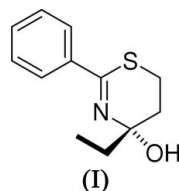
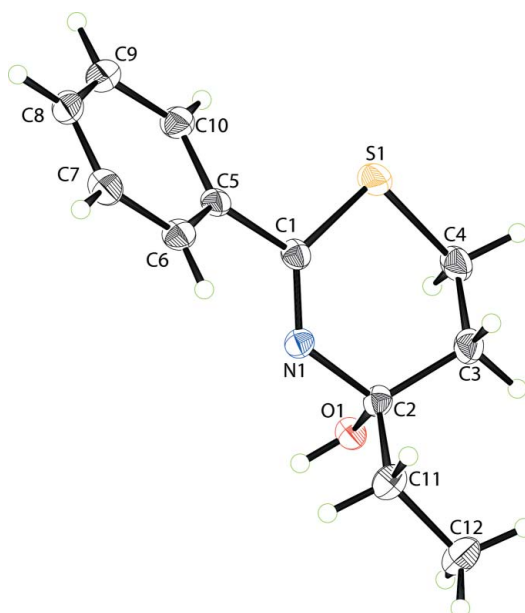


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koketsu@cc.gifu-u.ac.jp**Key indicators**Single-crystal X-ray study
 $T = 190$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.037
 wR factor = 0.093
Data-to-parameter ratio = 14.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**4-Ethyl-4-hydroxy-2-phenyl-5,6-dihydro-
4H-1,3-thiazine**In the title compound, $\text{C}_{12}\text{H}_{15}\text{NOS}$, the thiazine ring adopts a sofa conformation. Intermolecular $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds link centrosymmetrically related molecules into discrete pairs.Received 3 March 2006
Accepted 28 March 2006**Comment**The antimycobacterial properties of 5,6-dihydro-4H-1,3-thiazine derivatives have been investigated recently, showing that these compounds are active against *Mycobacterium tuberculosis* H37Rv (ATCC 27294) (Koketsu *et al.*, 2002). 4-Hydroxy-5,6-dihydro-4H-1,3-thiazines are synthesized by the $\text{BF}_3 \cdot \text{Et}_2\text{O}$ -catalysed reaction of primary thioamides with α,β -unsaturated ketones (Koketsu *et al.*, 1999, 2002).

The molecular structure of the title compound, (I), is shown in Fig. 1. The thiazine ring exhibits a sofa conformation with atom C3 deviating by 0.681 (3) Å from the least-squares mean plane of the remaining five atoms (r.m.s. deviation = 0.036 Å).

**Figure 1**

The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii.

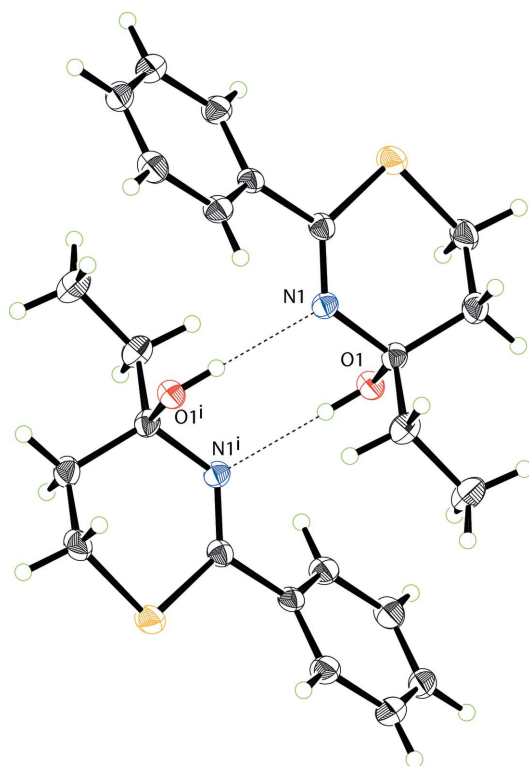


Figure 2
The hydrogen-bonded (dashed lines) dimeric structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

Intermolecular hydrogen bonds (Table 2) link centrosymmetrically related molecules into discrete pairs (Fig. 2).

Experimental

Ethyl vinyl ketone (0.42 g, 5.0 mmol) was added to a solution of thiobenzamide (0.69 g, 5.0 mmol) in dry dichloromethane (50 ml) at room temperature under an argon atmosphere. To this solution was added $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (1.2 mmol). The reaction mixture was stirred for 2 h, quenched with saturated sodium carbonate solution, and extracted with dichloromethane. The extracts were dried (Na_2SO_4) and evaporated to dryness. Recrystallization from diethyl ether/hexane (3:5) gave (I) as crystals (yield 0.95 g, 86%; m.p.: 370.3–371.2 K).

Crystal data

$\text{C}_{12}\text{H}_{15}\text{NOS}$	$D_x = 1.259 \text{ Mg m}^{-3}$
$M_r = 221.31$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3894 reflections
$a = 9.4353 (2) \text{ \AA}$	$\theta = 1.0\text{--}25.0^\circ$
$b = 6.7725 (2) \text{ \AA}$	$\mu = 0.25 \text{ mm}^{-1}$
$c = 18.3013 (6) \text{ \AA}$	$T = 190 (2) \text{ K}$
$\beta = 93.6060 (13)^\circ$	Prism, colorless
$V = 1167.15 (6) \text{ \AA}^3$	$0.34 \times 0.12 \times 0.06 \text{ mm}$
$Z = 4$	

Data collection

Nonius KappaCCD diffractometer	2055 independent reflections
φ and ω scans	1563 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SCALEPACK; Otwinowski & Minor, 1997)	$R_{\text{int}} = 0.040$
$T_{\text{min}} = 0.920$, $T_{\text{max}} = 0.985$	$\theta_{\text{max}} = 25.0^\circ$
7372 measured reflections	$h = -11 \rightarrow 11$
	$k = -8 \rightarrow 8$
	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0406P)^2 + 0.3082P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.093$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
2055 reflections	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$
142 parameters	Extinction correction: SHELXL97
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.010 (2)

Table 1

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

S1—C1	1.7561 (18)	C2—O1	1.418 (2)
S1—C4	1.8043 (19)	C2—C11	1.518 (3)
C1—N1	1.272 (2)	C2—C3	1.522 (3)
C1—C5	1.492 (2)	C3—C4	1.507 (3)
N1—C2	1.484 (2)		
C1—S1—C4	100.93 (9)	N1—C2—C11	105.64 (14)
N1—C1—C5	118.65 (16)	O1—C2—C3	106.06 (14)
N1—C1—S1	128.80 (14)	N1—C2—C3	113.53 (14)
C5—C1—S1	112.55 (13)	C11—C2—C3	112.51 (16)
C1—N1—C2	122.92 (15)	C4—C3—C2	112.36 (16)
O1—C2—N1	107.63 (14)	C3—C4—S1	110.80 (13)
O1—C2—C11	111.46 (14)		

Table 2

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

$D\text{—}H \cdots A$	$D\text{—}H$	$H \cdots A$	$D \cdots A$	$D\text{—}H \cdots A$
$\text{O1—H1A} \cdots \text{N1}^i$	0.84 (2)	2.03 (2)	2.866 (2)	176 (2)

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

The H atom of the hydroxyl group was located in an electron-density difference map and refined isotropically with an O—H distance restraint of 0.84 (1) \AA . C-bound H atoms were placed in idealized positions and treated as riding atoms, with C—H distances in the range 0.95–0.99 \AA and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms or $1.2U_{\text{eq}}(\text{C})$ for the remaining H atoms.

Data collection: COLLECT (Nonius, 2000); cell refinement: SCALEPACK (Otwinowski & Minor, 1997); data reduction: SCALEPACK and DENZO (Otwinowski & Minor, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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