Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*Z*)-*N*-(3-Nicotinoyl-1,3-thiazolidin-2-ylidene)cyanamide

Yun-Man Xie* and Yu-Min Li

Henan Chemical Industry Research Institute Co Ltd, Zhengzhou 450052, People's Republic of China
Correspondence e-mail: yunman_xie@yahoo.cn

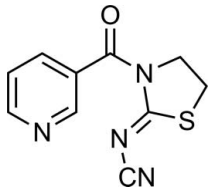
Received 18 April 2010; accepted 19 April 2010

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.095; data-to-parameter ratio = 12.4.

In the title compound, $C_{10}H_8N_4OS$, the dihedral angle between the pyridine and thiazolidine rings is 52.5 (5)°. Intermolecular C—H···N interactions help to stabilize the crystal structure.

Related literature

For related structures, see: Wang *et al.* (2008); Liu & Li (2009). For the biological activity of thiazolidine-containing compounds, see: Iwata *et al.* (1988); Ogawa (2000). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{10}H_8N_4OS$
M_r = 232.26
Monoclinic, $P2_1/c$
a = 5.9180 (12) Å
b = 15.182 (3) Å
c = 11.448 (2) Å
β = 94.62 (3)°
V = 1025.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 173 K
0.17 × 0.07 × 0.05 mm

Data collection

Rigaku Mercury CCD/AFC diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007)
T_{min} = 0.951, T_{max} = 0.985
7491 measured reflections
1799 independent reflections
1699 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.095
S = 1.15
1799 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···N4^{i}	0.93	2.52	3.383 (3)	154
C8—H8B···N1^{ii}	0.97	2.55	3.481 (3)	162

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

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: HG2674).

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.
Iwata, C., Watanabe, M., Okamoto, S., Fujimoto, M., Sakae, M., Katsurada, M. & Imanishi, T. (1988). *Synthesis*, pp. 261–262.
Liu, X.-L. & Li, Y.-M. (2009). *Acta Cryst.* E**65**, o1645.
Ogawa, T. (2000). Jpn Patent JP 2000226378.
Rigaku (2007). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, J.-G., Huang, L.-H. & Jian, F.-F. (2008). *Acta Cryst.* E**64**, o2321.

supporting information

Acta Cryst. (2010). E**66**, o1158 [https://doi.org/10.1107/S1600536810014406]

(*Z*)-*N*-(3-Nicotinoyl-1,3-thiazolidin-2-ylidene)cyanamide

Yun-Man Xie and Yu-Min Li

S1. 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; Ogawa, 2000). In order to search for new thiazolidine compounds with higher bioactivity, we synthesized the title compound and describe its structure here.

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). The dihedral angle between pyridine (C1—C5/N1) and thiazolidine (C7—C9/N2/S1) rings is 52.5 (5)°. The intermolecular C—H···N hydrogen bonds stabilize the structure.

S2. Experimental

A mixture of *N*-cyanoiminothiazolidine 10 mmol (1.27 g), nicotinoyl chloride (1.42 g, 10 mmol) and (1.01 g, 10 mmol) triethylamine is refluxed in absolute acetone (25 ml) for 4 h. On cooling, the product crystallizes and is filtered, and recrystallized from absolute EtOH, yield 2.13 g (92%). Single crystals suitable for X-ray measurements were obtained by recrystallization from dichloromethane 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).

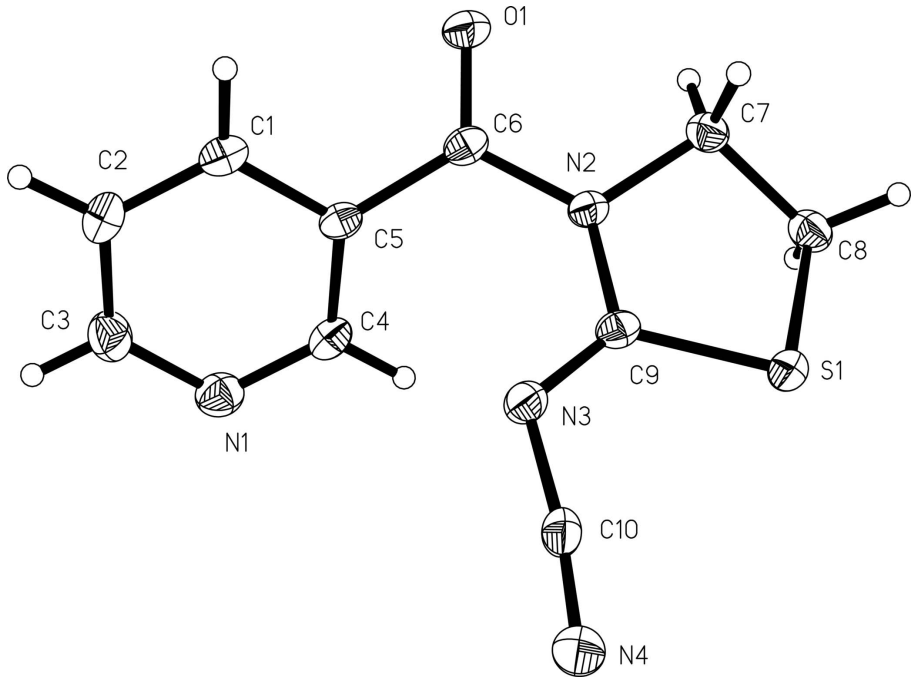


Figure 1

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

(*Z*)-*N*-(3-Nicotinoyl-1,3-thiazolidin-2-ylidene)cyanamide

Crystal data

$C_{10}H_8N_4OS$
$M_r = 232.26$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.9180\ (12)$ Å
$b = 15.182\ (3)$ Å
$c = 11.448\ (2)$ Å
$\beta = 94.62\ (3)°$
$V = 1025.2\ (4)$ Å^3
$Z = 4$
$F(000) = 480$
$D_x = 1.505$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3351 reflections
$\theta = 1.3–27.5°$
$\mu = 0.30$ mm^{-1}
$T = 173$ K
Needle, colorless
0.17 × 0.07 × 0.05 mm

Data collection

Rigaku Mercury CCD/AFC diffractometer
Radiation source: Sealed Tube
Graphite Monochromator monochromator
φ and ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2007)
$T_{min} = 0.951$, $T_{max} = 0.985$
7491 measured reflections
1799 independent reflections
1699 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -6\rightarrow7$
$k = -18\rightarrow18$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.095$
$S = 1.15$
1799 reflections
145 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
$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 0.7053P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.07382 (9)	0.71271 (4)	0.18314 (5)	0.02782 (18)
O1	0.6823 (2)	0.58746 (10)	−0.01165 (14)	0.0305 (4)
N1	0.0795 (3)	0.54439 (13)	−0.29129 (17)	0.0316 (5)
N2	0.3613 (3)	0.63953 (12)	0.05512 (15)	0.0230 (4)
N3	0.0875 (3)	0.72532 (12)	−0.05117 (15)	0.0253 (4)
N4	−0.2685 (4)	0.81222 (15)	−0.06511 (18)	0.0426 (6)
C1	0.5188 (4)	0.60983 (14)	−0.2489 (2)	0.0264 (5)
H1A	0.6663	0.6306	−0.2347	0.032*
C2	0.4329 (4)	0.58936 (16)	−0.3616 (2)	0.0318 (5)
H2A	0.5202	0.5972	−0.4248	0.038*
C3	0.2154 (4)	0.55716 (16)	−0.3780 (2)	0.0338 (6)
H3B	0.1591	0.5434	−0.4540	0.041*
C4	0.1635 (4)	0.56544 (14)	−0.1829 (2)	0.0262 (5)
H4A	0.0720	0.5573	−0.1214	0.031*
C5	0.3806 (3)	0.59877 (13)	−0.15738 (19)	0.0217 (5)
C6	0.4871 (4)	0.60973 (13)	−0.03604 (19)	0.0228 (5)
C7	0.4663 (4)	0.63253 (15)	0.17646 (18)	0.0254 (5)
H7A	0.5699	0.6811	0.1940	0.030*
H7B	0.5496	0.5777	0.1871	0.030*
C8	0.2732 (4)	0.63538 (15)	0.25500 (19)	0.0268 (5)
H8A	0.3252	0.6557	0.3329	0.032*
H8B	0.2048	0.5777	0.2611	0.032*
C9	0.1716 (3)	0.69261 (14)	0.04735 (19)	0.0222 (5)
C10	−0.1045 (4)	0.77156 (15)	−0.05189 (18)	0.0280 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0233 (3)	0.0389 (4)	0.0215 (3)	0.0052 (2)	0.0034 (2)	−0.0013 (2)
O1	0.0204 (9)	0.0388 (9)	0.0324 (9)	0.0057 (7)	0.0024 (6)	0.0012 (7)
N1	0.0276 (11)	0.0311 (11)	0.0363 (12)	−0.0026 (8)	0.0029 (9)	−0.0036 (9)
N2	0.0185 (9)	0.0278 (10)	0.0228 (10)	0.0038 (7)	0.0023 (7)	0.0007 (8)
N3	0.0237 (10)	0.0293 (10)	0.0232 (10)	0.0055 (8)	0.0044 (7)	0.0029 (8)
N4	0.0399 (13)	0.0566 (14)	0.0306 (12)	0.0207 (12)	−0.0015 (9)	−0.0012 (10)
C1	0.0205 (11)	0.0250 (11)	0.0342 (13)	−0.0001 (9)	0.0058 (9)	−0.0007 (10)
C2	0.0334 (14)	0.0362 (13)	0.0272 (13)	0.0006 (11)	0.0104 (10)	−0.0007 (10)
C3	0.0368 (14)	0.0371 (14)	0.0272 (13)	−0.0029 (11)	0.0006 (10)	−0.0058 (10)
C4	0.0252 (12)	0.0246 (11)	0.0300 (12)	0.0030 (9)	0.0088 (9)	0.0000 (9)
C5	0.0192 (11)	0.0197 (10)	0.0267 (11)	0.0029 (8)	0.0037 (8)	0.0000 (9)
C6	0.0202 (12)	0.0202 (11)	0.0286 (12)	−0.0009 (9)	0.0057 (9)	0.0007 (9)
C7	0.0232 (12)	0.0272 (11)	0.0252 (12)	0.0028 (9)	−0.0014 (9)	−0.0013 (9)
C8	0.0259 (12)	0.0303 (12)	0.0237 (12)	−0.0016 (10)	−0.0014 (9)	0.0030 (9)
C9	0.0176 (11)	0.0222 (10)	0.0270 (12)	−0.0015 (9)	0.0034 (9)	−0.0004 (9)
C10	0.0311 (13)	0.0344 (12)	0.0187 (11)	0.0057 (11)	0.0037 (9)	−0.0003 (9)

Geometric parameters (Å, º)

S1—C9	1.729 (2)	C1—H1A	0.9300
S1—C8	1.814 (2)	C2—C3	1.376 (3)
O1—C6	1.214 (3)	C2—H2A	0.9300
N1—C4	1.338 (3)	C3—H3B	0.9300
N1—C3	1.342 (3)	C4—C5	1.390 (3)
N2—C9	1.379 (3)	C4—H4A	0.9300
N2—C6	1.405 (3)	C5—C6	1.488 (3)
N2—C7	1.479 (3)	C7—C8	1.510 (3)
N3—C9	1.295 (3)	C7—H7A	0.9700
N3—C10	1.335 (3)	C7—H7B	0.9700
N4—C10	1.150 (3)	C8—H8A	0.9700
C1—C2	1.383 (3)	C8—H8B	0.9700
C1—C5	1.391 (3)		
C9—S1—C8	92.34 (10)	C1—C5—C6	117.34 (19)
C4—N1—C3	116.86 (19)	O1—C6—N2	118.05 (19)
C9—N2—C6	128.16 (18)	O1—C6—C5	120.49 (19)
C9—N2—C7	112.40 (17)	N2—C6—C5	121.28 (18)
C6—N2—C7	117.80 (17)	N2—C7—C8	106.01 (17)
C9—N3—C10	118.32 (18)	N2—C7—H7A	110.5
C2—C1—C5	118.8 (2)	C8—C7—H7A	110.5
C2—C1—H1A	120.6	N2—C7—H7B	110.5
C5—C1—H1A	120.6	C8—C7—H7B	110.5
C3—C2—C1	118.5 (2)	H7A—C7—H7B	108.7
C3—C2—H2A	120.8	C7—C8—S1	104.14 (14)
C1—C2—H2A	120.8	C7—C8—H8A	110.9

N1—C3—C2	124.1 (2)	S1—C8—H8A	110.9
N1—C3—H3B	118.0	C7—C8—H8B	110.9
C2—C3—H3B	118.0	S1—C8—H8B	110.9
N1—C4—C5	123.4 (2)	H8A—C8—H8B	108.9
N1—C4—H4A	118.3	N3—C9—N2	122.30 (19)
C5—C4—H4A	118.3	N3—C9—S1	125.63 (17)
C4—C5—C1	118.4 (2)	N2—C9—S1	112.01 (15)
C4—C5—C6	123.50 (19)	N4—C10—N3	172.7 (2)
C5—C1—C2—C3	−1.3 (3)	C1—C5—C6—N2	150.65 (19)
C4—N1—C3—C2	0.6 (4)	C9—N2—C7—C8	34.3 (2)
C1—C2—C3—N1	0.2 (4)	C6—N2—C7—C8	−159.14 (18)
C3—N1—C4—C5	−0.3 (3)	N2—C7—C8—S1	−36.57 (19)
N1—C4—C5—C1	−0.8 (3)	C9—S1—C8—C7	25.54 (16)
N1—C4—C5—C6	−170.6 (2)	C10—N3—C9—N2	175.9 (2)
C2—C1—C5—C4	1.6 (3)	C10—N3—C9—S1	−7.2 (3)
C2—C1—C5—C6	172.0 (2)	C6—N2—C9—N3	−2.5 (3)
C9—N2—C6—O1	157.6 (2)	C7—N2—C9—N3	162.4 (2)
C7—N2—C6—O1	−6.6 (3)	C6—N2—C9—S1	−179.73 (17)
C9—N2—C6—C5	−27.3 (3)	C7—N2—C9—S1	−14.8 (2)
C7—N2—C6—C5	168.55 (18)	C8—S1—C9—N3	175.7 (2)
C4—C5—C6—O1	135.5 (2)	C8—S1—C9—N2	−7.10 (17)
C1—C5—C6—O1	−34.3 (3)	C9—N3—C10—N4	−178 (2)
C4—C5—C6—N2	−39.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···N4^{i}	0.93	2.52	3.383 (3)	154
C8—H8*B*···N1^{ii}	0.97	2.55	3.481 (3)	162

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