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1,3-Thiazole-4-carbonitrile

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Keywords: crystal structure; thiazole; nitrile group; hydrogen bonding; π–π stacking interaction.

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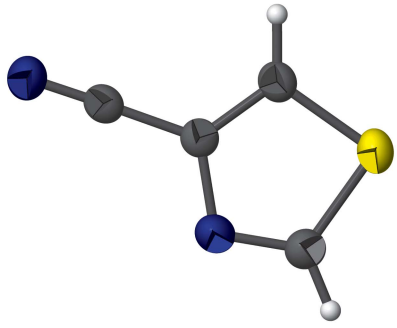
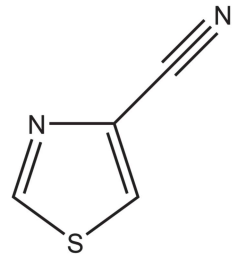
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_4H_2N_2S$, is a 1,3-thiazole substituted in the 4-position by a nitrile group. In the crystal, C—H···N hydrogen bonds and aromatic π–π stacking interactions are observed.

3D view



Chemical scheme



Structure description

The title compound, $C_4H_2N_2S$, consists of a 1,3-thiazole ring substituted in the 4-position by a nitrile group (Fig. 1). The whole molecule is nearly planar with a mean deviation from the best plane defined by all non-hydrogen atoms of 0.005 Å. All bond lengths are in the expected ranges (Allen *et al.*, 1987).

In the crystal, weak C—H···N hydrogen bonds arising from both C—H groupings build up a wavy layer of molecules in the (011) plane (Table 1, Fig. 2). The layers are stacked in the (100) direction by weak π–π stacking interactions between the 1,3-thiazole rings [centroid–centroid distance = 3.7924 (10) Å, ring slippage = 1.39 Å].

Synthesis and crystallization

Commercial powder of the title compound (Fluorochem, UK, catalogue No. # 076318) was purified by sublimation at normal pressure on a hot plate set to 55°C. The colourless crystals formed over two days on the covering watch glass. ^{1}H NMR (300.2 MHz, DMSO-d_6) δ 9.316, 9.310 (J = 1.82 Hz, H3), 8.908, 8.902 (J = 1.84 Hz, H2). ^{13}C NMR (75.5 MHz, DMSO-d_6) δ 157.4, 133.6, 125.9, 114.5. The NMR data are consistent with those previously published by Augustine *et al.* (2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

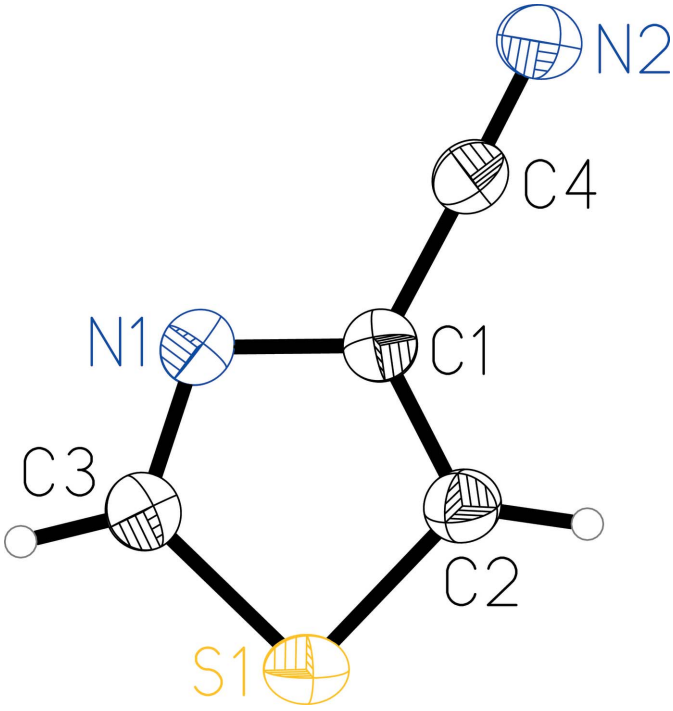


Figure 1
Molecular structure of the title compound with atom labelling and displacement ellipsoids drawn at 50% probability level.

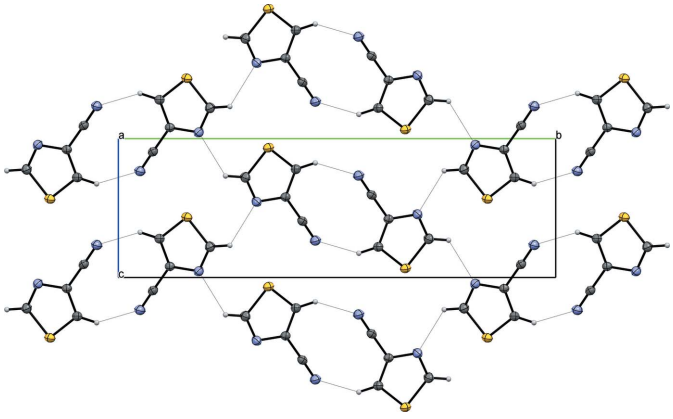


Figure 2
Packing diagram for the title compound along the *a* axis. Ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dotted lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N2^{i}	0.95	2.59	3.374 (2)	140
C3—H3···N1^{ii}	0.95	2.57	3.257 (2)	129

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_4H_2N_2S$
M_r	110.14
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	3.7924 (3), 19.8932 (18), 6.3155 (5)
β (°)	91.084 (6)
V (Å^3)	476.37 (7)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.77
Crystal size (mm)	0.24 × 0.18 × 0.08
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.40, 0.71
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4709, 854, 783
R_{int}	0.040
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.097, 1.09
No. of reflections	854
No. of parameters	64
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.23

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015), *XP* in *SHELXTL* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2021). **6**, x211332 [https://doi.org/10.1107/S2414314621013328]

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Crystal data

$C_4H_2N_2S$
M_r = 110.14
Monoclinic, $P2_1/n$
a = 3.7924 (3) Å
b = 19.8932 (18) Å
c = 6.3155 (5) Å
β = 91.084 (6)°
V = 476.37 (7) Å^3
Z = 4
$F(000)$ = 224
D_x = 1.536 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 2588 reflections
θ = 4.5–66.7°
μ = 4.77 mm^{-1}
T = 150 K
Plate, colourless
0.24 × 0.18 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: microfocus
Multilayer monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.40, T_{max} = 0.71
4709 measured reflections
854 independent reflections
783 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 66.7°, θ_{min} = 4.5°
h = −4→4
k = −23→23
l = −7→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.097
S = 1.09
854 reflections
64 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 0.0618P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8382 (4)	0.61784 (9)	0.5796 (3)	0.0306 (4)
C2	0.8897 (5)	0.59416 (9)	0.7795 (3)	0.0360 (4)
H2	0.838664	0.549800	0.825466	0.043*
C3	1.0479 (5)	0.70963 (10)	0.7216 (3)	0.0388 (5)
H3	1.124522	0.755015	0.731394	0.047*
C4	0.6933 (5)	0.57919 (9)	0.4057 (3)	0.0350 (4)
N1	0.9271 (4)	0.68396 (9)	0.5450 (3)	0.0400 (4)
N2	0.5794 (5)	0.54939 (9)	0.2660 (3)	0.0450 (4)
S1	1.06029 (11)	0.65664 (2)	0.93452 (7)	0.0367 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0280 (7)	0.0334 (9)	0.0306 (9)	0.0004 (7)	0.0030 (6)	0.0000 (6)
C2	0.0424 (10)	0.0352 (9)	0.0304 (9)	0.0020 (7)	0.0011 (7)	0.0000 (7)
C3	0.0400 (9)	0.0378 (9)	0.0383 (11)	−0.0060 (7)	−0.0022 (8)	0.0015 (7)
C4	0.0381 (9)	0.0364 (9)	0.0305 (9)	−0.0020 (7)	0.0040 (7)	0.0031 (7)
N1	0.0480 (10)	0.0372 (10)	0.0346 (9)	−0.0069 (6)	−0.0029 (7)	0.0049 (6)
N2	0.0559 (10)	0.0455 (9)	0.0336 (9)	−0.0102 (8)	0.0000 (7)	−0.0022 (7)
S1	0.0380 (3)	0.0426 (3)	0.0294 (3)	0.00213 (16)	−0.0020 (2)	−0.00236 (15)

Geometric parameters (Å, º)

C1—C2	1.358 (3)	C3—N1	1.302 (3)
C1—N1	1.376 (3)	C3—S1	1.7089 (19)
C1—C4	1.441 (3)	C3—H3	0.9500
C2—S1	1.7024 (19)	C4—N2	1.141 (3)
C2—H2	0.9500		
C2—C1—N1	116.58 (16)	N1—C3—S1	115.85 (15)
C2—C1—C4	124.71 (17)	N1—C3—H3	122.1
N1—C1—C4	118.70 (16)	S1—C3—H3	122.1
C1—C2—S1	109.13 (14)	N2—C4—C1	178.96 (19)
C1—C2—H2	125.4	C3—N1—C1	108.81 (16)
S1—C2—H2	125.4	C2—S1—C3	89.62 (9)
N1—C1—C2—S1	−0.4 (2)	C4—C1—N1—C3	179.24 (16)
C4—C1—C2—S1	−179.26 (14)	C1—C2—S1—C3	0.28 (15)
S1—C3—N1—C1	−0.1 (2)	N1—C3—S1—C2	−0.12 (16)
C2—C1—N1—C3	0.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···N2^{i}	0.95	2.59	3.374 (2)	140

C3—H3···N1^{ii}	0.95	2.57	3.257 (2)	129

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