0034 (5)
O3	0.0144 (5)	0.0226 (7)	0.0283 (6)	0.0009 (5)	0.0031 (5)	−0.0023 (6)
N1	0.0135 (6)	0.0230 (8)	0.0150 (6)	0.0015 (5)	0.0042 (5)	−0.0006 (6)
N2	0.0165 (6)	0.0166 (7)	0.0148 (6)	−0.0005 (5)	0.0049 (5)	0.0007 (5)
N3	0.0142 (6)	0.0210 (7)	0.0162 (6)	0.0020 (5)	0.0046 (5)	−0.0002 (6)
N4	0.0170 (6)	0.0167 (7)	0.0176 (6)	−0.0003 (5)	0.0075 (5)	0.0003 (5)
C1	0.0168 (7)	0.0155 (8)	0.0180 (8)	−0.0017 (6)	0.0069 (6)	0.0014 (6)
C2	0.0152 (7)	0.0135 (8)	0.0181 (7)	−0.0021 (6)	0.0066 (6)	0.0014 (6)
C3	0.0165 (7)	0.0247 (9)	0.0182 (8)	−0.0006 (6)	0.0062 (6)	−0.0005 (7)
C4	0.0162 (7)	0.0139 (8)	0.0179 (7)	−0.0031 (6)	0.0066 (6)	0.0008 (6)
C5	0.0175 (7)	0.0130 (8)	0.0212 (8)	−0.0013 (6)	0.0078 (6)	0.0005 (6)
C6	0.0179 (7)	0.0185 (9)	0.0200 (8)	−0.0027 (6)	0.0032 (6)	0.0014 (7)
C7	0.0253 (8)	0.0226 (9)	0.0177 (8)	−0.0057 (7)	0.0075 (7)	−0.0023 (7)
C8	0.0247 (8)	0.0211 (9)	0.0243 (8)	−0.0022 (7)	0.0136 (7)	−0.0031 (7)
C9	0.0167 (7)	0.0194 (8)	0.0209 (8)	−0.0015 (6)	0.0081 (6)	0.0008 (7)
C10	0.0186 (7)	0.0132 (8)	0.0176 (7)	−0.0033 (6)	0.0058 (6)	0.0015 (6)
C11	0.0193 (8)	0.0236 (9)	0.0226 (8)	−0.0014 (6)	0.0046 (7)	0.0001 (7)
C12	0.0212 (8)	0.0136 (8)	0.0170 (7)	−0.0025 (6)	0.0069 (6)	0.0014 (6)
C13	0.0206 (7)	0.0181 (8)	0.0172 (7)	−0.0049 (6)	0.0080 (6)	0.0006 (6)
C14	0.0190 (8)	0.0249 (9)	0.0243 (8)	−0.0027 (6)	0.0096 (7)	0.0006 (7)
C15	0.0319 (9)	0.0202 (9)	0.0263 (9)	−0.0032 (7)	0.0181 (7)	−0.0024 (7)
C16	0.0360 (9)	0.0202 (9)	0.0169 (8)	−0.0018 (7)	0.0105 (7)	−0.0019 (7)
C17	0.0248 (8)	0.0168 (8)	0.0186 (8)	0.0003 (6)	0.0050 (7)	0.0008 (7)

Geometric parameters (Å, °)

S1—C1	1.6754 (15)	C6—C7	1.380 (2)
O1—C5	1.3606 (19)	C6—H6	0.9500
O1—H1O	0.83 (2)	C7—C8	1.389 (2)
O2—C13	1.3550 (19)	C7—H7	0.9500
O2—H2O	0.82 (2)	C8—C9	1.382 (2)
O3—H3O	0.84 (2)	C8—H8	0.9500
O3—H4O	0.82 (2)	C9—H9	0.9500
N1—C1	1.355 (2)	C10—C12	1.470 (2)
N1—N2	1.3649 (18)	C10—C11	1.503 (2)
N1—H1N	0.865 (18)	C11—H11A	0.9800
N2—C2	1.290 (2)	C11—H11B	0.9800
N3—C1	1.356 (2)	C11—H11C	0.9800
N3—N4	1.3650 (18)	C12—C17	1.406 (2)
N3—H3N	0.876 (18)	C12—C13	1.416 (2)
N4—C10	1.2956 (19)	C13—C14	1.392 (2)
C2—C4	1.472 (2)	C14—C15	1.378 (2)
C2—C3	1.503 (2)	C14—H14	0.9500
C3—H3A	0.9800	C15—C16	1.391 (2)
C3—H3B	0.9800	C15—H15	0.9500
C3—H3C	0.9800	C16—C17	1.377 (2)
C4—C9	1.396 (2)	C16—H16	0.9500
C4—C5	1.420 (2)	C17—H17	0.9500
C5—C6	1.387 (2)		
C5—O1—H1O	108.2 (14)	C8—C7—H7	120.0
C13—O2—H2O	107.0 (14)	C9—C8—C7	119.54 (16)
H3O—O3—H4O	109 (2)	C9—C8—H8	120.2
C1—N1—N2	118.65 (13)	C7—C8—H8	120.2
C1—N1—H1N	121.2 (12)	C8—C9—C4	122.18 (14)
N2—N1—H1N	120.2 (12)	C8—C9—H9	118.9
C2—N2—N1	120.48 (12)	C4—C9—H9	118.9
C1—N3—N4	119.32 (13)	N4—C10—C12	115.31 (13)
C1—N3—H3N	117.4 (12)	N4—C10—C11	123.03 (15)
N4—N3—H3N	123.3 (12)	C12—C10—C11	121.65 (14)
C10—N4—N3	119.45 (13)	C10—C11—H11A	109.5
N1—C1—N3	111.55 (13)	C10—C11—H11B	109.5
N1—C1—S1	124.15 (12)	H11A—C11—H11B	109.5
N3—C1—S1	124.30 (12)	C10—C11—H11C	109.5
N2—C2—C4	114.84 (13)	H11A—C11—H11C	109.5
N2—C2—C3	123.59 (14)	H11B—C11—H11C	109.5
C4—C2—C3	121.55 (14)	C17—C12—C13	116.86 (15)
C2—C3—H3A	109.5	C17—C12—C10	121.22 (14)
C2—C3—H3B	109.5	C13—C12—C10	121.91 (14)
H3A—C3—H3B	109.5	O2—C13—C14	116.31 (14)
C2—C3—H3C	109.5	O2—C13—C12	123.28 (15)
H3A—C3—H3C	109.5	C14—C13—C12	120.40 (15)
H3B—C3—H3C	109.5	C15—C14—C13	120.93 (15)

C9—C4—C5	117.19 (14)	C15—C14—H14	119.5
C9—C4—C2	120.92 (13)	C13—C14—H14	119.5
C5—C4—C2	121.88 (14)	C14—C15—C16	119.74 (16)
O1—C5—C6	117.06 (14)	C14—C15—H15	120.1
O1—C5—C4	122.53 (14)	C16—C15—H15	120.1
C6—C5—C4	120.40 (15)	C17—C16—C15	119.75 (15)
C7—C6—C5	120.68 (15)	C17—C16—H16	120.1
C7—C6—H6	119.7	C15—C16—H16	120.1
C5—C6—H6	119.7	C16—C17—C12	122.27 (15)
C6—C7—C8	120.00 (15)	C16—C17—H17	118.9
C6—C7—H7	120.0	C12—C17—H17	118.9
C1—N1—N2—C2	179.58 (14)	C7—C8—C9—C4	−0.4 (3)
C1—N3—N4—C10	175.22 (15)	C5—C4—C9—C8	−0.4 (2)
N2—N1—C1—N3	−178.03 (13)	C2—C4—C9—C8	−179.56 (15)
N2—N1—C1—S1	1.7 (2)	N3—N4—C10—C12	−179.77 (13)
N4—N3—C1—N1	−178.53 (13)	N3—N4—C10—C11	−0.5 (2)
N4—N3—C1—S1	1.8 (2)	N4—C10—C12—C17	−176.26 (15)
N1—N2—C2—C4	−178.58 (13)	C11—C10—C12—C17	4.5 (2)
N1—N2—C2—C3	0.2 (2)	N4—C10—C12—C13	4.6 (2)
N2—C2—C4—C9	174.83 (15)	C11—C10—C12—C13	−174.62 (15)
C3—C2—C4—C9	−4.0 (2)	C17—C12—C13—O2	178.25 (15)
N2—C2—C4—C5	−4.3 (2)	C10—C12—C13—O2	−2.6 (2)
C3—C2—C4—C5	176.85 (15)	C17—C12—C13—C14	−2.9 (2)
C9—C4—C5—O1	−178.43 (14)	C10—C12—C13—C14	176.31 (15)
C2—C4—C5—O1	0.8 (2)	O2—C13—C14—C15	−178.53 (15)
C9—C4—C5—C6	1.0 (2)	C12—C13—C14—C15	2.5 (3)
C2—C4—C5—C6	−179.76 (15)	C13—C14—C15—C16	−0.5 (3)
O1—C5—C6—C7	178.47 (15)	C14—C15—C16—C17	−1.0 (3)
C4—C5—C6—C7	−1.0 (2)	C15—C16—C17—C12	0.6 (3)
C5—C6—C7—C8	0.3 (3)	C13—C12—C17—C16	1.4 (2)
C6—C7—C8—C9	0.4 (3)	C10—C12—C17—C16	−177.81 (15)

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···N2	0.83 (2)	1.79 (2)	2.5191 (17)	147 (2)
O1—H1O···S1	0.83 (2)	2.86 (2)	3.5126 (13)	138 (2)
O2—H2O···N4	0.82 (2)	1.81 (2)	2.542 (2)	148 (2)
O2—H2O···S1	0.82 (2)	2.96 (2)	3.6220 (15)	139 (2)
O3—H3O···O1	0.84 (2)	1.91 (2)	2.7525 (18)	174 (2)
O3—H4O···S1^{i}	0.82 (2)	2.76 (2)	3.5089 (14)	154 (2)
N1—H1N···O3^{ii}	0.87 (2)	2.04 (2)	2.8169 (19)	150.(2)
N3—H3N···O3^{ii}	0.88 (2)	2.04 (2)	2.854 (2)	154.(2)
C11—H11C···Cg1^{iii}	0.98	2.61	3.4497 (17)	144

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

Fig. 1

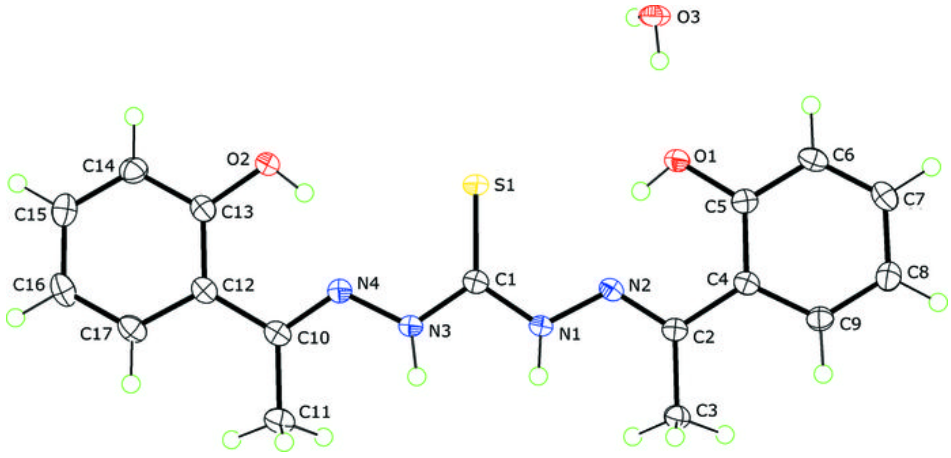
O3
O2
C14
C15
C13
C16
C12
C17
N4
C10
C11
S1
C1
N3
N1
N2
O1
C5
C6
C7
C4
C8
C9
C2
C3

Fig. 2