Crystal structure of 1-(thiazolo[5,4-*b*]pyridin-2-yl)hydrazine, $C_6H_6N_4S$

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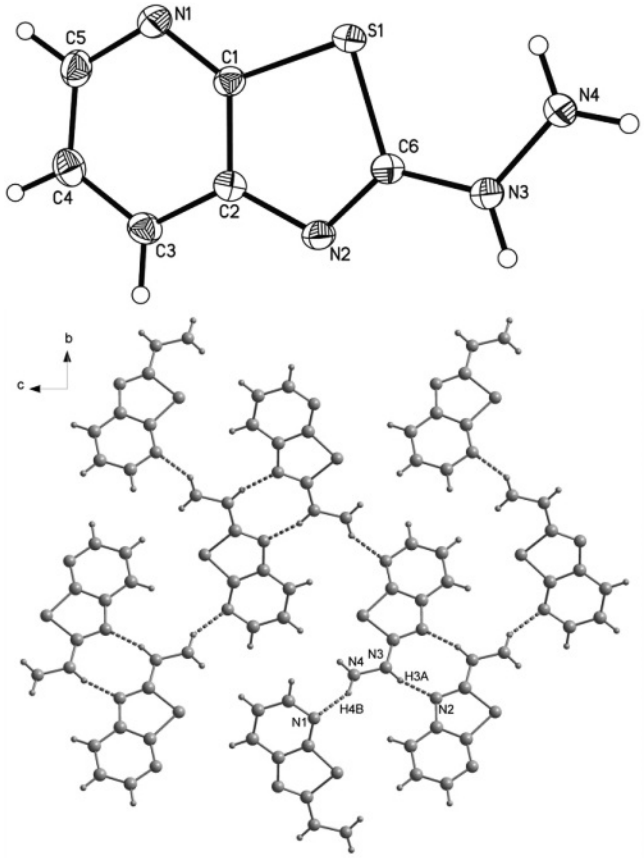

Abstract

$C_6H_6N_4S$, monoclinic, $P2_1/c$ (no. 14), a = 3.885(2) Å, b = 13.423(8) Å, c = 13.634(8) Å, β = 98.017(6)°, V = 704.1 Å^3, Z = 4, $R_{gt}(F)$ = 0.0376, $wR_{ref}(F^2)$ = 0.1127, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.17×0.22×0.38 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	3.88 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	50.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5287, 1313
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1157
$N(param)_{refined}$:	100
Programs:	SHELX [14]

Source of material

The title compound was obtained according to the literature method [13]. Single crystals suitable for X-ray diffraction were obtained by crystallization from methanol.

Experimental details

The hydrogen atoms were assigned with common isotropic displacement factors U_{iso}(H) = 1.2 times U_{eq}(C,N), and included in the final refinement by using geometrical restraints, with C–H = 0.93 Å and N–H = 0.86 Å.

Discussion

The thiazole ring has been found in many natural compounds that have useful biological activities [1-3]. Thiazoles and their derivatives have been demonstrated to possess a wide range of exercise physiology and pharmaceutical activities such as antitumor [4], anticonvulsant [5], antiviral [6], antibacterial [7], antimicrobial [8], and fungicidal activities [9]. On the other hand, hydrogen bonds play an important role in crystal engineering [10] and in the biological system [11]. Taking these results into account, we report the synthesis and crystal structure of the title compound in this paper. A view of the molecular structure of the title compound is given in Fig. top. The asymmetric unit contains one molecule of the title compound, which is constructed by the pyridine-thiazole moiety, and the hydrazine moiety. The whole molecule is almost planar with the maximum deviation of 0.0742(6) Å for S1. The C1–N1, C5–N1, C6–N2, and C6–N3 bond lengths are 1.329(3) Å, 1.348(3) Å, 1.312(3) Å, and 1.332(3) Å, respectively. The C1–S1 and C6–S1 bond lengths of 1.754(2) Å and 1.762(2) Å are intermediate between the double and single bonds. The shortening of the C–S bonds showing the partial double-bond character of the C–S bonds, which is agrees with the literature data [12]. The crystal packing of the title compound exhibits intermolecule N–H···N hydrogen bonds. The molecules of the title compound form centrosymmetric hydrogen-bonded dimers through a pair of N3–H3A···N2^{i} hydrogen bonds: d(H3A···N2) = 2.12 Å, d(N3···N2) = 2.925(3) Å, and ∠N3–H3A···N2 = 156.2° (symmetry code **i**: $-x+1, -y+1, -z$). The dimers are further connected into two-dimensional nets through N4–H4B...N1^{ii} hydrogen bonds: d(H4B···N1) = 2.43 Å, d(N4···N1) = 3.170(3) Å, and ∠N4–H4B···N1 = 144.4° (symmetry code **ii**: $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$), as shown in Fig. bottom.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(3)	4*e*	–0.0275	0.7396	–0.1220	0.044
H(4)	4*e*	–0.2689	0.8941	–0.0931	0.048
H(5)	4*e*	–0.3065	0.9440	0.0651	0.049
H(3A)	4*e*	0.4992	0.4471	0.0911	0.048
H(4A)	4*e*	0.5013	0.5055	0.2820	0.051
H(4B)	4*e*	0.6389	0.4075	0.2541	0.051

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	4*e*	0.0381(5)	0.7392(2)	0.1177(2)	0.028(1)	0.030(1)	0.029(1)	–0.0016(9)	0.0037(9)	–0.0027(9)
C(2)	4*e*	0.0784(6)	0.7021(2)	0.0235(2)	0.030(1)	0.029(1)	0.029(1)	–0.0035(9)	0.0053(9)	–0.0007(9)
C(3)	4*e*	–0.0429(6)	0.7610(2)	–0.0579(2)	0.043(1)	0.039(1)	0.028(1)	–0.001(1)	0.007(1)	0.003(1)
C(4)	4*e*	–0.1874(7)	0.8526(2)	–0.0404(2)	0.043(1)	0.035(1)	0.041(1)	0.000(1)	0.001(1)	0.009(1)
C(5)	4*e*	–0.2103(7)	0.8819(2)	0.0556(2)	0.042(1)	0.031(1)	0.048(2)	0.006(1)	0.002(1)	–0.000(1)
C(6)	4*e*	0.3109(6)	0.5762(2)	0.1132(2)	0.032(1)	0.028(1)	0.027(1)	–0.0018(9)	0.0062(9)	–0.0021(9)
N(1)	4*e*	–0.1022(5)	0.8263(2)	0.1364(2)	0.042(1)	0.032(1)	0.037(1)	0.0039(9)	0.0049(9)	–0.0041(9)
N(2)	4*e*	0.2356(5)	0.6097(2)	0.0224(1)	0.042(1)	0.031(1)	0.026(1)	0.0029(8)	0.0072(8)	–0.0014(8)
N(3)	4*e*	0.4579(6)	0.4881(2)	0.1365(2)	0.059(1)	0.034(1)	0.027(1)	0.011(1)	0.0060(9)	–0.0010(8)
N(4)	4*e*	0.5438(6)	0.4639(2)	0.2372(2)	0.064(1)	0.037(1)	0.028(1)	0.013(1)	0.007(1)	0.0041(9)
S(1)	4*e*	0.2034(2)	0.65320(4)	0.20908(4)	0.0410(4)	0.0359(4)	0.0230(3)	0.0050(2)	0.0057(2)	–0.0015(2)

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