

Çiğdem Yüksektepe,<sup>a</sup>  
Mustafa Serkan Soylu,<sup>a\*</sup>  
Hanife Saraçoğlu,<sup>a</sup> Ibrahim  
Yılmaz,<sup>b</sup> Alaaddin Çukurovalı<sup>b</sup>  
and Nezihe Çalışkan<sup>a</sup>

<sup>a</sup>Department of Physics, Arts and Sciences Faculty, Ondokuz Mayıs University, 55139 Samsun, Turkey, and <sup>b</sup>Department of Chemistry, Arts and Sciences Faculty, Firat University, 23119 Elazığ, Turkey

Correspondence e-mail: mssoylu@omu.edu.tr

#### Key indicators

Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$   
R factor = 0.035  
wR factor = 0.075  
Data-to-parameter ratio = 14.4

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

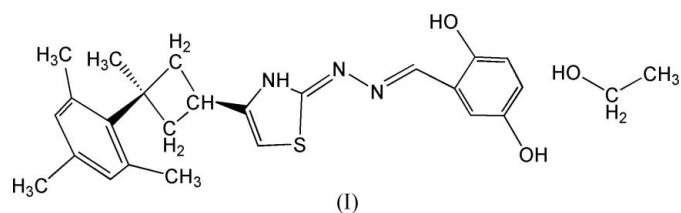
## 2-({4-[3-Methyl-3-(2,4,6-trimethylphenyl)cyclobutyl]-3H-thiazol-2-ylidene}hydrazonomethyl)benzene-1,4-diol ethanol solvate

In the title compound,  $\text{C}_{24}\text{H}_{27}\text{N}_3\text{O}_2\text{S}\cdot\text{C}_2\text{H}_6\text{O}$ , the dihedral angle between the least-squares planes of the 2,5-dihydroxybenzene ring and the mesityl group is  $78.59(6)^\circ$ . An intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond is observed in the molecular structure. Centrosymmetrically related molecules are linked by  $\text{N}-\text{H}\cdots\text{O}$  intermolecular hydrogen bonds to form a dimer. The dimers are interlinked by  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{N}$  intermolecular hydrogen bonds involving the ethanol molecule of crystallization to form chains along the *a* axis.

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#### Comment

Various hydrazone compounds possess strong bactericidal, herbicidal, insecticidal and fungicidal properties (Sahni *et al.*, 1977). In addition, hydrazones have analytical applications (Jensen & Pflaum, 1967). Most Schiff bases have antibacterial, anticancer, anti-inflammatory and antitoxic activities (Williams, 1972), and the sulfur-containing Schiff bases are particularly effective. Schiff bases have been used extensively as ligands in the field of coordination chemistry (Calligaris *et al.*, 1972). The intramolecular hydrogen bond between the O and N atoms plays an important role in the formation of metal complexes and Schiff base compounds in the solid state *via* proton transfer from the hydroxy O atom to the imine N atom (Hadjoudis *et al.*, 1987; Xu *et al.*, 1994). Benzothiazolium groups have been used in organic dyes as either electron-withdrawing or electron-donating substituents, depending on whether the N atom is cationic or not (Zollinger, 1991).



A view of the asymmetric unit with the atom-labelling scheme is shown in Fig. 1. The thiazole ring and mesityl group are each planar. In the mesityl group, atom C5 deviates by  $0.034(1) \text{ \AA}$  from the mean plane through the C5–C10 ring. In the thiazole ring, the S1–C16 and S1–C17 bond lengths (Table 1) are shorter than the accepted value for an  $\text{S}-\text{Csp}^2$  single bond ( $1.762 \text{ \AA}$  for C–S; Allen, 1984). Variations in C16=C15, C15–N1, N1–C17, C17=N2, N2–N3 and N3=C18 bond lengths (Table 1) confirm electron delocalization along the  $-\text{C16}=\text{C15}-\text{N1}-\text{C17}=\text{N2}-\text{N3}=\text{C18}-$ segment. The dihedral angles between 2,5-dihydroxybenzene

plane *A* (C19–C24), thiazole plane *B* (N1/S1/C15–C17) and mesityl plane *C* (C5–C10) are  $A/B = 12.64 (12)^\circ$ ,  $A/C = 78.59 (6)^\circ$  and  $C/D = 76.70 (6)^\circ$ . In the cyclobutane ring, the C4/C1/C2 plane forms a dihedral angle of  $26.8 (2)^\circ$  with the C2/C3/C4 plane. Literature values for the puckering of the cyclobutane ring are  $23.5^\circ$  (Swenson *et al.*, 1997) and  $29.03 (13)^\circ$  (Yüksektepe *et al.*, 2004).

An intramolecular O–H···N hydrogen bond is observed in the molecular structure. Atom N1 of the thiazole ring behaves as a donor in N–H···O intermolecular hydrogen bonds around inversion centres, forming dimers (Table 2). The dimers are interlinked *via* an ethanol molecule of crystallization by O–H···O and O–H···N intermolecular hydrogen bonds into chains along the *a* axis (Fig. 2).

## Experimental

To a suspension of 1-(2,5-dihydroxybenzylidene)thiosemicarbazide (1.056 g, 5 mmol) in DMSO (30 ml), a solution of 1-methyl-1-mesityl-3-(2-chloro-1-oxoethyl)cyclobutane (1.3225 g, 5 mmol) in absolute ethanol (20 ml) was added dropwise at *ca* 303–313 K with continuous stirring. After the addition of the  $\alpha$ -haloketone, the temperature was raised to 323–328 K. The solution was then made alkaline with an aqueous solution of  $\text{NH}_3$  (5%), and an orange precipitate separated. The precipitate was filtered off, washed with aqueous  $\text{NH}_3$  solution several times and dried in air. Suitable single crystals for crystal structure determination were obtained by slow evaporation of an ethanol solution.

### Crystal data

$\text{C}_{24}\text{H}_{27}\text{N}_3\text{O}_2\text{S}\cdot\text{C}_2\text{H}_6\text{O}$   
 $M_r = 467.61$   
 Triclinic,  $P\bar{1}$   
 $a = 7.5304 (9) \text{ \AA}$   
 $b = 12.5739 (16) \text{ \AA}$   
 $c = 14.5935 (18) \text{ \AA}$   
 $\alpha = 65.678 (9)^\circ$   
 $\beta = 84.257 (10)^\circ$   
 $\gamma = 89.335 (10)^\circ$   
 $V = 1252.2 (3) \text{ \AA}^3$

$Z = 2$   
 $D_x = 1.240 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 8264 reflections  
 $\theta = 1.5\text{--}26.6^\circ$   
 $\mu = 0.16 \text{ mm}^{-1}$   
 $T = 293 (2) \text{ K}$   
 Prism, yellow  
 $0.30 \times 0.28 \times 0.27 \text{ mm}$

### Data collection

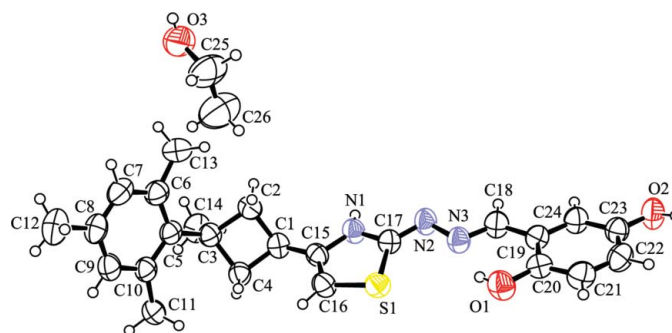
Stoe IPDS-II diffractometer  
 $\varphi$  scans  
 Absorption correction: integration  
 (*X-RED32*; Stoe & Cie, 2002)  
 $T_{\min} = 0.953$ ,  $T_{\max} = 0.958$   
 16 210 measured reflections  
 4402 independent reflections

2329 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.050$   
 $\theta_{\text{max}} = 25.0^\circ$   
 $h = -8 \rightarrow 8$   
 $k = -14 \rightarrow 14$   
 $l = -17 \rightarrow 17$

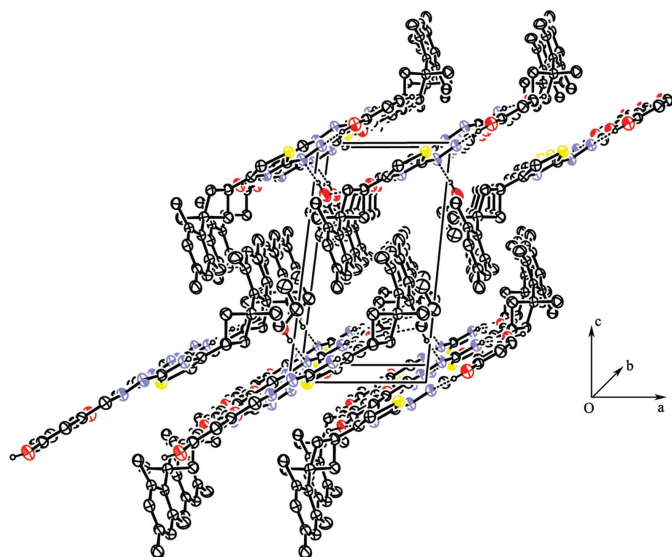
### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.075$   
 $S = 0.80$   
 4402 reflections  
 306 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.034P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$



**Figure 1**  
 An ORTEP-3 (Farrugia, 1997) drawing of the asymmetric unit, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



**Figure 2**  
 Packing of the title compound, viewed down the *b* axis, showing hydrogen-bonded chains. Hydrogen bonds are indicated by dashed lines. H atoms have been omitted.

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

S1–C17	1.734 (2)	C1–C15	1.477 (3)
S1–C16	1.738 (2)	C1–C4	1.526 (3)
N1–C17	1.359 (2)	C1–C2	1.543 (3)
N1–C15	1.388 (2)	C2–C3	1.558 (3)
N2–C17	1.299 (2)	C3–C4	1.561 (2)
N2–N3	1.399 (2)	C15–C16	1.333 (2)
N3–C18	1.286 (2)		
C17–S1–C16	90.50 (10)	C1–C2–C3	89.74 (15)
C17–N1–C15	115.95 (17)	C2–C3–C4	85.89 (14)
C17–N2–N3	111.07 (16)	C1–C4–C3	90.24 (14)
C4–C1–C2	87.61 (14)		
C17–N2–N3–C18	171.75 (17)	N2–N3–C18–C19	178.66 (18)
N3–N2–C17–S1	2.8 (3)	N3–C18–C19–C20	−6.3 (3)

**Table 2**  
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1N\cdots O2^i$	0.83 (2)	2.30 (2)	3.099 (2)	164 (2)
$O2-H2O\cdots O3^{ii}$	0.82	1.87	2.678 (2)	167
$O3-H3\cdots N2^{iii}$	0.82	2.26	2.844 (2)	128
$O1-H1O\cdots N3$	0.82	1.98	2.700 (2)	147

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

Atom H1N was located in a difference Fourier map and refined isotropically. All other H atoms were placed in calculated positions ( $O-H = 0.82$  Å and  $C-H = 0.93-0.98$  Å) and refined using a riding model. Their  $U_{iso}(H)$  values were constrained to be 1.2 (1.5 for hydroxy and methyl groups) times  $U_{eq}$  of the parent atom.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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