Crystal structure of 2-(methylthio)thiazolo[5,4-*b*]pyridine, $C_7H_6N_2S_2$

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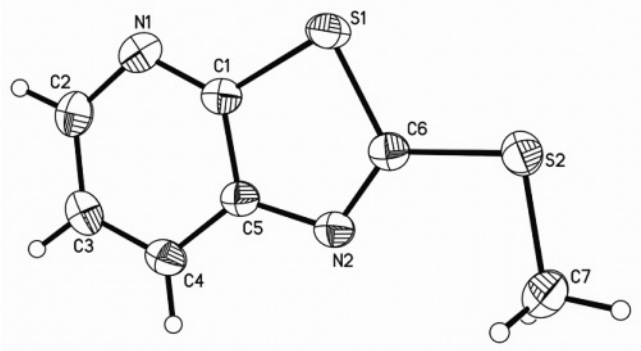

Abstract

$C_7H_6N_2S_2$, orthorhombic, $P2_12_12_1$ (no. 19), a = 4.9698(13) Å, b = 10.634(3) Å, c = 15.259(4) Å, V = 806.4 Å^3, Z = 4, $R_{gt}(F)$ = 0.0256, $wR_{ref}(F^2)$ = 0.0597, T = 296 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.17×0.21×0.26 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	5.89 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6001, 1493
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1383
$N(param)_{refined}$:	101
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, aromatic ring), and U_{iso}(H) = 1.5 times U_{eq}(C, methyl). The final refinement by using geometrical restraints, with C–H = 0.93 Å (aromatic ring), and C–H = 0.96 Å (methyl).

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, weak hydrogen bonds from C–H groups have received great attention in recent years since these 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 a new thiazole in this paper. A view of the molecular structure of the title compound is given in the figure. The asymmetric unit contains one molecule of the title compound, which is constructed by the pyridine-thiazole moiety, and the methylsulfide group. All non hydrogen atoms of the title compound are almost planar with a maximum deviation of 0.0739(3) Å for C7. The C1–S1, C6–S1, and C6–S2 bond lengths are 1.744(2) Å, 1.760(2) Å, and 1.741(2) Å, respectively. The values are intermediate between the double and single bonds. The shortening of these C–S bonds showing the partial double–bond character of the C–S bonds, which is agrees with the literature data [12]. The C7–S2 bond length is 1.790(3) Å, which is close to the expected single bond value of 1.82 Å.

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

Atom	Site	x	y	z	U_{iso}
H(2)	4*e*	–0.3834	–0.7760	–0.7827	0.068
H(3)	4*e*	–0.3958	–0.6736	–0.6510	0.066
H(4)	4*e*	–0.6761	–0.7431	–0.5405	0.061
H(7A)	4*e*	–1.4549	–0.9781	–0.4470	0.106
H(7B)	4*e*	–1.2331	–1.0670	–0.4083	0.106
H(7C)	4*e*	–1.5362	–1.1076	–0.4057	0.106

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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*	–0.8115(4)	–0.9430(2)	–0.6937(1)	0.039(1)	0.044(1)	0.042(1)	0.0072(9)	–0.0068(9)	–0.003(1)
C(2)	4*e*	–0.5005(6)	–0.8054(2)	–0.7398(2)	0.050(1)	0.061(1)	0.059(1)	–0.001(1)	0.003(1)	0.010(1)
C(3)	4*e*	–0.5055(5)	–0.7433(2)	–0.6600(2)	0.051(1)	0.045(1)	0.070(1)	–0.004(1)	–0.006(1)	0.005(1)
C(4)	4*e*	–0.6707(5)	–0.7840(2)	–0.5943(2)	0.055(1)	0.045(1)	0.051(1)	0.001(1)	–0.007(1)	–0.008(1)
C(5)	4*e*	–0.8307(4)	–0.8887(2)	–0.6107(1)	0.040(1)	0.040(1)	0.041(1)	0.0072(9)	–0.0031(9)	–0.0021(8)
C(6)	4*e*	–1.1247(4)	–1.0398(2)	–0.5910(1)	0.040(1)	0.041(1)	0.046(1)	0.0086(9)	–0.0010(9)	–0.0020(9)
C(7)	4*e*	–1.4015(6)	–1.0641(3)	–0.4391(2)	0.078(2)	0.080(2)	0.053(1)	–0.012(2)	0.012(1)	0.001(1)
N(1)	4*e*	–0.6543(4)	–0.9053(2)	–0.7589(1)	0.051(1)	0.065(1)	0.046(1)	0.004(1)	0.0012(9)	–0.0006(9)
N(2)	4*e*	–1.0101(3)	–0.9452(2)	–0.5536(1)	0.049(1)	0.0437(9)	0.0427(9)	0.0031(9)	0.0001(9)	–0.0055(7)
S(1)	4*e*	–1.0310(1)	–1.07066(5)	–0.70011(4)	0.0516(3)	0.0533(3)	0.0479(3)	–0.0037(3)	0.0003(3)	–0.0145(2)
S(2)	4*e*	–1.3648(1)	–1.13798(5)	–0.54388(4)	0.0548(3)	0.0495(3)	0.0586(3)	–0.0048(3)	0.0034(3)	–0.0005(3)

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