

C(7)—O(1)—C(8)	119.2 (3)	O(1)—C(7)—O(2)	123.5 (4)
C(2)—C(1)—C(6)	121.1 (5)	O(1)—C(7)—C(6)	112.5 (4)
C(1)—C(2)—C(3)	117.5 (5)	O(2)—C(7)—C(6)	124.0 (5)
F(1)—C(3)—C(2)	117.6 (5)	O(1)—C(8)—C(9)	121.0 (4)
F(1)—C(3)—C(4)	118.7 (5)	O(1)—C(8)—C(13)	116.8 (4)
C(2)—C(3)—C(4)	123.7 (4)	C(9)—C(8)—C(13)	122.2 (4)
C(3)—C(4)—C(5)	118.0 (4)	C(8)—C(9)—C(10)	118.8 (4)
C(4)—C(5)—C(6)	120.0 (4)	C(9)—C(10)—C(11)	119.9 (5)
C(1)—C(6)—C(5)	119.7 (4)	C(10)—C(11)—C(12)	120.6 (4)
C(1)—C(6)—C(7)	118.0 (4)	C(11)—C(12)—C(13)	120.1 (5)
C(5)—C(6)—C(7)	122.3 (4)	C(8)—C(13)—C(12)	118.4 (5)

## PB

O(1)—C(7)	1.351 (2)	C(5)—C(6)	1.386 (2)
O(1)—C(8)	1.415 (2)	C(6)—C(7)	1.481 (2)
O(2)—C(7)	1.195 (2)	C(8)—C(9)	1.364 (3)
C(1)—C(2)	1.376 (3)	C(8)—C(13)	1.371 (3)
C(1)—C(6)	1.383 (2)	C(9)—C(10)	1.384 (3)
C(2)—C(3)	1.368 (3)	C(10)—C(11)	1.375 (3)
C(3)—C(4)	1.373 (3)	C(11)—C(12)	1.373 (3)
C(4)—C(5)	1.382 (3)	C(12)—C(13)	1.381 (3)
C(7)—O(1)—C(8)	118.1 (1)	O(1)—C(7)—C(6)	111.5 (1)
C(2)—C(1)—C(6)	120.3 (2)	O(2)—C(7)—C(6)	125.4 (2)
C(1)—C(2)—C(3)	120.1 (2)	O(1)—C(8)—C(9)	121.2 (2)
C(2)—C(3)—C(4)	120.3 (2)	O(1)—C(8)—C(13)	116.8 (2)
C(3)—C(4)—C(5)	120.2 (2)	C(9)—C(8)—C(13)	121.9 (2)
C(4)—C(5)—C(6)	119.6 (2)	C(8)—C(9)—C(10)	119.0 (2)
C(1)—C(6)—C(5)	119.6 (2)	C(9)—C(10)—C(11)	119.9 (2)
C(1)—C(6)—C(7)	118.2 (2)	C(10)—C(11)—C(12)	120.1 (2)
C(5)—C(6)—C(7)	122.2 (2)	C(11)—C(12)—C(13)	120.3 (2)
O(1)—C(7)—O(2)	123.1 (2)	C(8)—C(13)—C(12)	118.7 (2)

The structures were solved by direct methods using *SAPI91* (Fan, 1991) and expanded using *DIRDIF92* (Beurskens *et al.*, 1992). H atoms were placed at calculated positions (C—H 0.95 Å). The displacement factors of the H atoms were kept fixed at the isotropic value of the parent atoms. All calculations were performed using the *TEXSAN* crystallographic software package (Molecular Structure Corporation, 1985).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, interatomic distances, bond distances involving H atoms and torsion angles have been deposited with the IUCr (Reference: AS1092). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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*Acta Cryst.* (1995). C51, 330–333

### 3,4,5-Trimethoxybenzaldehyde Thiosemicarbazone Monohydrate

M. K. KOKILA AND PUTTARAJA\*

*Department of Physics, Bangalore University, Bangalore 560 056, India*

M. V. KULKARNI

*Department of Chemistry, Karnatak University, Dharwad 580 003, India*

SARALA THAMPI

*Department of Organic Chemistry, Government College of Pharmacy, Bangalore 560 027, India*

(Received 10 March 1993; accepted 14 December 1993)

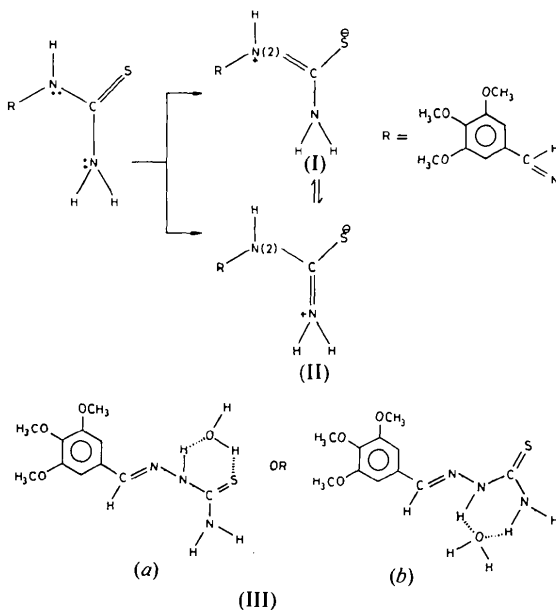
## Abstract

The structure of the title compound, C<sub>11</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub>S·H<sub>2</sub>O (III), has been determined. The molecule as a whole is not planar, though the phenyl ring is planar and makes a dihedral angle of 73.8 (2)° with the methoxy group at C(4). Molecules are linked through intermolecular N—H···S and N—H···O hydrogen bonds.

## Comment

Thiosemicarbazones (TSCs) are derivatives of carbonyl compounds which exhibit wide ranging biological activities. These include antituberculosis, antiviral, antileukaemic and antitumour activities and are given below with their appropriate TSC. Combinations of metal complexes with pyridoxal thiosemicarbazone (Ferrari Belicchi, Fava Gasparri, Leporati, Pelizzi, Tarasconi & Tosi, 1986) possess interesting spectroscopic properties. Non-bonded interactions of thiophene derivatives, observed in 2-formylthiophene semicarbazone (Anna, Palenik & Palenik, 1988), include a novel intramolecular S···N attraction. 4-Formylpyridine thiosemicarbazone (4FPYTSC) possesses both antitumour (Hagenbach & Gysin, 1952) and antiviral activity (Jones, Slack, Squires & Woolridge, 1965), 2-formylpyridine thiosemicarbazone (French & Blanz, 1966) is a tumor inhibitor and *P. Colinalde* thiosemicarbazone (Brockman & Thomson, 1956) possesses anti-leukaemic activity. Extensive delocalization involving the heteroaromatic ring system and the thiosemicarbazide side chain (Palenik, Rendle & Carter, 1974) takes place and this is responsible for various

intra- and intermolecular interactions. Recently, a nickel complex of salicylaldehyde thiosemicarbazone has been reported as a functional model for hydrogenases (Zimmer, Schulte, Luo & Crabtree, 1991). Furthermore, the 3,4,5-trimethoxyphenyl group is present in the clinically useful drug trimethoprim (Pinder, 1970). In the light of these observations, a three-dimensional structure analysis of the title compound, (III), was undertaken.



The C(7)—N(1) [1.277 (3) Å], C(8)—N(2) [1.343 (3) Å] and C(8)—N(3) [1.325 (3) Å] bond distances of the title compound are comparable with the C(6)—N(2) [1.275 (3) Å], C(7)—N(3) [1.354 (3) Å] and C(7)—N(4) [1.329 (3) Å] bond distances of 4-formylpyridine thiosemicarbazone (4FPYTSC) (Restivo & Palenik, 1970) and indicate that C(7)—N(1) [1.277 (3) Å] is a double bond and the distances C(8)—N(2) and C(8)—N(3) possess partial double-bond character due to resonance, as shown in forms (I) and (II) above. This appears to be a common feature in all TSCs. The contribution due to resonance calls for a change in the location of the water molecule [see (III) above]. Hence the bond C(8)—N(2) [1.343 (3) Å] is longer than C(8)—N(3) [1.325 (3) Å] indicating that the contribution from resonance form (II) is more significant in the title compound than in other TSCs. Also, this difference is reasonable (Palenik, Rendle & Carter, 1974) since in the case of N(2), the NH group is attached to the O atom of the water molecule, and for N(3), the NH<sub>2</sub> group is attached to the S atom of the other molecule.

The N(1)—N(2) [1.374 (2) Å] distance is close to the N—N distance of 1.376 (6) Å in 2-keto-3-ethoxybutyraldehyde thiosemicarbazone (KTS)

(Gabe, Taylor, Glusker, Minkin & Patterson, 1969) and may be due to an extensively delocalized group attached to the N atom. This resonance seems to have no effect on the bond lengths of the benzene ring but accounts for the shortening of the N—N distance in contrast to that of 1.399 (6) Å in thiosemicarbazide (Domanio, Gasparri, Nardelli & Sgarabotto, 1969), but C(1)—C(7) [1.454 (3) Å] is short compared to C(5)—C(6) [1.467 (3) Å] (Restivo & Palenik, 1970) which supports the above resonance.

The C(8)—S [1.688 (2) Å] bond is longer than the C—S distance of 1.678 (3) Å given by Restivo & Palenik (1970) and is intermediate between the C—S single-bond distance (1.82 Å) and the C—S double-bond distance (1.56 Å) (Sutton, 1965), indicating that it possesses only partial double-bond character.

The molecule, as a whole, is not planar and consists of a planar benzene ring with an extended zigzag side chain of non-planar thiosemicarbazone. The O and C atoms of the methoxy groups attached to the benzene ring show no deviation from the mean plane. The bond lengths and bond angles within the benzene ring are normal and those of the methoxy groups agree with corresponding values observed in related structures. The bond angles of thiosemicarbazone are close to the bond angles of 4FPYTSC (Restivo & Palenik, 1970).

The average value of the O(2)—C(3)—C(4) and C(4)—C(5)—O(1) angles is 115.2 (2)° and the average value of O(2)—C(3)—C(2) and O(1)—C(5)—C(6) is 124.6 (2)°. This difference might be due to the *cis* orientation of the O(2)—C(9) and C(2)—C(3) bonds about the O(2)—C(3) bond, and the O(1)—C(11) and C(5)—C(6) bonds about the O(1)—C(5) bond which causes repulsion between C(9) and C(2), and C(11) and C(6) (Sakaki, Sogo, Wakahara, Kanai, Fujiwara & Tomito, 1976).

The methoxy groups attached to C(3) and C(5) of the six-membered ring are nearly coplanar with the plane of the ring (Karthan, Ahmed & Barner, 1962);

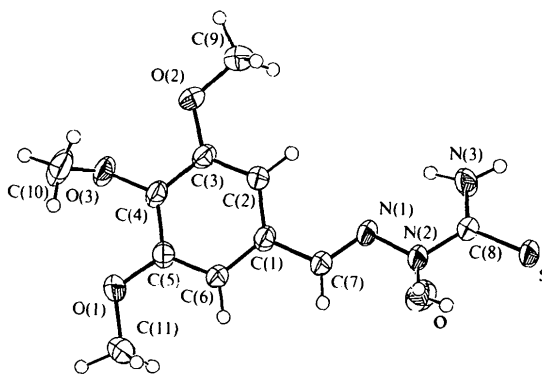


Fig. 1. PLATON (Spek, 1990) plot of the title compound. Displacement ellipsoids are shown at the 50% probability level.

torsion angles as defined by Klyne & Prelog (1960) are 3.8 (2) and 1.3 (2)° for C(11)—O(1)—C(5)—C(6) and C(9)—O(2)—C(3)—C(2), respectively. The torsion angle C(10)—O(3)—C(4)—C(5) of -74.5 (2)° shows that C(10) is almost normal to the plane of the six-membered ring. The bond angles at C(4) have an average value of 120.0 (2)°, indicating no steric hindrance on C(10). The torsion angle H(N2)—N(2)—C(8)—N(3) of -180.0 (2)° indicates that N—H is *trans* to C—N about the N(2)—C(8) bond. The torsion angle C(1)—C(7)—N(1)—N(2) of -174.8 (2)° indicates that the 3,4,5-trimethoxyphenyl group is *anti* to the thiocarbamide group and corresponds to an *E* configuration.

The molecular packing viewed down the *a* axis is shown in Fig. 2. The molecules are linked by N—H...S bonds across the centre of symmetry. The water molecule takes part in bonding through N—H...O bonds. The details of the hydrogen bonding are given in Table 3.

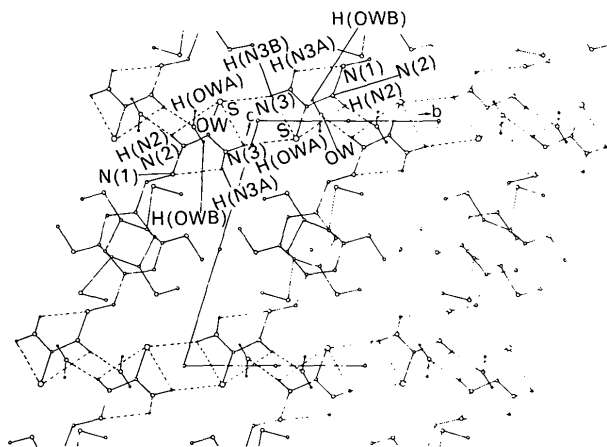


Fig. 2. The molecular packing of the title compound viewed down the *a* axis.

## Experimental

### Crystal data

C<sub>11</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub>S.H<sub>2</sub>O

*M<sub>r</sub>* = 287.33

Triclinic

*P*1̄

*a* = 7.428 (1) Å

*b* = 9.652 (1) Å

*c* = 11.102 (2) Å

α = 73.29 (2)°

β = 70.89 (2)°

γ = 70.49 (2)°

*V* = 694.6 (2) Å<sup>3</sup>

*Z* = 2

*D<sub>x</sub>* = 1.374 Mg m<sup>-3</sup>

*D<sub>m</sub>* = 1.359 Mg m<sup>-3</sup>

*D<sub>m</sub>* measured by flotation in KI solution

Cu Kα radiation

λ = 1.5418 Å

Cell parameters from 25

reflections

θ = 0–25°

μ = 2.17 mm<sup>-1</sup>

*T* = 300 K

Needle

0.75 × 0.38 × 0.25 mm

Colourless

### Data collection

Enraf–Nonius CAD-4

diffractometer

ω/2θ scans

Absorption correction:

none

2767 measured reflections

2528 independent reflections

2398 observed reflections

[*I* ≥ 2.5σ(*I*)]

### Refinement

Refinement on *F*

*R* = 0.036

*wR* = 0.039

*S* = 1.92

240 parameters

Only H-atom *U*'s refined

*w* = 1/σ<sup>2</sup>(*F*)

(Δ/σ)<sub>max</sub> = 0.159

Δρ<sub>max</sub> = 0.28 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.20 e Å<sup>-3</sup>

*R*<sub>int</sub> = 0.000 (11)

θ<sub>max</sub> = 65°

*h* = -8 → 8

*k* = 0 → 11

*l* = -12 → 13

3 standard reflections

monitored every 50

reflections

intensity decay: none

Extinction correction:

secondary

Extinction coefficient:

0.85 (2)

Atomic scattering factors

from *International Tables*

for X-ray Crystallography

(1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å<sup>2</sup>)

$$B_{\text{eq}} = (4/3) \sum_i \sum_j \beta_{ij} \mathbf{a}_i \cdot \mathbf{a}_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> <sub>eq</sub>
S	0.2861 (1)	0.2032 (1)	0.0725 (1)	3.00 (3)
O(W)	0.1342 (3)	0.6514 (1)	0.0194	4.40 (9)
O(1)	0.7992 (2)	1.0191 (2)	-0.5415 (2)	3.20 (7)
O(2)	0.9153 (2)	0.5923 (2)	-0.7017 (1)	3.44 (8)
O(3)	0.9685 (2)	0.8582 (2)	-0.7312 (3)	3.37 (7)
N(1)	0.5518 (3)	0.4656 (2)	-0.2180 (2)	2.73 (8)
N(2)	0.4337 (3)	0.4147 (2)	-0.1003 (2)	2.86 (8)
N(3)	0.6005 (3)	0.1768 (2)	-0.1294 (2)	3.97 (10)
C(1)	0.6442 (3)	0.6724 (2)	-0.3755 (2)	2.48 (9)
C(2)	0.7278 (3)	0.5934 (2)	-0.4767 (2)	2.66 (9)
C(3)	0.8300 (3)	0.6583 (2)	-0.5956 (2)	2.65 (9)
C(4)	0.8541 (3)	0.8014 (2)	-0.6149 (2)	2.63 (9)
C(5)	0.7683 (3)	0.8808 (2)	-0.5141 (2)	2.53 (8)
C(6)	0.6630 (3)	0.8167 (2)	-0.3956 (2)	2.55 (9)
C(7)	0.5376 (3)	0.6062 (2)	-0.2484 (2)	2.64 (9)
C(8)	0.4505 (3)	0.2667 (2)	-0.0607 (2)	2.67 (9)
C(9)	0.8925 (4)	0.4471 (3)	-0.6876 (3)	3.76 (12)
C(10)	0.8611 (5)	0.9752 (4)	-0.8148 (3)	5.08 (15)
C(11)	0.7267 (4)	1.0985 (3)	-0.4373 (3)	3.66 (12)

Table 2. Selected geometric parameters (Å, °)

S—C(8)	1.688 (2)	C(1)—C(2)	1.396 (3)
C(2)—C(3)	1.378 (3)	C(1)—C(6)	1.392 (3)
O(1)—C(5)	1.361 (2)	C(3)—C(4)	1.398 (3)
O(1)—C(11)	1.429 (3)	C(4)—C(5)	1.396 (3)
O(2)—C(3)	1.367 (2)	C(5)—C(6)	1.380 (3)
O(2)—C(9)	1.426 (3)	O(3)—C(4)	1.370 (2)
O(3)—C(10)	1.434 (3)	N(1)—N(2)	1.374 (2)
N(1)—C(7)	1.277 (3)	N(2)—C(8)	1.343 (3)
N(3)—C(8)	1.325 (3)	C(1)—C(7)	1.454 (3)
C(5)—O(1)—C(11)	117.0 (2)	C(3)—O(2)—C(9)	117.0 (2)
C(4)—O(3)—C(10)	115.0 (2)	N(2)—N(1)—C(7)	116.6 (2)
N(1)—N(2)—C(8)	119.0 (2)	C(2)—C(1)—C(6)	119.9 (2)
C(2)—C(1)—C(7)	121.0 (2)	C(6)—C(1)—C(7)	119.1 (2)
C(1)—C(2)—C(3)	119.7 (2)	O(2)—C(3)—C(2)	124.7 (2)
O(2)—C(3)—C(4)	114.8 (2)	C(2)—C(3)—C(4)	120.5 (2)
O(3)—C(4)—C(3)	119.0 (2)	O(3)—C(4)—C(5)	121.3 (2)
C(3)—C(4)—C(5)	119.6 (2)	O(1)—C(5)—C(4)	115.6 (2)
O(1)—C(5)—C(6)	124.6 (2)	C(4)—C(5)—C(6)	120.0 (2)
C(1)—C(6)—C(5)	120.5 (2)	N(1)—C(7)—C(1)	120.6 (2)
S—C(8)—N(2)	120.0 (2)	S—C(8)—N(3)	123.1 (2)
N(2)—C(8)—N(3)	117.0 (2)		

Table 3. *Inter- and intramolecular hydrogen-bonding geometry* ( $\text{\AA}$ ,  $^\circ$ )

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N(2)-H(N2) \cdots S$	0.88 (3)	2.68 (3)	2.630 (2)	77 (2)
$N(3)-H(N3B) \cdots S$	0.87 (4)	2.68 (3)	2.654 (2)	79 (2)
$N(3)-H(N3B) \cdots N$	0.97 (3)	2.25 (3)	2.618 (3)	101 (2)
$N(2)-H(N2) \cdots O(W)$	0.88 (3)	2.03 (3)	2.890 (3)	167 (2)
$N(3)-H(N3B) \cdots S^1$	0.87 (4)	2.55 (4)	3.393 (22)	163 (2)

Symmetry code: (i)  $1 - x, -y, -z$ .

Data were corrected for Lorentz-polarization effects. The structure was solved using *SHELXS86* (Sheldrick, 1985). All the H atoms were located from difference Fourier maps. Full-matrix least-squares refinement with anisotropic displacement parameters for non-H and isotropic for H atoms was performed using the *NRCVAX* crystal structure system (Larson, Lee, Le Page, Webster, Charland, Gabe & White, 1990).

The authors wish to thank Dr N. C. Shivaprakash, ISU, X-RD laboratory, IISc, Bangalore, India, for the data. One of the authors, MKK, thanks Professor J. Shashidharaprasad, Department of Postgraduate Studies in Physics, Manasagangothri, Mysore, India, for providing the computational facilities.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CR1072). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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*Acta Cryst.* (1995). **C51**, 333–336

## 4-Amino-N-(2-pyrimidinyl)-benzenesulfonamide

M. K. KOKILA AND PUTTARAJA

*Department of Physics, Bangalore University, Bangalore 560 056, India*

M. V. KULKARNI

*Department of Chemistry, Karnatak University, Dharwad 580 003, India*

SARALA THAMPI

*Department of Organic Chemistry, Government College of Pharmacy, Bangalore 560 027, India*

(Received 9 March 1993; accepted 17 December 1993)

## Abstract

The structure of the title compound,  $C_{10}H_{10}N_4O_2S$ , has been determined. The two six-membered rings are planar and folded towards each other making an acute angle of  $74.9(2)^\circ$ . The molecules are linked by intermolecular  $N-H \cdots O$  and  $N-H \cdots N$  bonds.

## Comment

4-Amino-N-(2-pyrimidinyl)benzenesulfonamide, (I), ( $R = H$ ) is one of the most important 'sulpha' drugs and is useful in the treatment of bacterial infections and extraluminal urinary-tract infections (Aurthur Osol, 1990); its higher homologue ( $R = CH_3$ ), known as sulphamerazine, has been used in combination with other antibiotics (Aurthur Osol, 1990). Crystal structure studies of sulfonamides have revealed the nature of their intermolecular hydrogen bonding (O'Connell & Maslen, 1967), their interaction with protic solvents (Rambaud, Maury, Pauvert, Audran, Lasserre, Berge & Declercq, 1985) and their binding with specific proteins (Acharya, Kuchela & Kartha, 1982). The crystal structure of sulphadiazine (I) ( $R = H$ ) has been reported (Ihn, Kim & Koo, 1975) and interesting variations of its solid-state conformation have been found in its silver and zinc complexes (Cook & Turner, 1975; Brown, Cook &