Crystal structure of 1-(*p*-methyl benzylidene)-2-(thiazolo[5,4-*b*]pyridin-2-yl)hydrazine, $C_{14}H_{12}N_4S$

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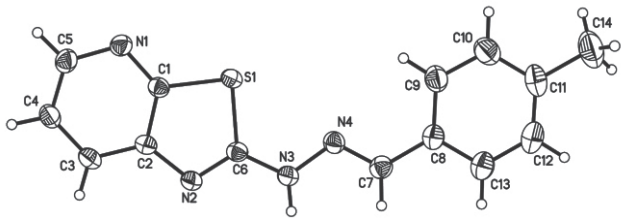
Received December 11, 2014, accepted June 01, 2015, available online June 09, 2015, CCDC no. 1267/4319



Abstract

$C_{14}H_{12}N_4S$, monoclinic, $P2_1/c$ (no. 14), a = 17.119(5) Å, b = 6.813(2) Å, c = 11.505(3) Å, β = 98.947(4)°, V = 1325.5 Å^3, Z = 4, $R_{gt}(F)$ = 0.0469, $wR_{ref}(F^2)$ = 0.1189, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.17×0.21×0.29 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.35 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9535, 2465
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1676
$N(param)_{refined}$:	173
Programs:	SHELX [14]

Source of material

The title compound was obtained according to the literature method [12]. 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) = 1.2 times U_{eq}(N and aromatic ring C), or U_{iso}(H) = 1.5 times U_{eq}(methyl C) and included in the final refinement by using geometrical restraints, with C–H = 0.93 Å (aromatic ring) or C–H = 0.96 Å (methyl), 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], antimicro-bial [8], and fungicidal activities [9]. On the other hand, hydrogen bonds play an important role in crystal engineering [10] and in biological system [11]. Therefore, we report on the synthesis and crystal structure of the title compound as part of our continuing interest in these systems [12, 13]. A view of the molecular structure of the title compound is given in the figure. The independent part of the unit cell contains one molecule of the title compound, which is constructed by the pyridine-thiazole moiety, the hydrazone linker, and the *p*-methyl benzaldehyde moiety. All non-hydrogen atoms of the title compound are almost planar with the maximum deviation is 0.1080(7) Å for C5. The C6–N3, N3–N4, and C7–N4 bond lengths are 1.343(3) Å, 1.366(3) Å, and 1.280(3) Å, respectively. The C1–S1 and C6–S1 bond lengths of 1.744(3) Å and 1.750(3) Å are intermediate between the double and single bonds. The crystal packing of the title compound exhibits intermolecule N–H···N hydrogen bonds. Adjacent molecules are linked by the N3–H3A···N1^{i} hydrogen bonds into one-dimensional chain. The distance of H3A···N1 is 2.02 Å, the distance of N3···N1 is 2.881(3) Å, and the angle of N3–H3A···N1 is 178.6°. Symmetry code i: x, $-y+\frac{3}{2}$, $z+\frac{1}{2}$.

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

Atom	Site	x	y	z	U_{iso}
H(3)	4*e*	0.0192	1.1287	0.7194	0.058
H(4)	4*e*	0.0136	1.3690	0.5768	0.063
H(5)	4*e*	0.0866	1.3397	0.4278	0.063
H(7)	4*e*	0.2392	0.2179	0.8338	0.061
H(9)	4*e*	0.3336	0.2403	0.5779	0.075
H(10)	4*e*	0.4156	0.0066	0.5190	0.090
H(12)	4*e*	0.3934	–0.3199	0.7984	0.086
H(13)	4*e*	0.3118	–0.0887	0.8605	0.074
H(14A)	4*e*	0.5207	–0.3085	0.6452	0.168
H(14B)	4*e*	0.4616	–0.3322	0.5274	0.168
H(14C)	4*e*	0.4522	–0.4631	0.6364	0.168
H(3A)	4*e*	0.1712	0.4895	0.8172	0.061

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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*	0.1372(1)	0.9476(4)	0.5534(2)	0.043(1)	0.041(2)	0.038(1)	–0.003(1)	0.007(1)	–0.005(1)
C(2)	4*e*	0.0974(1)	0.9572(4)	0.6512(2)	0.038(1)	0.044(2)	0.038(1)	–0.005(1)	0.009(1)	–0.005(1)
C(3)	4*e*	0.0488(2)	1.1175(4)	0.6585(2)	0.045(2)	0.058(2)	0.044(2)	0.006(1)	0.010(1)	–0.008(1)
C(4)	4*e*	0.0454(2)	1.2590(4)	0.5734(2)	0.058(2)	0.053(2)	0.046(2)	0.015(2)	0.004(1)	–0.008(1)
C(5)	4*e*	0.0888(2)	1.2392(4)	0.4829(2)	0.066(2)	0.047(2)	0.042(2)	0.004(2)	–0.001(1)	0.001(1)
C(6)	4*e*	0.1600(2)	0.6798(4)	0.6915(2)	0.045(2)	0.039(2)	0.040(2)	–0.006(1)	0.012(1)	–0.002(1)
C(7)	4*e*	0.2591(2)	0.2416(4)	0.7644(2)	0.056(2)	0.046(2)	0.052(2)	–0.004(1)	0.008(1)	0.001(1)
C(8)	4*e*	0.3130(2)	0.1013(4)	0.7259(3)	0.048(2)	0.043(2)	0.057(2)	–0.002(1)	0.002(1)	–0.002(1)
C(9)	4*e*	0.3453(2)	0.1277(5)	0.6230(3)	0.062(2)	0.052(2)	0.075(2)	0.006(2)	0.018(2)	0.002(2)
C(10)	4*e*	0.3945(2)	–0.0128(5)	0.5879(3)	0.068(2)	0.078(2)	0.083(2)	0.008(2)	0.024(2)	–0.002(2)
C(11)	4*e*	0.4133(2)	–0.1823(5)	0.6526(3)	0.054(2)	0.062(2)	0.092(3)	0.012(2)	–0.000(2)	–0.012(2)
C(12)	4*e*	0.3815(2)	–0.2069(5)	0.7539(3)	0.070(2)	0.055(2)	0.083(3)	0.008(2)	–0.011(2)	0.003(2)
C(13)	4*e*	0.3323(2)	–0.0685(4)	0.7912(3)	0.060(2)	0.051(2)	0.070(2)	–0.002(2)	–0.001(2)	0.001(2)
C(14)	4*e*	0.4668(2)	–0.3355(6)	0.6116(4)	0.103(3)	0.103(3)	0.129(4)	0.044(3)	0.016(3)	–0.014(3)
N(1)	4*e*	0.1342(1)	1.0822(3)	0.4701(2)	0.058(1)	0.044(1)	0.039(1)	–0.002(1)	0.008(1)	–0.001(1)
N(2)	4*e*	0.1116(1)	0.8027(3)	0.7296(2)	0.049(1)	0.046(1)	0.044(1)	0.002(1)	0.017(1)	0.001(1)
N(3)	4*e*	0.1865(1)	0.5175(3)	0.7514(2)	0.066(2)	0.044(1)	0.047(1)	0.006(1)	0.023(1)	0.003(1)
N(4)	4*e*	0.2380(1)	0.3976(3)	0.7058(2)	0.053(1)	0.040(1)	0.051(1)	–0.001(1)	0.012(1)	–0.002(1)
S(1)	4*e*	0.19176(4)	0.7310(1)	0.55728(6)	0.0554(4)	0.0440(4)	0.0434(4)	0.0033(3)	0.0203(3)	–0.0014(3)

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