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3-Phenyl-2-thioxo-1,3-thiazolidin-4-one

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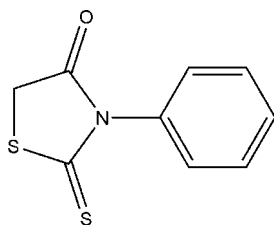
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.040; wR factor = 0.080; data-to-parameter ratio = 15.3.

In the molecule of the title compound, $\text{C}_9\text{H}_7\text{NOS}_2$, the heterocycle and the phenyl ring are oriented at a dihedral angle of 72.3 (1)°. Adjacent molecules are connected through $\text{C}-\text{H}\cdots\text{O}$ interactions.

Related literature

For the synthesis of 3-phenylrhodanine, see: Brown *et al.* (1956). For the therapeutic properties of rhodanine-based molecules, including anticonvulsant, antibacterial, antiviral and antidiabetic properties, see: Momose *et al.* (1991); HCV protease, Sudo *et al.* (1997); HCV NS3 protease, Sing *et al.* (2001); aldols reductase, Bruno *et al.* (2002); factor protease, Sherida *et al.* (2006).



Experimental

Crystal data

$\text{C}_9\text{H}_7\text{NOS}_2$
 $M_r = 209.28$
 Monoclinic, $P2_1/c$

$a = 12.9941$ (13) Å
 $b = 5.6111$ (6) Å
 $c = 12.7271$ (13) Å

$\beta = 93.847$ (3)°
 $V = 925.86$ (17) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.53$ mm⁻¹
 $T = 296$ (2) K
 $0.20 \times 0.15 \times 0.05$ mm

Data collection

Bruker APEXII diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2000)
 $T_{\min} = 0.91$, $T_{\max} = 0.97$

10918 measured reflections
 1800 independent reflections
 1146 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.066$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.080$
 $S = 1.00$
 1800 reflections

118 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.25$ e Å⁻³
 $\Delta\rho_{\min} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C5}-\text{H5}\cdots\text{O1}^i$	0.93	2.51	3.410 (3)	163
$\text{C8}-\text{H8}\cdots\text{O1}^{ii}$	0.93	2.46	3.386 (3)	171

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2120).

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3-Phenyl-2-thioxo-1,3-thiazolidin-4-one

Feng-Xia Zhu, Jian-Feng Zhou and Gui-Xia Gong

S1. Comment

Rhodanine derivatives are attractive compounds owing to their outstanding biological activities. They have undergone rapid development as a result of their use in anticonvulsant, antibacterial, antiviral and antidiabetic treatments (Momose *et al.*, 1991). As an extension of these studies, we report herein on the structure of 3-phenylrhodanine (3-phenyl-2-thioxo-thiazolidin-4-one).

A 3-phenylrhodanine molecule, which is the asymmetric unit of the structure, is shown in Fig. 1. All the bond distances and bond angles are within the normal ranges. The two parts of the molecule, the five-member heterocycle and the phenyl ring, are oriented at a dihedral angle of 72.3 (1)°. Adjacent molecules are connected through C—H—O hydrogen bonds (Table 1).

S2. Experimental

3-phenylrhodanine was synthesized according to the literature (Brown *et al.*, 1956), and was recrystallized using a mixed solvent of ether and 95% ethanol (1:1 by volume). Yellow sheet crystals are obtained.

S3. Refinement

All non-hydrogen atoms were found in Fourier maps, and were refined anisotropically. Hydrogen atoms were positioned geometrically, and the isotropic vibration parameters related to the atoms which they are bonded to with $U_{\text{iso}} = 1.2 U_{\text{eq}}$.

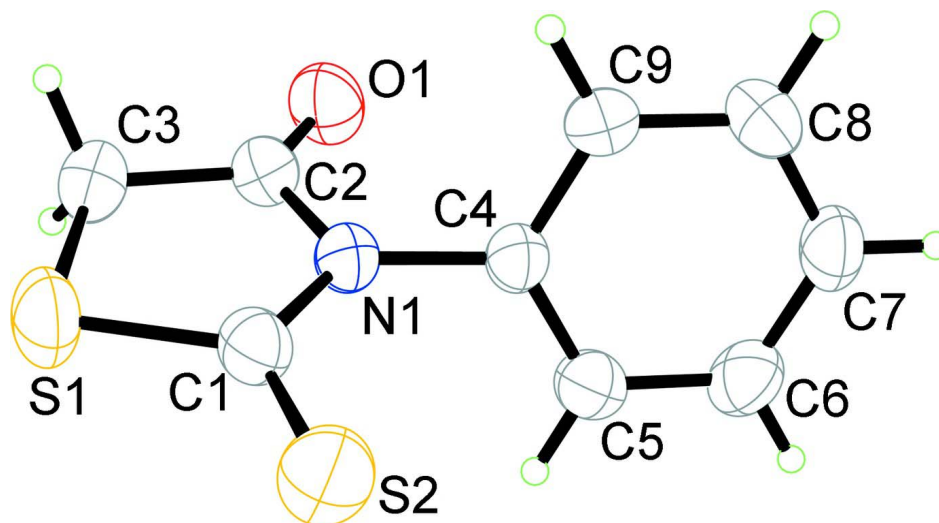


Figure 1

The asymmetric unit of 3-benzylrhodanine with atom labels and 50% probability displacement ellipsoids for non-H atoms.

3-Phenyl-2-thioxo-1,3-thiazolidin-4-one

Crystal data

C₉H₇NOS₂ $M_r = 209.28$ Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

 $a = 12.9941 (13) \text{ \AA}$ $b = 5.6111 (6) \text{ \AA}$ $c = 12.7271 (13) \text{ \AA}$ $\beta = 93.847 (3)^\circ$ $V = 925.86 (17) \text{ \AA}^3$ $Z = 4$ $F(000) = 432$ $D_x = 1.501 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1321 reflections

 $\theta = 3.1\text{--}21.1^\circ$ $\mu = 0.53 \text{ mm}^{-1}$ $T = 296 \text{ K}$

Plate, yellow

 $0.20 \times 0.15 \times 0.05 \text{ mm}$

Data collection

Bruker APEXII

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8 pixels mm^{-1} ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2000)

 $T_{\min} = 0.91, T_{\max} = 0.97$

10918 measured reflections

1800 independent reflections

1146 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.066$ $\theta_{\max} = 26.0^\circ, \theta_{\min} = 1.6^\circ$ $h = -14 \rightarrow 15$ $k = -6 \rightarrow 6$ $l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.040$ $wR(F^2) = 0.080$ $S = 1.00$

1800 reflections

118 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 0.2182P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.25 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.23 \text{ e \AA}^{-3}$

Special details

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.35704 (19)	0.8242 (4)	0.64373 (18)	0.0412 (6)
C2	0.2485 (2)	0.5060 (4)	0.58348 (17)	0.0413 (6)
C3	0.32529 (19)	0.5020 (4)	0.50099 (19)	0.0495 (7)
H3A	0.2908	0.5231	0.4317	0.059*

H3B	0.3616	0.3508	0.5024	0.059*
C4	0.20680 (17)	0.7118 (4)	0.74476 (17)	0.0351 (6)
C5	0.13898 (18)	0.8984 (4)	0.74630 (18)	0.0433 (6)
H5	0.1376	1.0140	0.6938	0.052*
C6	0.07285 (19)	0.9134 (5)	0.8263 (2)	0.0478 (7)
H6	0.0262	1.0389	0.8275	0.057*
C7	0.0756 (2)	0.7437 (5)	0.90434 (19)	0.0484 (7)
H7	0.0309	0.7549	0.9582	0.058*
C8	0.1438 (2)	0.5586 (5)	0.90295 (19)	0.0512 (7)
H8	0.1455	0.4441	0.9559	0.061*
C9	0.21025 (19)	0.5414 (4)	0.82277 (18)	0.0444 (6)
H9	0.2569	0.4158	0.8216	0.053*
N1	0.27190 (14)	0.6844 (3)	0.65849 (14)	0.0364 (5)
O1	0.17588 (14)	0.3754 (3)	0.58706 (13)	0.0541 (5)
S1	0.41400 (5)	0.74161 (13)	0.52991 (6)	0.0566 (2)
S2	0.40143 (5)	1.03944 (13)	0.71931 (6)	0.0583 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0359 (15)	0.0436 (15)	0.0446 (14)	0.0026 (12)	0.0059 (11)	0.0053 (12)
C2	0.0456 (16)	0.0411 (15)	0.0378 (13)	0.0024 (13)	0.0066 (12)	0.0023 (12)
C3	0.0501 (16)	0.0522 (17)	0.0475 (14)	0.0041 (14)	0.0124 (12)	-0.0048 (13)
C4	0.0342 (14)	0.0356 (14)	0.0362 (12)	-0.0006 (11)	0.0077 (11)	-0.0010 (11)
C5	0.0440 (16)	0.0407 (15)	0.0458 (15)	0.0024 (13)	0.0069 (13)	0.0055 (11)
C6	0.0403 (16)	0.0461 (16)	0.0577 (16)	0.0089 (13)	0.0089 (13)	-0.0033 (13)
C7	0.0474 (16)	0.0539 (17)	0.0458 (14)	-0.0049 (15)	0.0182 (12)	-0.0063 (14)
C8	0.0614 (18)	0.0489 (16)	0.0445 (15)	-0.0046 (15)	0.0125 (14)	0.0097 (13)
C9	0.0497 (16)	0.0370 (14)	0.0472 (14)	0.0093 (12)	0.0090 (12)	0.0044 (12)
N1	0.0359 (12)	0.0356 (11)	0.0386 (11)	-0.0007 (9)	0.0088 (9)	-0.0003 (9)
O1	0.0594 (13)	0.0506 (11)	0.0532 (11)	-0.0147 (10)	0.0107 (9)	-0.0059 (9)
S1	0.0465 (4)	0.0673 (5)	0.0588 (4)	-0.0072 (4)	0.0228 (3)	-0.0061 (4)
S2	0.0511 (5)	0.0561 (5)	0.0682 (5)	-0.0128 (4)	0.0081 (4)	-0.0131 (4)

Geometric parameters (Å, °)

C1—N1	1.379 (3)	C4—N1	1.439 (3)
C1—S2	1.626 (3)	C5—C6	1.378 (3)
C1—S1	1.733 (2)	C5—H5	0.9300
C2—O1	1.198 (3)	C6—C7	1.375 (3)
C2—N1	1.402 (3)	C6—H6	0.9300
C2—C3	1.496 (3)	C7—C8	1.366 (3)
C3—S1	1.793 (3)	C7—H7	0.9300
C3—H3A	0.9700	C8—C9	1.384 (3)
C3—H3B	0.9700	C8—H8	0.9300
C4—C5	1.370 (3)	C9—H9	0.9300
C4—C9	1.377 (3)		

N1—C1—S2	126.73 (18)	C6—C5—H5	120.3
N1—C1—S1	110.68 (17)	C7—C6—C5	120.3 (2)
S2—C1—S1	122.59 (15)	C7—C6—H6	119.9
O1—C2—N1	123.1 (2)	C5—C6—H6	119.9
O1—C2—C3	125.5 (2)	C8—C7—C6	120.2 (2)
N1—C2—C3	111.4 (2)	C8—C7—H7	119.9
C2—C3—S1	107.11 (17)	C6—C7—H7	119.9
C2—C3—H3A	110.3	C7—C8—C9	120.0 (2)
S1—C3—H3A	110.3	C7—C8—H8	120.0
C2—C3—H3B	110.3	C9—C8—H8	120.0
S1—C3—H3B	110.3	C4—C9—C8	119.5 (2)
H3A—C3—H3B	108.5	C4—C9—H9	120.3
C5—C4—C9	120.7 (2)	C8—C9—H9	120.3
C5—C4—N1	120.3 (2)	C1—N1—C2	116.9 (2)
C9—C4—N1	118.9 (2)	C1—N1—C4	124.14 (19)
C4—C5—C6	119.4 (2)	C2—N1—C4	119.0 (2)
C4—C5—H5	120.3	C1—S1—C3	93.86 (12)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C5—H5 \cdots O1 ⁱ	0.93	2.51	3.410 (3)	163
C8—H8 \cdots O1 ⁱⁱ	0.93	2.46	3.386 (3)	171

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