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***N*-(*Z*)-3-(4-Chlorobenzoyl)-1,3-thiazolidin-2-ylidene]cyanamide**Jian-Gang Wang,^a Li-Hua Huang^b and Fang-Fang Jian^{c*}

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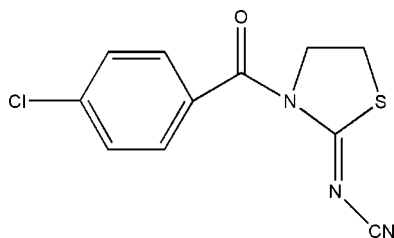
Received 8 October 2008; accepted 7 November 2008

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.026; wR factor = 0.066; data-to-parameter ratio = 13.0.

The title compound, $\text{C}_{11}\text{H}_8\text{ClN}_3\text{OS}$, was prepared by the reaction of *N*-cyanoiminothiazolidine, 2-aminoethanethiol and triethylamine at 350 K. The dihedral angle between the two rings is 62.5 (8)°.

Related literature

For the biological activities of thiazolidine compounds, see: Iwata *et al.* (1988); Huang & Shi (1990). For related structures, see Jian *et al.* (2006); Schroth *et al.* (1997).



Experimental

Crystal data

$\text{C}_{11}\text{H}_8\text{ClN}_3\text{OS}$
 $M_r = 265.72$
 Monoclinic, $P2_1/c$
 $a = 16.442$ (3) Å
 $b = 5.6798$ (11) Å
 $c = 13.313$ (3) Å
 $\beta = 112.76$ (3)°
 $V = 1146.5$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.50$ mm⁻¹
 $T = 293$ (2) K
 $0.34 \times 0.21 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Absorption correction: none
 8343 measured reflections
 2016 independent reflections
 1915 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.066$
 $S = 1.13$
 2016 reflections
 155 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2128).

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supplementary materials

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N-[(*Z*)-3-(4-Chlorobenzoyl)-1,3-thiazolidin-2-ylidene]cyanamide

J.-G. Wang, L.-H. Huang and F.-F. Jian

Comment

Thiazolidine is an important group in organic chemistry. Many compounds containing thiazolidine groups possess a broad spectrum of biological activities (Iwata *et al.*, 1988; Huang & Shi, 1990).

In the crystal structure (Fig. 1), the torsion angle formed by atoms N1, C8, C9 and S1 was 34.5 (9)°. The dihedral angle formed by the the ring (N1, C8, C9, C10 and S1) and the phenyl ring (C1-C6) was 62.5 (8)°. The C=N bond length (1.299 (2) Å) is in agreement with that observed before (Jian *et al.*, 2006). The C—S bond length (1.734 (7) and 1.808 (2) Å) are in agreement with those observed before (Schroth *et al.*, 1997). Intermolecular C—H···N interactions help to stabilize the crystal structure.

Experimental

A mixture of *N*-cyanoiminothiazolidine 10 mmol (1.27 g), 2-amino-ethanethiol (1.75 g, 10 mmol) and (1.01 g, 10 mmol) triethylamine was refluxed in absolute acetone (25 ml) for 4 h. On cooling, the product crystallized, was filtered, and recrystallized from absolute EtOH (yield 2.42 g (91%)). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances of 0.93–0.97 Å, respectively, and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}$ of the parent atoms.

Figures

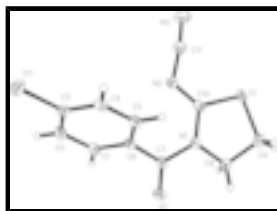


Fig. 1. The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 40% probability level.

N-[(*Z*)-3-(4-Chlorobenzoyl)-1,3-thiazolidin-2-ylidene]cyanamide

Crystal data

$\text{C}_{11}\text{H}_8\text{ClN}_3\text{OS}$

$M_r = 265.72$

Monoclinic, $P2_1/c$

$F_{000} = 544$

$D_x = 1.539 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

supplementary materials

Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 16.442 (3) \text{ \AA}$	Cell parameters from 1021 reflections
$b = 5.6798 (11) \text{ \AA}$	$\theta = 2.9\text{--}26.4^\circ$
$c = 13.313 (3) \text{ \AA}$	$\mu = 0.50 \text{ mm}^{-1}$
$\beta = 112.76 (3)^\circ$	$T = 293 (2) \text{ K}$
$V = 1146.5 (5) \text{ \AA}^3$	Block, colorless
$Z = 4$	$0.34 \times 0.21 \times 0.15 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	1915 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.030$
Monochromator: graphite	$\theta_{\text{max}} = 25.0^\circ$
$T = 293(2) \text{ K}$	$\theta_{\text{min}} = 3.1^\circ$
φ and ω scans	$h = -19 \rightarrow 19$
Absorption correction: none	$k = -6 \rightarrow 6$
8343 measured reflections	$l = -15 \rightarrow 15$
2016 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.026$	$w = 1/[\sigma^2(F_o^2) + (0.017P)^2 + 0.7287P]$
$wR(F^2) = 0.066$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2016 reflections	$\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
155 parameters	$\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.031 (2)

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.07965 (3)	0.52934 (7)	0.33331 (3)	0.02469 (14)
C11	0.46689 (3)	0.71315 (8)	0.06338 (3)	0.03512 (15)
O1	0.27367 (8)	1.17756 (19)	0.37317 (10)	0.0302 (3)
N2	0.16368 (9)	0.5912 (2)	0.19639 (11)	0.0244 (3)
C3	0.40564 (10)	0.7898 (3)	0.13961 (12)	0.0229 (3)
N1	0.20390 (8)	0.8283 (2)	0.35254 (10)	0.0216 (3)
C10	0.15500 (10)	0.6503 (3)	0.28595 (12)	0.0201 (3)
C4	0.40148 (10)	0.6326 (3)	0.21690 (12)	0.0232 (3)
H4A	0.4315	0.4901	0.2281	0.028*
N3	0.08333 (10)	0.2509 (3)	0.08619 (14)	0.0426 (4)
C7	0.26182 (10)	0.9843 (3)	0.33103 (12)	0.0220 (3)
C6	0.30963 (9)	0.9060 (3)	0.26219 (12)	0.0197 (3)
C8	0.16984 (11)	0.9017 (3)	0.43566 (13)	0.0263 (4)
H8A	0.1270	1.0272	0.4077	0.032*
H8B	0.2176	0.9574	0.5007	0.032*
C1	0.31667 (10)	1.0641 (3)	0.18625 (13)	0.0227 (3)
H1A	0.2896	1.2106	0.1779	0.027*
C9	0.12728 (11)	0.6865 (3)	0.46101 (13)	0.0268 (4)
H9A	0.0820	0.7312	0.4872	0.032*
H9B	0.1708	0.5901	0.5158	0.032*
C11	0.11795 (11)	0.4075 (3)	0.14112 (14)	0.0275 (4)
C5	0.35225 (10)	0.6895 (3)	0.27740 (12)	0.0222 (3)
H5A	0.3477	0.5833	0.3281	0.027*
C2	0.36370 (10)	1.0057 (3)	0.12284 (13)	0.0244 (3)
H2B	0.3669	1.1093	0.0704	0.029*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0224 (2)	0.0236 (2)	0.0314 (2)	-0.00304 (16)	0.01415 (17)	0.00002 (16)
C11	0.0368 (3)	0.0412 (3)	0.0340 (2)	0.00200 (19)	0.02096 (19)	-0.00607 (19)
O1	0.0369 (7)	0.0210 (6)	0.0374 (7)	-0.0065 (5)	0.0194 (5)	-0.0072 (5)
N2	0.0252 (7)	0.0244 (7)	0.0252 (7)	-0.0060 (6)	0.0115 (6)	-0.0039 (6)
C3	0.0187 (7)	0.0266 (8)	0.0226 (8)	-0.0038 (6)	0.0071 (6)	-0.0060 (6)
N1	0.0246 (7)	0.0207 (7)	0.0217 (6)	-0.0036 (5)	0.0114 (5)	-0.0012 (5)
C10	0.0185 (7)	0.0167 (7)	0.0243 (8)	0.0018 (6)	0.0075 (6)	0.0039 (6)
C4	0.0194 (8)	0.0190 (7)	0.0273 (8)	0.0006 (6)	0.0047 (6)	-0.0016 (6)
N3	0.0337 (8)	0.0427 (10)	0.0586 (11)	-0.0120 (8)	0.0257 (8)	-0.0256 (9)
C7	0.0218 (8)	0.0201 (8)	0.0229 (8)	-0.0012 (6)	0.0072 (6)	0.0024 (6)
C6	0.0171 (7)	0.0187 (7)	0.0219 (7)	-0.0047 (6)	0.0062 (6)	-0.0019 (6)
C8	0.0293 (8)	0.0284 (8)	0.0244 (8)	-0.0013 (7)	0.0140 (7)	-0.0026 (7)
C1	0.0209 (8)	0.0171 (7)	0.0289 (8)	-0.0013 (6)	0.0082 (6)	0.0017 (6)
C9	0.0248 (8)	0.0326 (9)	0.0236 (8)	-0.0002 (7)	0.0101 (7)	0.0028 (7)
C11	0.0230 (8)	0.0303 (9)	0.0348 (9)	-0.0025 (7)	0.0172 (7)	-0.0056 (8)

supplementary materials

C5	0.0226 (8)	0.0192 (8)	0.0227 (8)	-0.0029 (6)	0.0064 (6)	0.0022 (6)
C2	0.0242 (8)	0.0248 (8)	0.0245 (8)	-0.0030 (7)	0.0099 (6)	0.0040 (7)

Geometric parameters (Å, °)

S1—C10	1.7347 (15)	N3—C11	1.152 (2)
S1—C9	1.8082 (17)	C7—C6	1.488 (2)
C11—C3	1.7390 (16)	C6—C1	1.390 (2)
O1—C7	1.2136 (19)	C6—C5	1.391 (2)
N2—C10	1.299 (2)	C8—C9	1.510 (2)
N2—C11	1.329 (2)	C8—H8A	0.9700
C3—C2	1.382 (2)	C8—H8B	0.9700
C3—C4	1.384 (2)	C1—C2	1.388 (2)
N1—C10	1.379 (2)	C1—H1A	0.9300
N1—C7	1.409 (2)	C9—H9A	0.9700
N1—C8	1.4804 (19)	C9—H9B	0.9700
C4—C5	1.383 (2)	C5—H5A	0.9300
C4—H4A	0.9300	C2—H2B	0.9300
C10—S1—C9	92.05 (8)	N1—C8—H8A	110.5
C10—N2—C11	118.14 (14)	C9—C8—H8A	110.5
C2—C3—C4	121.83 (14)	N1—C8—H8B	110.5
C2—C3—C11	119.55 (12)	C9—C8—H8B	110.5
C4—C3—C11	118.61 (12)	H8A—C8—H8B	108.7
C10—N1—C7	127.01 (13)	C2—C1—C6	120.72 (14)
C10—N1—C8	113.06 (12)	C2—C1—H1A	119.6
C7—N1—C8	117.11 (13)	C6—C1—H1A	119.6
N2—C10—N1	122.40 (14)	C8—C9—S1	105.01 (11)
N2—C10—S1	125.37 (12)	C8—C9—H9A	110.7
N1—C10—S1	112.17 (11)	S1—C9—H9A	110.7
C5—C4—C3	119.40 (14)	C8—C9—H9B	110.7
C5—C4—H4A	120.3	S1—C9—H9B	110.7
C3—C4—H4A	120.3	H9A—C9—H9B	108.8
O1—C7—N1	118.36 (14)	N3—C11—N2	172.67 (18)
O1—C7—C6	121.78 (14)	C4—C5—C6	119.80 (14)
N1—C7—C6	119.80 (13)	C4—C5—H5A	120.1
C1—C6—C5	119.87 (14)	C6—C5—H5A	120.1
C1—C6—C7	117.87 (14)	C3—C2—C1	118.32 (14)
C5—C6—C7	122.08 (14)	C3—C2—H2B	120.8
N1—C8—C9	106.32 (13)	C1—C2—H2B	120.8
C11—N2—C10—N1	175.68 (14)	N1—C7—C6—C1	138.53 (15)
C11—N2—C10—S1	-7.2 (2)	O1—C7—C6—C5	130.83 (17)
C7—N1—C10—N2	6.7 (2)	N1—C7—C6—C5	-46.3 (2)
C8—N1—C10—N2	167.01 (14)	C10—N1—C8—C9	29.96 (17)
C7—N1—C10—S1	-170.72 (12)	C7—N1—C8—C9	-167.65 (13)
C8—N1—C10—S1	-10.44 (16)	C5—C6—C1—C2	1.9 (2)
C9—S1—C10—N2	172.92 (14)	C7—C6—C1—C2	177.18 (14)
C9—S1—C10—N1	-9.73 (12)	N1—C8—C9—S1	-34.60 (15)
C2—C3—C4—C5	1.7 (2)	C10—S1—C9—C8	25.81 (12)
C11—C3—C4—C5	-179.26 (11)	C3—C4—C5—C6	-1.8 (2)

supplementary materials

C10—N1—C7—O1	152.51 (15)	C1—C6—C5—C4	0.0 (2)
C8—N1—C7—O1	-7.1 (2)	C7—C6—C5—C4	-175.00 (14)
C10—N1—C7—C6	-30.2 (2)	C4—C3—C2—C1	0.2 (2)
C8—N1—C7—C6	170.18 (13)	C11—C3—C2—C1	-178.80 (12)
O1—C7—C6—C1	-44.3 (2)	C6—C1—C2—C3	-2.1 (2)

Fig. 1

