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1-(Biphenyl-4-ylmethylidene)thiosemicarbazide monohydrate

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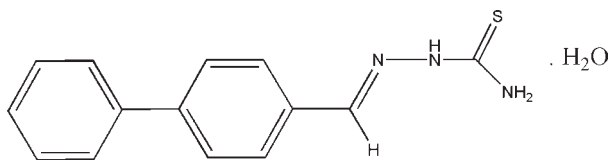
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å;
R factor = 0.044; wR factor = 0.145; data-to-parameter ratio = 11.4.

In the title compound, $\text{C}_{14}\text{H}_{13}\text{N}_3\text{S}\cdot\text{H}_2\text{O}$, the thiosemicarbazide group is nearly planar, with a maximum deviation of 0.072 (2) Å from the ideal least-squares plane, and shows an *E* conformation. In the crystal packing, the water molecules are involved in an extensive intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen-bond network, assisted by $\text{O}-\text{H}\cdots\text{S}$ interactions, which link the independent molecules into chains extended along *b* axis. An intramolecular hydrogen $\text{N}-\text{H}\cdots\text{N}$ bond helps to stabilize the molecular conformation.

Related literature

For the biological activity and potential medical applications of thiosemicarbazides, see: West *et al.* (1991). For thiosemicarbazides as ligands, see: Kowol *et al.* (2007).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{13}\text{N}_3\text{S}\cdot\text{H}_2\text{O}$
 $M_r = 273.36$
 Monoclinic, $P2_1/c$
 $a = 14.428$ (5) Å
 $b = 6.350$ (5) Å
 $c = 15.276$ (4) Å
 $\beta = 99.750$ (5)°

$V = 1379.3$ (12) Å³
 $Z = 4$
 Cu $K\alpha$ radiation
 $\mu = 2.05$ mm⁻¹
 $T = 293$ K
 $0.28 \times 0.22 \times 0.19$ mm

Data collection

Oxford Diffraction Xcalibur Gemini S diffractometer
 Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
 $T_{\min} = 0.659$, $T_{\max} = 1.000$
 8823 measured reflections
 2652 independent reflections
 2208 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.145$
 $S = 1.12$
 2652 reflections
 233 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.34$ e Å⁻³
 $\Delta\rho_{\min} = -0.32$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H14}\cdots\text{O1}$	0.92 (3)	1.91 (3)	2.819 (3)	172 (3)
$\text{N3}-\text{H15}\cdots\text{N1}$	0.91 (3)	2.14 (3)	2.585 (3)	110 (2)
$\text{N3}-\text{H16}\cdots\text{S1}^{\text{i}}$	0.86 (4)	2.59 (4)	3.422 (3)	163 (3)
$\text{O1}-\text{H17}\cdots\text{S1}^{\text{ii}}$	0.86 (5)	2.44 (5)	3.287 (3)	169 (4)
$\text{O1}-\text{H18}\cdots\text{S1}^{\text{iii}}$	0.77 (5)	2.60 (5)	3.352 (3)	164 (5)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2023).

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supplementary materials

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1-(Biphenyl-4-ylmethylidene)thiosemicarbazide monohydrate

R. Mendoza-Meroño, L. Menéndez-Taboada, E. Fernández-Zapico and S. García-Granda

Comment

Thiosemicarbazides, a class of compounds possessing a wide spectrum of potential medicinal applications, have been studied for their antitumoral, antiviral, antibacterial, antimalarial, antifungal, anti-inflammatory and anti-HIV activities (West *et al.*, 1991). These properties are thought to arise from the metal-chelating ability of these ligands. In almost all cases, the ligands are bidentate and bind to the metal through the S and hydrazinic N atoms, although there are examples of them acting as monodentate ligands binding only through sulfur (Kowol *et al.*, 2007).

The title compound $C_{14}H_{13}N_3S \cdot H_2O$ was synthesized and its crystal structure is reported here. This compound is likely to have biomedical properties similar to other nitrogen-sulfur donor ligands. The asymmetric unit consists of a single molecule (I), shown in Figure 1. The thiosemicarbazide adopts an E conformation with a *trans* configuration observed about the C=N bond. The thiosemicarbazide moiety is planar, the C(14)—N(2) (1.341 (3) Å) and N(1)—N(2) (1.371 (3) Å) bond lengths imply significant electron delocalization and the C13/N1/N2/C14/S1 fragment is close to planar (max. deviation = 0.072 (2) Å). The dihedral angle between benzene ring C7/C8/C9/C10/C11/C12 and the moiety C13/N1/N2/C14/S1 is 4.67 (1)°. This value suggests that they are nearly coplanar, and π -electrons are delocalized in the benzaldehyde thiosemicarbazide fragment.

The water molecules are involved in an extensive intermolecular N(2)—H(14)⋯O(1) hydrogen bonds and O(1)—H(17)⋯S(1) interactions (Table 1), which link the molecules into chains extended along the *b* axis. Sulfur atom S(1) is also involved in N(3)—H(16)⋯S(1) intermolecular interactions, favoring the crystal grown in the *ac* plane. An intramolecular N(3)—H(15)⋯N(1) hydrogen bond (Table 1) contributes to stabilize the molecular conformation. The intermolecular distance value between ring centroids in the *b* axis direction (6.350 Å), suggests that there is no π -stacking interaction between parallel molecules (Figure 2).

Experimental

A solution of 4-biphenylcarboxaldehyde (1.822 g, 0.01 mol) and thiosemicarbazide (0.91 g, 0.01 mol) in absolute methanol (50 ml) was refluxing for 4 h, in the presence of *p*-toluenesulfonic acid (0.005 g) as catalyst, with continuous stirring. Completeness of the reaction was TLC controlled indicating the disappearance of the aldehyde spot. On cooling to room temperature the precipitate was filtered off, washed with copious cold methanol and dried in air (yield: 1.581 g, 61%; m.p. 475 K). Yellow single crystals compound were obtained after recrystallization from a solution of chloroform/methanol (3:7 v/v) after 10 days at room temperature.

Refinement

At the end of the refinement the highest peak in the electron density was $0.3350 \text{ e \AA}^{-3}$, while the deepest hole was $-0.3210 \text{ e \AA}^{-3}$.

Figures

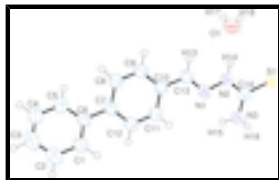


Fig. 1. A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

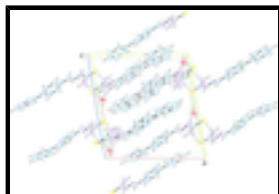


Fig. 2. Packing diagram viewed parallel to the *b* axis. Hydrogen bonds and other intermolecular interactions are indicated by dashed lines.

1-(Biphenyl-4-ylmethylidene)thiosemicarbazide monohydrate

Crystal data

$C_{14}H_{13}N_3S \cdot H_2O$

$M_r = 273.36$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.428 (5) \text{ \AA}$

$b = 6.350 (5) \text{ \AA}$

$c = 15.276 (4) \text{ \AA}$

$\beta = 99.750 (5)^\circ$

$V = 1379.3 (12) \text{ \AA}^3$

$Z = 4$

$F(000) = 576$

$D_x = 1.316 \text{ Mg m}^{-3}$

Melting point: 475 K

Cu $K\alpha$ radiation, $\lambda = 1.54180 \text{ \AA}$

Cell parameters from 3594 reflections

$\theta = 3.9\text{--}71.2^\circ$

$\mu = 2.05 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Needle, yellow

$0.28 \times 0.22 \times 0.19 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur Gemini S diffractometer

Radiation source: Enhance (Cu) X-ray Source graphite

Detector resolution: $10.2673 \text{ pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan (CrysAlis Pro; Oxford Diffraction, 2009)

$T_{\min} = 0.659$, $T_{\max} = 1.000$

8823 measured reflections

2652 independent reflections

2208 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 71.3^\circ$, $\theta_{\min} = 5.9^\circ$

$h = -17 \rightarrow 17$

$k = -6 \rightarrow 7$

$l = -17 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$$R[F^2 > 2\sigma(F^2)] = 0.044$$

$$wR(F^2) = 0.145$$

$$S = 1.12$$

2652 reflections

233 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0724P)^2 + 0.4128P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.34 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -0.32 \text{ e } \text{Å}^{-3}$$

Extinction correction: SHELXL97 (Sheldrick, 2008),

$$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Extinction coefficient: 0.0022 (5)

Special details

Experimental. CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.34.9 (release 08-12-2009 CrysAlis171 .NET)(compiled Dec 8 2009,17:31:18). Empirical absorption correction using spherical harmonics,implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	1.03245 (4)	-0.35800 (9)	0.35948 (4)	0.0569 (2)
N2	0.87783 (13)	-0.1308 (3)	0.31541 (13)	0.0506 (5)
N1	0.79162 (12)	-0.0958 (3)	0.26420 (12)	0.0512 (5)
O1	0.95339 (19)	0.1981 (4)	0.42955 (18)	0.0826 (7)
C9	0.62409 (16)	0.3346 (4)	0.22359 (17)	0.0554 (6)
C14	0.92353 (15)	-0.3091 (4)	0.30268 (15)	0.0518 (5)
N3	0.87879 (17)	-0.4428 (4)	0.24280 (16)	0.0687 (6)
C7	0.48473 (14)	0.2361 (4)	0.12056 (15)	0.0490 (5)
C13	0.75391 (15)	0.0839 (4)	0.27165 (16)	0.0526 (5)
C10	0.66283 (15)	0.1342 (3)	0.21913 (15)	0.0506 (5)
C11	0.61170 (16)	-0.0131 (4)	0.16261 (17)	0.0546 (5)
C8	0.53638 (16)	0.3841 (4)	0.17552 (16)	0.0543 (6)
C6	0.39026 (15)	0.2860 (4)	0.07042 (15)	0.0516 (5)
C12	0.52453 (16)	0.0367 (4)	0.11508 (16)	0.0545 (6)
C5	0.36951 (18)	0.4859 (4)	0.03497 (19)	0.0639 (6)
C1	0.31911 (17)	0.1354 (4)	0.05726 (18)	0.0609 (6)
C2	0.22957 (19)	0.1843 (5)	0.01258 (19)	0.0707 (7)
C4	0.2796 (2)	0.5341 (5)	-0.0100 (2)	0.0748 (8)
C3	0.2100 (2)	0.3841 (6)	-0.02047 (18)	0.0728 (8)

supplementary materials

H8	0.5121 (18)	0.525 (5)	0.1814 (18)	0.063 (7)*
H12	0.4912 (18)	-0.064 (4)	0.0746 (17)	0.060 (7)*
H5	0.421 (2)	0.590 (5)	0.041 (2)	0.078 (9)*
H1	0.3329 (17)	-0.005 (4)	0.0831 (18)	0.060 (7)*
H9	0.6583 (17)	0.436 (4)	0.2642 (17)	0.057 (7)*
H13	0.7819 (17)	0.187 (4)	0.3128 (17)	0.052 (6)*
H11	0.638 (2)	-0.147 (4)	0.1583 (19)	0.066 (8)*
H3	0.146 (2)	0.420 (5)	-0.053 (2)	0.085 (9)*
H4	0.267 (2)	0.679 (6)	-0.036 (2)	0.094 (10)*
H2	0.180 (2)	0.076 (6)	0.004 (2)	0.094 (11)*
H14	0.907 (2)	-0.033 (5)	0.3552 (19)	0.066 (8)*
H15	0.825 (2)	-0.392 (5)	0.211 (2)	0.072 (8)*
H16	0.907 (2)	-0.553 (6)	0.229 (2)	0.082 (9)*
H17	0.975 (3)	0.304 (8)	0.404 (3)	0.129 (16)*
H18	0.959 (3)	0.210 (7)	0.481 (3)	0.120 (17)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0468 (3)	0.0545 (4)	0.0666 (4)	0.0023 (2)	0.0016 (3)	0.0058 (3)
N2	0.0410 (9)	0.0526 (10)	0.0555 (11)	0.0008 (8)	0.0005 (8)	-0.0025 (8)
N1	0.0417 (9)	0.0596 (11)	0.0509 (10)	0.0024 (8)	0.0035 (7)	-0.0017 (8)
O1	0.1079 (17)	0.0666 (12)	0.0679 (14)	-0.0285 (12)	-0.0003 (12)	-0.0015 (11)
C9	0.0459 (12)	0.0556 (13)	0.0621 (14)	-0.0015 (10)	0.0020 (10)	-0.0123 (11)
C14	0.0498 (12)	0.0509 (12)	0.0562 (13)	-0.0018 (9)	0.0134 (10)	0.0014 (10)
N3	0.0610 (13)	0.0635 (14)	0.0759 (15)	0.0105 (11)	-0.0048 (11)	-0.0176 (11)
C7	0.0431 (10)	0.0533 (12)	0.0500 (11)	-0.0014 (9)	0.0066 (9)	-0.0015 (9)
C13	0.0444 (11)	0.0564 (13)	0.0560 (13)	-0.0008 (10)	0.0052 (9)	-0.0058 (11)
C10	0.0422 (11)	0.0541 (12)	0.0552 (12)	-0.0006 (9)	0.0073 (9)	-0.0027 (10)
C11	0.0490 (12)	0.0500 (12)	0.0630 (14)	0.0034 (10)	0.0046 (10)	-0.0039 (10)
C8	0.0485 (12)	0.0516 (13)	0.0614 (14)	0.0038 (10)	0.0057 (10)	-0.0061 (10)
C6	0.0457 (11)	0.0598 (13)	0.0490 (12)	0.0023 (10)	0.0067 (9)	-0.0032 (10)
C12	0.0491 (12)	0.0536 (13)	0.0577 (13)	-0.0037 (10)	0.0004 (10)	-0.0081 (10)
C5	0.0558 (14)	0.0617 (15)	0.0714 (16)	0.0053 (12)	0.0030 (11)	0.0020 (12)
C1	0.0488 (12)	0.0681 (16)	0.0627 (15)	-0.0034 (11)	0.0007 (10)	0.0016 (12)
C2	0.0510 (14)	0.092 (2)	0.0656 (16)	-0.0049 (14)	0.0009 (11)	-0.0072 (14)
C4	0.0709 (17)	0.0776 (19)	0.0721 (18)	0.0199 (15)	0.0007 (13)	0.0035 (14)
C3	0.0559 (15)	0.102 (2)	0.0566 (15)	0.0155 (15)	-0.0005 (11)	-0.0039 (14)

Geometric parameters (\AA , $^\circ$)

S1—C14	1.690 (2)	C13—H13	0.95 (3)
N2—C14	1.341 (3)	C10—C11	1.396 (3)
N2—N1	1.371 (3)	C11—C12	1.378 (3)
N2—H14	0.92 (3)	C11—H11	0.94 (3)
N1—C13	1.278 (3)	C8—H8	0.97 (3)
O1—H17	0.86 (5)	C6—C1	1.393 (4)
O1—H18	0.77 (5)	C6—C5	1.393 (4)
C9—C8	1.387 (3)	C12—H12	0.96 (3)

C9—C10	1.397 (3)	C5—C4	1.396 (4)
C9—H9	0.97 (3)	C5—H5	0.98 (3)
C14—N3	1.332 (3)	C1—C2	1.390 (4)
N3—H15	0.90 (3)	C1—H1	0.98 (3)
N3—H16	0.86 (4)	C2—C3	1.377 (5)
C7—C8	1.390 (3)	C2—H2	0.98 (4)
C7—C12	1.399 (3)	C4—C3	1.374 (5)
C7—C6	1.480 (3)	C4—H4	1.01 (4)
C13—C10	1.454 (3)	C3—H3	0.99 (3)
C14—N2—N1	118.4 (2)	C10—C11—H11	118.6 (17)
C14—N2—H14	119.4 (17)	C9—C8—C7	121.0 (2)
N1—N2—H14	122.1 (17)	C9—C8—H8	118.1 (16)
C13—N1—N2	116.9 (2)	C7—C8—H8	120.9 (16)
H17—O1—H18	113 (4)	C1—C6—C5	117.7 (2)
C8—C9—C10	121.1 (2)	C1—C6—C7	121.3 (2)
C8—C9—H9	120.6 (15)	C5—C6—C7	121.0 (2)
C10—C9—H9	118.1 (15)	C11—C12—C7	121.5 (2)
N3—C14—N2	116.4 (2)	C11—C12—H12	120.0 (16)
N3—C14—S1	122.39 (19)	C7—C12—H12	118.4 (16)
N2—C14—S1	121.19 (18)	C6—C5—C4	120.8 (3)
C14—N3—H15	114.4 (19)	C6—C5—H5	118.1 (18)
C14—N3—H16	120 (2)	C4—C5—H5	121.1 (18)
H15—N3—H16	124 (3)	C2—C1—C6	121.2 (3)
C8—C7—C12	117.7 (2)	C2—C1—H1	120.6 (15)
C8—C7—C6	121.3 (2)	C6—C1—H1	118.1 (15)
C12—C7—C6	121.0 (2)	C3—C2—C1	120.1 (3)
N1—C13—C10	120.4 (2)	C3—C2—H2	120 (2)
N1—C13—H13	122.5 (15)	C1—C2—H2	120 (2)
C10—C13—H13	117.1 (15)	C3—C4—C5	120.4 (3)
C11—C10—C9	117.8 (2)	C3—C4—H4	121 (2)
C11—C10—C13	121.9 (2)	C5—C4—H4	119 (2)
C9—C10—C13	120.3 (2)	C4—C3—C2	119.7 (3)
C12—C11—C10	120.8 (2)	C4—C3—H3	119.5 (19)
C12—C11—H11	120.6 (17)	C2—C3—H3	120.8 (19)
C14—N2—N1—C13	-173.4 (2)	C12—C7—C6—C1	35.4 (3)
N1—N2—C14—N3	-2.6 (3)	C8—C7—C6—C5	36.1 (3)
N1—N2—C14—S1	176.85 (16)	C12—C7—C6—C5	-144.8 (3)
N2—N1—C13—C10	179.54 (19)	C10—C11—C12—C7	0.9 (4)
C8—C9—C10—C11	1.9 (4)	C8—C7—C12—C11	0.3 (4)
C8—C9—C10—C13	-178.5 (2)	C6—C7—C12—C11	-178.8 (2)
N1—C13—C10—C11	3.1 (4)	C1—C6—C5—C4	1.7 (4)
N1—C13—C10—C9	-176.4 (2)	C7—C6—C5—C4	-178.1 (2)
C9—C10—C11—C12	-2.0 (4)	C5—C6—C1—C2	-1.9 (4)
C13—C10—C11—C12	178.5 (2)	C7—C6—C1—C2	177.9 (2)
C10—C9—C8—C7	-0.7 (4)	C6—C1—C2—C3	0.7 (4)
C12—C7—C8—C9	-0.4 (4)	C6—C5—C4—C3	-0.3 (4)
C6—C7—C8—C9	178.8 (2)	C5—C4—C3—C2	-1.0 (4)
C8—C7—C6—C1	-143.7 (2)	C1—C2—C3—C4	0.8 (4)

supplementary materials

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H14 \cdots O1	0.92 (3)	1.91 (3)	2.819 (3)	172 (3)
N3—H15 \cdots N1	0.91 (3)	2.14 (3)	2.585 (3)	110 (2)
N3—H16 \cdots S1 ⁱ	0.86 (4)	2.59 (4)	3.422 (3)	163 (3)
O1—H17 \cdots S1 ⁱⁱ	0.86 (5)	2.44 (5)	3.287 (3)	169 (4)
O1—H18 \cdots S1 ⁱⁱⁱ	0.77 (5)	2.60 (5)	3.352 (3)	164 (5)

Symmetry codes: (i) $-x+2, y-1/2, -z+1/2$; (ii) $x, y+1, z$; (iii) $-x+2, -y, -z+1$.

Fig. 1

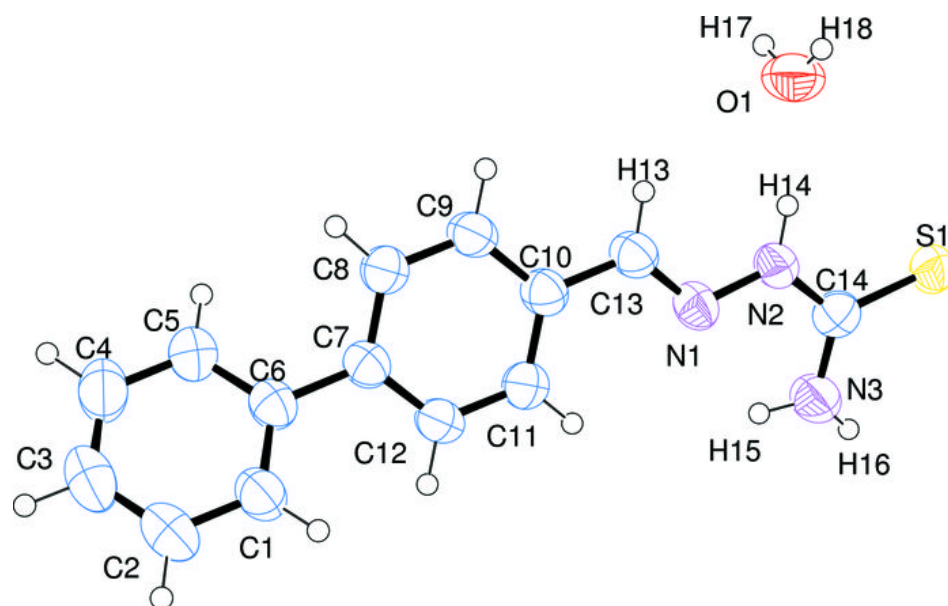


Fig. 2

