Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*Z*)-5-(3-Nitrobenzylidene)-1,3-thiazolidine-2,4-dione

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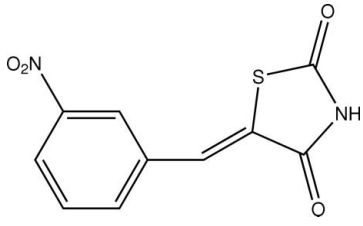
Received 15 October 2007; accepted 18 October 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.077; wR factor = 0.194; data-to-parameter ratio = 12.9.

In the title compound, $C_{10}H_6N_2O_4S$, the benzene and thiazolidine rings are oriented at a dihedral angle of 8.8 (5)° to one another. In the crystal structure, intramolecular C—H···O and C—H···S hydrogen bonds are present; intermolecular N—H···O and C—H···O hydrogen bonds link the molecules into rows down the *a* axis.

Related literature

For background to thiazolidine compounds, see: Barreca & Balzarini (2002); Botti *et al.* (1996). For a related structure, see: Guo *et al.* (2006). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{10}H_6N_2O_4S$
M_r = 250.23
Triclinic, $P\overline{1}$
a = 4.7270 (9) Å
b = 10.936 (2) Å
c = 11.276 (2) Å
α = 117.41 (3)°
β = 97.93 (3)°
γ = 93.36 (3)°
V = 507.6 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 293 (2) K
0.30 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.909, T_{max} = 0.968
2246 measured reflections
1992 independent reflections
1409 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.194
S = 1.01
1992 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O4^{i}	0.86	2.00	2.846 (6)	167
C4—H4A···S	0.93	2.54	3.246 (6)	132
C6—H6A···O2^{ii}	0.93	2.54	3.387 (7)	152
C7—H7A···O4	0.93	2.49	2.856 (7)	104
C7—H7A···O2^{ii}	0.93	2.51	3.390 (7)	157

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo,1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens,1996); software used to prepare material for publication: *SHELXL97*.

The authors thank the Center for Testing and Analysis, Nanjing University, for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2379).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Barreca, M. L. & Balzarini, J. G. K. (2002). *J. Med. Chem.* **45**, 5410–5413.
Botti, P. T., Pallin, D. & Tam, J. P. (1996). *J. Am. Chem. Soc.* **118**, 10018–10024.
Enraf–Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Guo, C., Zhang, D.-M., Tang, Q.-G. & Sun, H.-S. (2006). *Acta Cryst.* E**62**, o3994–o3995.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

 doi:10.1107/S1600536807051653

supplementary materials

Acta Cryst. (2007). E**63**, o4425 [**doi:10.1107/S1600536807051653**]

(*Z*)-5-(3-Nitrobenzylidene)-1,3-thiazolidine-2,4-dione

H. Sun, W. He, Y. Xu, S. Tang and C. Guo

Comment

Thiazolidines are an important class of heteroaromatic compounds and have widespread applications from pharmaceuticals (Barreca & Balzarini, 2002) to materials (Botti *et al.*, 1996). As part of our studies in this area (Guo *et al.*, 2006), we report herein the synthesis and crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings A (C1—C6) and B (C8/C10/N/C9/S) are planar and oriented at a dihedral angle of 8.8 (5)° to one another.

In the crystal structure, intramolecular C—H···O and C—H···S hydrogen bonds affect the conformation of the molecule while intermolecular N—H···O and C—H···O hydrogen bonds (Table 1) link the molecules into rows down the *a* axis (Fig. 2).

Experimental

Thiazolidine-2,4-dione(10 mmol) and 3-nitrobenzaldehyde(10 mmol) were dissolved in ethanol (10 ml) in a 50 mL round-bottomed flask and 5 drops of piperidine were added. The flask was heated in a modified domestic microwave oven at 300 W for 5 minutes. After cooling, the mixture was poured into water, the crude compound (I) filtered out, and recrystallized from ethanol. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Refinement

H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93, 0.98 and 0.96 Å for aromatic, methine and methyl H, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*N*), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

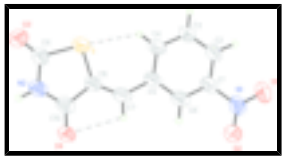


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and intramolecular hydrogen bonds are drawn as dashed lines.

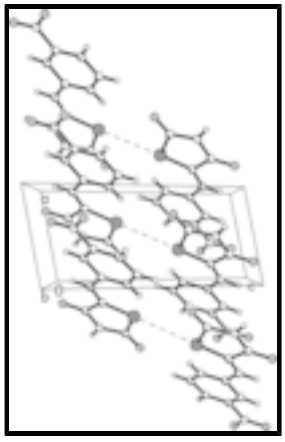


Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

(*Z*)-5-(3-Nitrobenzylidene)-1,3-thiazolidine-2,4-dione

Crystal data

$C_{10}H_6N_2O_4S$	$Z = 2$
$M_r = 250.23$	$F_{000} = 256$
Triclinic, $P\overline{1}$	$D_x = 1.637$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 4.7270$ (9) Å	Cell parameters from 25 reflections
$b = 10.936$ (2) Å	$\theta = 9$–13º
$c = 11.276$ (2) Å	$\mu = 0.32$ mm^{-1}
$\alpha = 117.41$ (3)º	$T = 293$ (2) K
$\beta = 97.93$ (3)º	Block, colorless
$\gamma = 93.36$ (3)º	0.30 × 0.10 × 0.10 mm
$V = 507.6$ (2) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.044$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.0$º
Monochromator: graphite	$\theta_{min} = 2.1$º
$T = 293(2)$ K	$h = -5 \rightarrow 5$
$\omega/2\theta$ scans	$k = -13 \rightarrow 11$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = 0 \rightarrow 13$
$T_{min} = 0.909$, $T_{max} = 0.968$	3 standard reflections
2246 measured reflections	every 200 reflections
1992 independent reflections	intensity decay: none
1409 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.077$	H-atom parameters constrained
$wR(F^2) = 0.194$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1.7P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
1992 reflections	$\Delta\rho_{max} = 0.67$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S	0.3581 (3)	0.59718 (13)	0.63995 (13)	0.0598 (4)
C1	−0.3675 (11)	0.2519 (5)	0.7606 (5)	0.0531 (12)
N1	−0.5780 (11)	0.2091 (4)	0.8249 (5)	0.0633 (12)
O1	−0.6747 (10)	0.0859 (4)	0.7697 (4)	0.0766 (12)
O2	−0.6415 (10)	0.2990 (4)	0.9278 (4)	0.0765 (12)
N2	0.5030 (10)	0.8520 (4)	0.8274 (4)	0.0593 (11)
H2A	0.5898	0.9360	0.8731	0.071*
C2	−0.2926 (12)	0.1520 (5)	0.6454 (5)	0.0568 (13)
H2B	−0.3610	0.0583	0.6112	0.068*
O3	0.7236 (10)	0.7914 (4)	0.6431 (4)	0.0825 (13)
C3	−0.1128 (12)	0.1953 (5)	0.5825 (5)	0.0611 (14)
H3A	−0.0614	0.1303	0.5028	0.073*
O4	0.2315 (9)	0.8721 (3)	0.9849 (4)	0.0656 (11)
C4	−0.0071 (12)	0.3341 (5)	0.6359 (5)	0.0567 (13)
H4A	0.1131	0.3610	0.5908	0.068*
C5	−0.0757 (11)	0.4342 (5)	0.7550 (5)	0.0501 (12)
C6	−0.2752 (11)	0.3898 (5)	0.8169 (5)	0.0533 (12)
H6A	−0.3393	0.4536	0.8934	0.064*

C7	0.0334 (12)	0.5816 (5)	0.8209 (5)	0.0548 (13)
H7A	−0.0274	0.6345	0.9024	0.066*
C8	0.2062 (11)	0.6537 (5)	0.7841 (5)	0.0502 (11)
C9	0.5580 (12)	0.7639 (5)	0.7014 (5)	0.0586 (13)
C10	0.3069 (12)	0.8021 (5)	0.8776 (5)	0.0549 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0842 (10)	0.0441 (7)	0.0461 (7)	0.0083 (6)	0.0215 (6)	0.0146 (6)
C1	0.069 (3)	0.037 (2)	0.044 (3)	0.008 (2)	0.005 (2)	0.012 (2)
N1	0.091 (3)	0.044 (2)	0.058 (3)	0.010 (2)	0.010 (2)	0.027 (2)
O1	0.101 (3)	0.044 (2)	0.080 (3)	−0.002 (2)	0.017 (2)	0.027 (2)
O2	0.112 (3)	0.049 (2)	0.073 (3)	0.017 (2)	0.043 (2)	0.026 (2)
N2	0.084 (3)	0.035 (2)	0.055 (2)	0.017 (2)	0.024 (2)	0.0147 (19)
C2	0.074 (4)	0.035 (2)	0.055 (3)	0.008 (2)	0.010 (3)	0.017 (2)
O3	0.113 (3)	0.062 (2)	0.078 (3)	0.007 (2)	0.052 (3)	0.029 (2)
C3	0.083 (4)	0.038 (3)	0.049 (3)	0.005 (2)	0.020 (3)	0.008 (2)
O4	0.096 (3)	0.0364 (18)	0.056 (2)	0.0065 (17)	0.032 (2)	0.0109 (16)
C4	0.076 (4)	0.043 (3)	0.046 (3)	0.013 (2)	0.019 (2)	0.015 (2)
C5	0.068 (3)	0.033 (2)	0.041 (2)	0.012 (2)	0.011 (2)	0.0099 (19)
C6	0.067 (3)	0.040 (3)	0.047 (3)	0.017 (2)	0.010 (2)	0.015 (2)
C7	0.077 (4)	0.042 (3)	0.040 (3)	0.018 (2)	0.014 (2)	0.014 (2)
C8	0.067 (3)	0.036 (2)	0.046 (3)	0.013 (2)	0.017 (2)	0.015 (2)
C9	0.070 (3)	0.044 (3)	0.057 (3)	0.004 (2)	0.013 (3)	0.020 (2)
C10	0.069 (3)	0.045 (3)	0.051 (3)	0.015 (2)	0.012 (2)	0.022 (2)

Geometric parameters (Å, °)

S—C8	1.729 (5)	O3—C9	1.197 (6)
S—C9	1.775 (5)	C3—C4	1.379 (7)
C1—C6	1.353 (7)	C3—H3A	0.9300
C1—C2	1.368 (7)	O4—C10	1.215 (6)
C1—N1	1.482 (7)	C4—C5	1.384 (6)
N1—O2	1.218 (6)	C4—H4A	0.9300
N1—O1	1.220 (5)	C5—C6	1.433 (7)
N2—C10	1.359 (7)	C5—C7	1.453 (6)
N2—C9	1.374 (6)	C6—H6A	0.9300
N2—H2A	0.8600	C7—C8	1.334 (7)
C2—C3	1.371 (7)	C7—H7A	0.9300
C2—H2B	0.9300	C8—C10	1.472 (7)
C8—S—C9	91.7 (2)	C4—C5—C6	117.6 (4)
C6—C1—C2	124.7 (5)	C4—C5—C7	125.2 (5)
C6—C1—N1	116.8 (4)	C6—C5—C7	117.2 (4)
C2—C1—N1	118.4 (4)	C1—C6—C5	117.9 (5)
O2—N1—O1	125.4 (5)	C1—C6—H6A	121.1
O2—N1—C1	117.7 (4)	C5—C6—H6A	121.1
O1—N1—C1	116.9 (4)	C8—C7—C5	130.8 (5)

C10—N2—C9	117.8 (4)	C8—C7—H7A	114.6
C10—N2—H2A	121.1	C5—C7—H7A	114.6
C9—N2—H2A	121.1	C7—C8—C10	119.5 (4)
C1—C2—C3	117.3 (5)	C7—C8—S	129.5 (4)
C1—C2—H2B	121.3	C10—C8—S	110.9 (4)
C3—C2—H2B	121.3	O3—C9—N2	126.1 (5)
C2—C3—C4	120.9 (5)	O3—C9—S	124.4 (4)
C2—C3—H3A	119.6	N2—C9—S	109.4 (4)
C4—C3—H3A	119.6	O4—C10—N2	123.6 (5)
C3—C4—C5	121.5 (5)	O4—C10—C8	126.3 (5)
C3—C4—H4A	119.3	N2—C10—C8	110.1 (4)
C5—C4—H4A	119.3		
C6—C1—N1—O2	−3.9 (7)	C6—C5—C7—C8	−176.0 (5)
C2—C1—N1—O2	179.6 (5)	C5—C7—C8—C10	−174.0 (5)
C6—C1—N1—O1	175.7 (5)	C5—C7—C8—S	1.8 (9)
C2—C1—N1—O1	−0.7 (7)	C9—S—C8—C7	−175.0 (5)
C6—C1—C2—C3	−0.5 (8)	C9—S—C8—C10	1.2 (4)
N1—C1—C2—C3	175.6 (5)	C10—N2—C9—O3	−180.0 (6)
C1—C2—C3—C4	1.6 (9)	C10—N2—C9—S	−3.0 (6)
C2—C3—C4—C5	0.6 (9)	C8—S—C9—O3	177.9 (6)
C3—C4—C5—C6	−3.7 (8)	C8—S—C9—N2	0.9 (4)
C3—C4—C5—C7	177.8 (5)	C9—N2—C10—O4	−176.6 (5)
C2—C1—C6—C5	−2.6 (8)	C9—N2—C10—C8	3.9 (7)
N1—C1—C6—C5	−178.8 (4)	C7—C8—C10—O4	−5.8 (9)
C4—C5—C6—C1	4.6 (7)	S—C8—C10—O4	177.6 (5)
C7—C5—C6—C1	−176.7 (5)	C7—C8—C10—N2	173.6 (5)
C4—C5—C7—C8	2.5 (9)	S—C8—C10—N2	−3.0 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O4^{i}	0.86	2.00	2.846 (6)	167
C4—H4A···S	0.93	2.54	3.246 (6)	132
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Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+2; (ii) −*x*−1, −*y*+1, −*z*+2.

Fig. 1

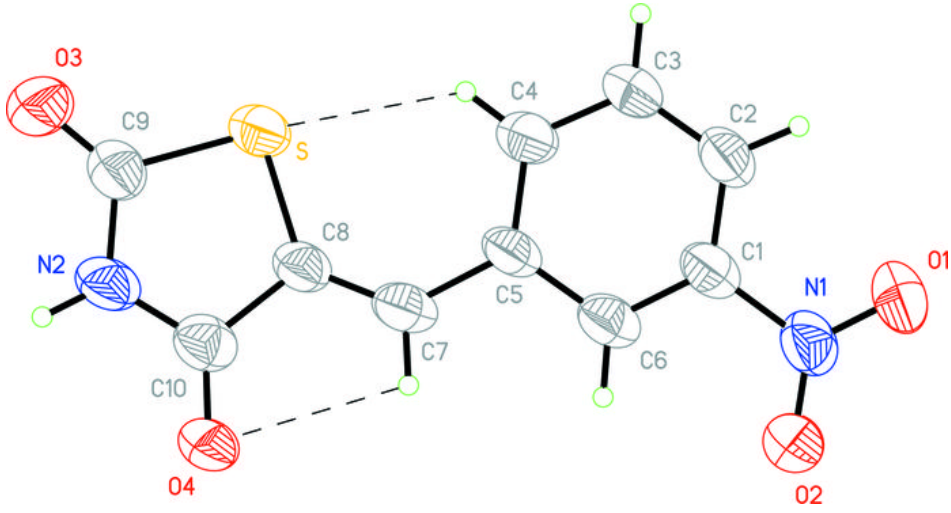

Fig. 2