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

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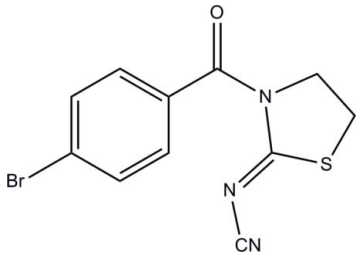
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.037; $wR$ factor = 0.108; data-to-parameter ratio = 13.4.

In the title compound, $C_{11}H_8BrN_3OS$, the dihedral angle between the benzene and thiazolidine rings is 63.4 (2)°. Intermolecular C—H···N interactions help to stabilize the crystal structure.

## Related literature

For related structures, see: Wang *et al.* (2008); Liu & Li (2009); Xie & Li (2010). For the biological activity of thiazolidine-containing compounds, see: Iwata *et al.* (1988). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{11}H_8BrN_3OS$
$M_r$ = 310.17
Monoclinic, $P2_1/c$
$a$ = 16.579 (3) Å
$b$ = 5.6471 (11) Å
$c$ = 13.611 (3) Å
$\beta$ = 112.91 (3)°
$V$ = 1173.9 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 3.67 mm$^{-1}$
$T$ = 173 K
0.25 × 0.20 × 0.06 mm

### Data collection

Rigaku Mercury CCD/AFC diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007)
$T_{min}$ = 0.461, $T_{max}$ = 0.810
8232 measured reflections
2067 independent reflections
1960 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.108
$S$ = 1.28
2067 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C9—H9$A$···N3$^{i}$ | 0.97 | 2.51 | 3.281 (5) | 137 |

Symmetry code: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrystalClear* (Rigaku, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: HG2746).

## References

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# supporting information

*Acta Cryst.* (2010). E**66**, o3206 [https://doi.org/10.1107/S1600536810046520]

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

**Jiu-Ming Li, Jian-Ping Yong, Feng-lan Huang, Li-mei Sun and Ling Xu**

### S1. Comment

Thiazolidine is an important kind of group in organic chemistry. Many compounds containing thiazolidine groups possess a broad spectrum of biological activities (Iwata *et al.*, 1988). Here, we report the crystal structure of (I).

In title compound, all bond lengths in the molecular are normal (Allen *et al.*, 1987) and in a good agreement with those reported previously (Wang *et al.*, 2008; Liu & Li, 2009; Xie & Li, 2010). The dihedral angle between benzene (C1—C6) and thiazolidine (C8—C10/N1/S2) rings is 63.4 (2) °. The intermolecular C—H···N hydrogen bonds stabilize the structure.

### S2. Experimental

A mixture of *N*-cyanoiminothiazolidine 10 mmol (1.27 g), 4-bromobenzoyl chloride (2.19 g, 10 mmol) and (1.01 g, 10 mmol) triethylamine was refluxed in absolute acetone (25 ml) for 3 h. On cooling, the product crystallized, was filtered, and recrystallized from absolute EtOH; yield 2.48 g (80.0%). Single crystals suitable for X-ray measurements were obtained by recrystallization from acetonitrile at room temperature.

### S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 or 0.97 Å and with $U_{iso}$(H) = 1.2 times $U_{eq}$(C).

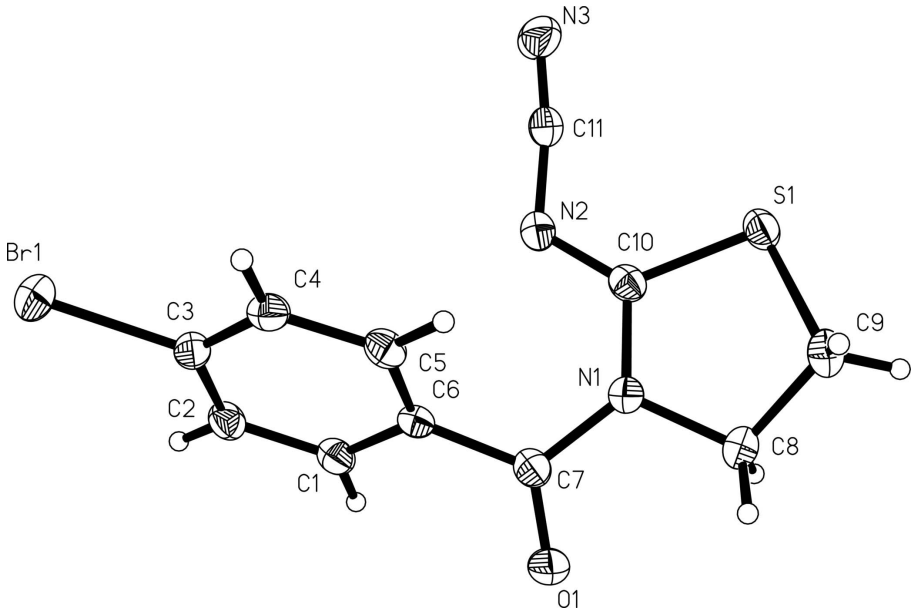


**Figure 1**

The molecular structure of (I), with atom labels and 40% probability displacement ellipsoids for non-H atoms.

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

*Crystal data*

$C_{11}H_8BrN_3OS$
$M_r = 310.17$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 16.579$ (3) Å
$b = 5.6471$ (11) Å
$c = 13.611$ (3) Å
$\beta = 112.91$ (3)°
$V = 1173.9$ (4) Å$^3$
$Z = 4$
$F(000) = 616$
$D_x = 1.755$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3665 reflections
$\theta = 1.3$–27.5°
$\mu = 3.67$ mm$^{-1}$
$T = 173$ K
Plate, colorless
0.25 × 0.20 × 0.06 mm

*Data collection*

Rigaku Mercury CCD/AFC diffractometer
Radiation source: Sealed Tube
Graphite Monochromator monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007)
$T_{min} = 0.461$, $T_{max} = 0.810$
8232 measured reflections
2067 independent reflections
1960 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.3°$
$h = -17\rightarrow19$
$k = -6\rightarrow6$
$l = -16\rightarrow13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.108$
$S = 1.28$
2067 reflections
154 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
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 0.437P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.46$ e Å$^{-3}$
$\Delta\rho_{min} = -0.35$ e Å$^{-3}$

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.46599 (2) | 0.71386 (7) | 0.56642 (3) | 0.03845 (19) |
| S1 | 0.07775 (6) | 0.52236 (16) | 0.83336 (8) | 0.0307 (2) |
| O1 | 0.26798 (18) | 1.1823 (4) | 0.8767 (2) | 0.0362 (6) |
| N1 | 0.19890 (18) | 0.8299 (5) | 0.8536 (2) | 0.0268 (6) |
| N2 | 0.15701 (19) | 0.6055 (6) | 0.6966 (2) | 0.0316 (7) |
| N3 | 0.0788 (2) | 0.2687 (6) | 0.5834 (3) | 0.0483 (10) |
| C1 | 0.3110 (2) | 1.0740 (6) | 0.6926 (3) | 0.0281 (7) |
| H1A | 0.2843 | 1.2215 | 0.6845 | 0.034* |
| C2 | 0.3582 (2) | 1.0153 (6) | 0.6309 (3) | 0.0288 (8) |
| H2B | 0.3614 | 1.1193 | 0.5796 | 0.035* |
| C3 | 0.3999 (2) | 0.7995 (6) | 0.6478 (3) | 0.0267 (8) |
| C4 | 0.3960 (2) | 0.6399 (6) | 0.7235 (3) | 0.0280 (8) |
| H4A | 0.4261 | 0.4969 | 0.7347 | 0.034* |
| C5 | 0.3469 (2) | 0.6969 (6) | 0.7817 (3) | 0.0274 (8) |
| H5A | 0.3427 | 0.5903 | 0.8315 | 0.033* |
| C6 | 0.3036 (2) | 0.9141 (6) | 0.7661 (3) | 0.0251 (7) |
| C7 | 0.2562 (2) | 0.9906 (6) | 0.8339 (3) | 0.0276 (8) |
| C8 | 0.1669 (2) | 0.8942 (7) | 0.9375 (3) | 0.0323 (8) |
| H8A | 0.1231 | 1.0182 | 0.9126 | 0.039* |
| H8B | 0.2148 | 0.9492 | 1.0011 | 0.039* |
| C9 | 0.1273 (2) | 0.6690 (7) | 0.9608 (3) | 0.0332 (8) |
| H9A | 0.0837 | 0.7059 | 0.9897 | 0.040* |
| H9B | 0.1723 | 0.5702 | 1.0114 | 0.040* |
| C10 | 0.1498 (2) | 0.6544 (6) | 0.7864 (3) | 0.0259 (7) |
| C11 | 0.1122 (2) | 0.4235 (7) | 0.6401 (3) | 0.0339 (8) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0425 (3) | 0.0437 (3) | 0.0358 (3) | −0.00069 (16) | 0.0225 (2) | −0.00648 (16) |
| S1 | 0.0292 (5) | 0.0296 (5) | 0.0375 (5) | −0.0023 (4) | 0.0175 (4) | 0.0020 (4) |
| O1 | 0.0422 (15) | 0.0270 (14) | 0.0456 (17) | −0.0066 (11) | 0.0239 (13) | −0.0086 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N1 | 0.0302 (16) | 0.0262 (15) | 0.0266 (16) | −0.0027 (12) | 0.0139 (13) | −0.0015 (12) |
| N2 | 0.0337 (16) | 0.0340 (17) | 0.0317 (16) | −0.0060 (13) | 0.0178 (14) | −0.0028 (13) |
| N3 | 0.039 (2) | 0.053 (2) | 0.061 (3) | −0.0111 (17) | 0.0277 (19) | −0.0232 (19) |
| C1 | 0.0256 (17) | 0.0238 (17) | 0.035 (2) | −0.0017 (14) | 0.0117 (15) | 0.0009 (15) |
| C2 | 0.0318 (18) | 0.0275 (18) | 0.0287 (19) | −0.0046 (14) | 0.0135 (16) | 0.0031 (14) |
| C3 | 0.0254 (18) | 0.0306 (19) | 0.0246 (19) | −0.0041 (14) | 0.0103 (15) | −0.0045 (14) |
| C4 | 0.0283 (18) | 0.0237 (17) | 0.0308 (19) | −0.0007 (14) | 0.0101 (15) | −0.0020 (14) |
| C5 | 0.0295 (19) | 0.0231 (17) | 0.0283 (19) | −0.0017 (14) | 0.0097 (16) | 0.0054 (14) |
| C6 | 0.0236 (16) | 0.0248 (17) | 0.0261 (18) | −0.0061 (14) | 0.0088 (14) | −0.0043 (14) |
| C7 | 0.0258 (17) | 0.0257 (18) | 0.0324 (19) | −0.0002 (13) | 0.0125 (15) | 0.0017 (14) |
| C8 | 0.0360 (19) | 0.036 (2) | 0.030 (2) | −0.0016 (16) | 0.0185 (16) | −0.0030 (16) |
| C9 | 0.0301 (19) | 0.041 (2) | 0.032 (2) | −0.0001 (16) | 0.0158 (17) | 0.0038 (17) |
| C10 | 0.0239 (17) | 0.0228 (16) | 0.0311 (19) | 0.0013 (14) | 0.0106 (15) | 0.0031 (14) |
| C11 | 0.0310 (19) | 0.035 (2) | 0.043 (2) | −0.0043 (16) | 0.0229 (17) | −0.0055 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C3 | 1.899 (4) | C2—C3 | 1.376 (5) |
| S1—C10 | 1.729 (3) | C2—H2B | 0.9300 |
| S1—C9 | 1.806 (4) | C3—C4 | 1.389 (5) |
| O1—C7 | 1.208 (4) | C4—C5 | 1.375 (5) |
| N1—C10 | 1.379 (4) | C4—H4A | 0.9300 |
| N1—C7 | 1.412 (4) | C5—C6 | 1.396 (5) |
| N1—C8 | 1.480 (4) | C5—H5A | 0.9300 |
| N2—C10 | 1.302 (5) | C6—C7 | 1.491 (5) |
| N2—C11 | 1.325 (5) | C8—C9 | 1.520 (5) |
| N3—C11 | 1.154 (5) | C8—H8A | 0.9700 |
| C1—C6 | 1.388 (5) | C8—H8B | 0.9700 |
| C1—C2 | 1.392 (5) | C9—H9A | 0.9700 |
| C1—H1A | 0.9300 | C9—H9B | 0.9700 |
| | | | |
| C10—S1—C9 | 92.05 (17) | C1—C6—C7 | 118.3 (3) |
| C10—N1—C7 | 127.0 (3) | C5—C6—C7 | 121.7 (3) |
| C10—N1—C8 | 113.1 (3) | O1—C7—N1 | 118.7 (3) |
| C7—N1—C8 | 117.3 (3) | O1—C7—C6 | 122.1 (3) |
| C10—N2—C11 | 118.3 (3) | N1—C7—C6 | 119.1 (3) |
| C6—C1—C2 | 120.5 (3) | N1—C8—C9 | 105.6 (3) |
| C6—C1—H1A | 119.7 | N1—C8—H8A | 110.6 |
| C2—C1—H1A | 119.7 | C9—C8—H8A | 110.6 |
| C3—C2—C1 | 118.3 (3) | N1—C8—H8B | 110.6 |
| C3—C2—H2B | 120.8 | C9—C8—H8B | 110.6 |
| C1—C2—H2B | 120.8 | H8A—C8—H8B | 108.7 |
| C2—C3—C4 | 122.2 (3) | C8—C9—S1 | 104.8 (3) |
| C2—C3—Br1 | 119.7 (3) | C8—C9—H9A | 110.8 |
| C4—C3—Br1 | 118.1 (3) | S1—C9—H9A | 110.8 |
| C5—C4—C3 | 118.9 (3) | C8—C9—H9B | 110.8 |
| C5—C4—H4A | 120.5 | S1—C9—H9B | 110.8 |
| C3—C4—H4A | 120.5 | H9A—C9—H9B | 108.9 |

| | | | |
|---|---|---|---|
| C4—C5—C6 | 120.2 (3) | N2—C10—N1 | 122.0 (3) |
| C4—C5—H5A | 119.9 | N2—C10—S1 | 125.7 (3) |
| C6—C5—H5A | 119.9 | N1—C10—S1 | 112.2 (2) |
| C1—C6—C5 | 119.8 (3) | N3—C11—N2 | 171.8 (4) |
| | | | |
| C6—C1—C2—C3 | −2.6 (5) | C1—C6—C7—N1 | 138.8 (3) |
| C1—C2—C3—C4 | 0.3 (5) | C5—C6—C7—N1 | −47.2 (4) |
| C1—C2—C3—Br1 | −179.3 (2) | C10—N1—C8—C9 | 30.9 (4) |
| C2—C3—C4—C5 | 1.7 (5) | C7—N1—C8—C9 | −165.9 (3) |
| Br1—C3—C4—C5 | −178.7 (2) | N1—C8—C9—S1 | −35.6 (3) |
| C3—C4—C5—C6 | −1.4 (5) | C10—S1—C9—C8 | 26.6 (3) |
| C2—C1—C6—C5 | 2.9 (5) | C11—N2—C10—N1 | 175.3 (3) |
| C2—C1—C6—C7 | 177.0 (3) | C11—N2—C10—S1 | −7.3 (5) |
| C4—C5—C6—C1 | −0.8 (5) | C7—N1—C10—N2 | 5.6 (5) |
| C4—C5—C6—C7 | −174.7 (3) | C8—N1—C10—N2 | 166.7 (3) |
| C10—N1—C7—O1 | 151.9 (3) | C7—N1—C10—S1 | −172.1 (3) |
| C8—N1—C7—O1 | −8.6 (5) | C8—N1—C10—S1 | −11.0 (4) |
| C10—N1—C7—C6 | −31.3 (5) | C9—S1—C10—N2 | 172.4 (3) |
| C8—N1—C7—C6 | 168.2 (3) | C9—S1—C10—N1 | −10.0 (3) |
| C1—C6—C7—O1 | −44.6 (5) | C10—N2—C11—N3 | −171 (3) |
| C5—C6—C7—O1 | 129.4 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9*A*···N3$^{i}$ | 0.97 | 2.51 | 3.281 (5) | 137 |

Symmetry code: (i) −*x*, *y*+1/2, −*z*+3/2.