Crystal structure of 1-(propan-2-ylidene)-2-(thiazolo[5,4-*b*]pyridin-2-yl)-hydrazine, $C_9H_{10}N_4S$

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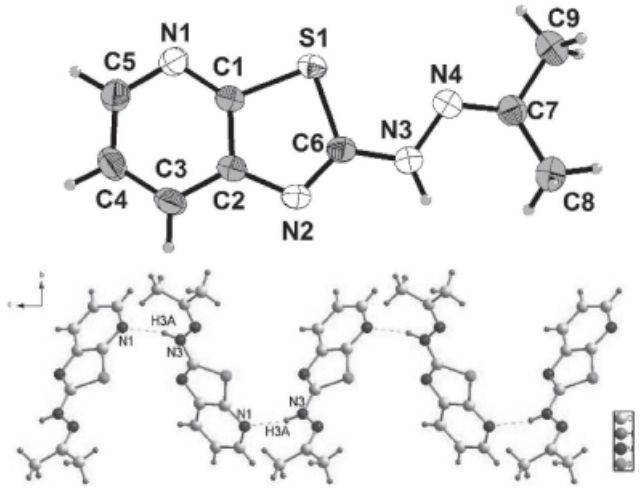

Abstract

$C_9H_{10}N_4S$, monoclinic, $P2_1/c$ (no. 14), a = 13.076(3) Å, b = 6.654(2) Å, c = 11.230(3) Å, β = 92.740(3)°, V = 976.0 Å^3, Z = 4, $R_{gt}(F)$ = 0.0330, $wR_{ref}(F^2)$ = 0.0876, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.21×0.32×0.36 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.95 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6919, 1801
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1546
$N(param)_{refined}$:	129
Programs:	SHELX [15]

Source of material

The title compound was obtained from 2-amin-3-chloropyridine according to the literature method [14]. Single crystals suitable for X-ray diffraction were obtained by crystallization of the title compound from methanol.

Experimental details

All of the non-hydrogen atoms were refined anisotropically. The hydrogen atoms were assigned with common isotropic displacement factors U_{iso}(H) = 1.2U_{eq} (N and pyridine C), or U_{iso}(H) = 1.5U_{eq} (methyl C) and included in the final refinement by using geometrical restraints, with C–H = 0.93 Å (pyridine) or C–H = 0.96 Å (methyl), and N–H = 0.86 Å.

Discussion

Hydrazones are an emerging class of materials, which have been demonstrated to possess a wide range of biological and pharmaceutical activities such as antimicrobial [1], anti-convulsant [2], antifungal [3], anticancer [4], antitubercular [5], antiviral [6], antibacterial [7], and antioxidant [8] activities. Meanwhile, hydrazones have also interesting properties because of the presence of several coordination sites, and thus their metal complexes are important for their possible biological applications [9]. The thiazole ring is present in various biologically active molecules. Thiazoles and their derivatives possess activities such as antitumor [10], antiviral [11], and antibacterial [12]. In this paper we report the synthesis and crystal structure of a novel thiazole-hyrazone compound. The asymmetric unit contains one molecule of the title compound, which is constructed by the pyridine-thiazole moiety, the hydrazone linker, and the bimethyl moiety. The C(6)–N(3), N(3)–N(4), and C(7)–N(4) bond lengths are 1.353(2) Å, 1.387(2) Å, and 1.278(2) Å, respectively, which is observed in similar compound [13]. The C(1)–S(1) and C(6)–S(1) bond lengths of 1.749(1) Å and 1.762(2) Å are shorter than the expected single bond value, showing some double bond character. The C(1)–S(1)–C(6) angle is 87.31(7)°, which is smaller than in simple thiazoles. All non-hydrogen atoms are almost planar in the title structure with a maxium deviation of 0.117(2) Å for C(9). In the crystal structure, adjacent molecules are linked by intermolecular N(3)–H(3A)···N(1)^{i} hydrogen bond into one-dimensional chains along the c axis (Fig. bottom).The distance of H(3A)···N(1) is 2.15 Å, the distance of N(3)···N(1) is 2.987(2) Å, and the angle of N(3)–H(3A)···N(1) is 165.3°, symmetry code **i**: x, -y+$\frac{1}{2}$, z+$\frac{1}{2}$.

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

Atom	Site	x	y	z	U_{iso}
H(3)	4*e*	0.0177	–0.0792	0.7195	0.052
H(4)	4*e*	0.0061	–0.3393	0.5821	0.058
H(5)	4*e*	0.1097	–0.3447	0.4235	0.057
H(8A)	4*e*	0.2991	0.9335	0.7985	0.093
H(8B)	4*e*	0.4154	0.9461	0.8384	0.093
H(8C)	4*e*	0.3503	0.7598	0.8745	0.093
H(9A)	4*e*	0.4838	0.7567	0.5654	0.086
H(9B)	4*e*	0.5340	0.8448	0.6838	0.086
H(9C)	4*e*	0.4543	0.9728	0.6076	0.086
H(3A)	4*e*	0.2466	0.5522	0.7845	0.050

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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*	0.1900(1)	0.0532(2)	0.5372(1)	0.0338(8)	0.0348(9)	0.0335(8)	0.0021(7)	0.0052(6)	0.0034(7)
C(2)	4*e*	0.1321(1)	0.0674(2)	0.6390(1)	0.0327(8)	0.0395(9)	0.0328(8)	0.0003(7)	0.0036(6)	0.0039(7)
C(3)	4*e*	0.0599(1)	–0.0825(3)	0.6552(2)	0.043(1)	0.052(1)	0.0360(9)	–0.0083(8)	0.0070(7)	0.0076(8)
C(4)	4*e*	0.0530(2)	–0.2360(3)	0.5729(2)	0.054(1)	0.044(1)	0.046(1)	–0.0152(8)	–0.0012(8)	0.0085(8)
C(5)	4*e*	0.1153(2)	–0.2375(3)	0.4766(2)	0.060(1)	0.039(1)	0.042(1)	–0.0068(8)	–0.0002(8)	–0.0008(8)
C(6)	4*e*	0.2258(1)	0.3377(2)	0.6673(1)	0.0334(8)	0.0376(9)	0.0346(8)	0.0029(7)	0.0058(6)	0.0010(7)
C(7)	4*e*	0.3876(1)	0.7525(2)	0.7019(2)	0.0417(9)	0.0362(9)	0.0417(9)	0.0007(7)	0.0003(7)	0.0045(7)
C(8)	4*e*	0.3607(2)	0.8573(3)	0.8132(2)	0.073(1)	0.052(1)	0.061(1)	–0.016(1)	0.013(1)	–0.013(1)
C(9)	4*e*	0.4725(2)	0.8395(3)	0.6336(2)	0.056(1)	0.053(1)	0.062(1)	–0.013(1)	0.010(1)	0.003(1)
N(1)	4*e*	0.1833(1)	–0.0926(2)	0.4558(1)	0.0493(9)	0.0378(8)	0.0365(7)	–0.0003(6)	0.0058(6)	–0.0016(6)
N(2)	4*e*	0.1536(1)	0.2316(2)	0.7123(1)	0.0384(8)	0.0437(8)	0.0342(7)	–0.0036(6)	0.0104(6)	–0.0030(6)
N(3)	4*e*	0.2672(1)	0.5047(2)	0.7187(1)	0.0452(8)	0.0419(8)	0.0396(8)	–0.0068(7)	0.0109(6)	–0.0065(6)
N(4)	4*e*	0.3453(1)	0.5941(2)	0.6581(1)	0.0406(8)	0.0412(8)	0.0393(8)	–0.0037(6)	0.0065(6)	0.0012(6)
S(1)	4*e*	0.27408(3)	0.25702(6)	0.53161(4)	0.0429(3)	0.0406(3)	0.0392(3)	–0.0059(2)	0.0165(2)	–0.0023(2)

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