Crystal structure of 1-(diphenylmethylene)-2-(thiazolo[4,5-*b*]pyridin-2(3*H*)-ylidene)hydrazine, $C_{19}H_{14}N_4S$

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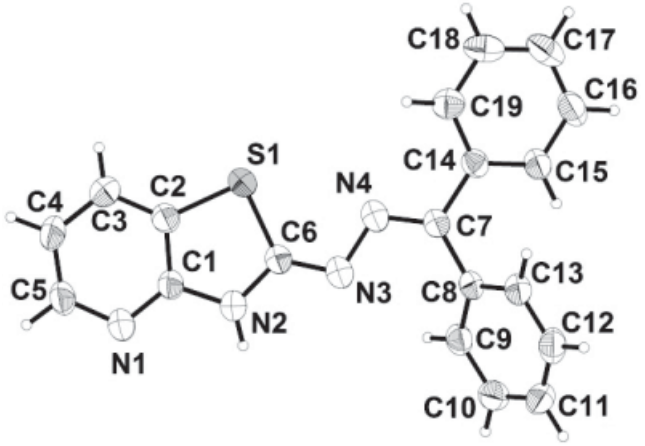

Abstract

$C_{19}H_{14}N_4S$, monoclinic, *C*2/*c* (no. 15), $a = 35.98(1)$ Å, $b = 5.671(2)$ Å, $c = 17.658(7)$ Å, $\beta = 115.608(4)°$, $V = 3249$ Å^3, $Z = 8$, $R_{gt}(F) = 0.0403$, $wR_{ref}(F^2) = 0.1462$, $T = 296$ K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.32×0.43×0.50 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.06 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8142, 2985
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2233
$N(param)_{refined}$:	217
Programs:	SHELX [13]

Source of material

The title compound was obtained from 2-amino-3-chloropyridine according to the literature method [12]. 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

Hydrazones are an emerging class of materials, which have been demonstrated to possess a wide range of exercise physiology and pharmaceutical activities such as fatigue resistance [1], anticonvulsant [2], antioxidant [3], antimicrobial [4], antifungal [5], anticancer [6], antitubercular [7], antiviral [8], and antibacterial [9] activities. Meanwhile, hydrazones have also interesting ligation properties because of the presence of several coordination sites, and thus their metal complexes are important for their possible biological applications [10]. The asymmetric unit contains one molecule of the title compound, which is constructed by the pyridine-dihydrothiazole moiety, the hydrazone linker, and the biaryl moiety. The C6–N3 and C7–N4 bond length of 1.295(3) Å and 1.297(3) Å, conform to the value for a double bond, while the C6–N2 bond length of 1.350(3) Å conforms to the value for a single bond. The C2–S1 and C6–S1 bond lengths of 1.758(2) Å and 1.773(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 agrees with the literature [11]. The pyridine-dihydrothiazole fragment (P1) is almost planar with the maximum deviation of 0.050(2) Å for C6. Furthermore, the atoms N3, N4, C7 are almost coplanar with P1 with the deviations 0.083(2) Å, 0.035(2) Å, 0.102(2) Å, respectively. The phenyl rings C8-C13 (P2) and C14-C19 (P3) are not coplanar with P1. The dihedral angles P1/P2, P1/P3, and P2/P3 are 47.388(5)°, 20.873(5)°, and 67.334(6)°, respectively. The molecules of the title compound form centrosymmetric hydrogen-bonded dimers through a pair of N2–H2···N1^{i} hydrogen bonds: d(H2···N1) = 2.00 Å, d(N2···N1) = 2.855(3) Å, and ∠N2–H2···N1 = 173.2° (symmetry code i: $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$).

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

Atom	Site	x	y	z	U_{iso}
H(3)	8*f*	0.3042	0.9848	0.1993	0.069
H(4)	8*f*	0.3503	0.9129	0.1413	0.071
H(5)	8*f*	0.3396	0.6034	0.0518	0.065
H(9)	8*f*	0.1305	–0.0095	0.0635	0.054
H(10)	8*f*	0.0884	–0.2619	–0.0409	0.068
H(11)	8*f*	0.0202	–0.1709	–0.1207	0.070
H(12)	8*f*	–0.0066	0.1786	–0.0978	0.067
H(13)	8*f*	0.0354	0.4315	0.0068	0.055
H(15)	8*f*	0.0594	0.2210	0.1623	0.057
H(16)	8*f*	0.0373	0.3412	0.2602	0.069
H(17)	8*f*	0.0592	0.6982	0.3284	0.076
H(18)	8*f*	0.1028	0.9319	0.2971	0.073
H(19)	8*f*	0.1264	0.8105	0.2011	0.059
H(2)	8*f*	0.2207	0.2819	0.0297	0.060

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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)	8*f*	0.26176(6)	0.5324(4)	0.0826(1)	0.033(1)	0.051(1)	0.043(1)	–0.0041(9)	0.0167(9)	–0.003(1)
C(2)	8*f*	0.26631(7)	0.7151(4)	0.1390(1)	0.039(1)	0.058(1)	0.041(1)	–0.003(1)	0.018(1)	–0.005(1)
C(3)	8*f*	0.29996(7)	0.8608(5)	0.1620(2)	0.049(1)	0.068(2)	0.053(1)	–0.014(1)	0.021(1)	–0.017(1)
C(4)	8*f*	0.32734(7)	0.8167(5)	0.1278(2)	0.038(1)	0.080(2)	0.060(2)	–0.019(1)	0.021(1)	–0.013(1)
C(5)	8*f*	0.32057(7)	0.6302(5)	0.0736(2)	0.034(1)	0.079(2)	0.053(1)	–0.007(1)	0.022(1)	–0.007(1)
C(6)	8*f*	0.20208(6)	0.4777(4)	0.0975(1)	0.038(1)	0.053(1)	0.046(1)	–0.003(1)	0.021(1)	–0.006(1)
C(7)	8*f*	0.11288(6)	0.4065(3)	0.1146(1)	0.037(1)	0.042(1)	0.043(1)	0.0004(9)	0.021(1)	0.0011(9)
C(8)	8*f*	0.08716(6)	0.2402(4)	0.0463(1)	0.039(1)	0.044(1)	0.042(1)	–0.0051(9)	0.024(1)	0.0004(9)
C(9)	8*f*	0.10297(7)	0.0292(4)	0.0313(1)	0.045(1)	0.045(1)	0.055(1)	–0.003(1)	0.029(1)	0.002(1)
C(10)	8*f*	0.07771(8)	–0.1220(4)	–0.0312(2)	0.071(2)	0.047(1)	0.069(2)	–0.013(1)	0.046(2)	–0.011(1)
C(11)	8*f*	0.03693(8)	–0.0675(5)	–0.0790(2)	0.060(2)	0.066(2)	0.055(2)	–0.026(1)	0.030(1)	–0.016(1)
C(12)	8*f*	0.02093(7)	0.1403(5)	–0.0653(2)	0.043(1)	0.075(2)	0.051(1)	–0.013(1)	0.022(1)	0.001(1)
C(13)	8*f*	0.04627(7)	0.2917(4)	–0.0026(1)	0.041(1)	0.050(1)	0.050(1)	–0.003(1)	0.024(1)	0.000(1)
C(14)	8*f*	0.09562(6)	0.4999(4)	0.1712(1)	0.035(1)	0.044(1)	0.040(1)	0.0041(9)	0.0166(9)	0.0010(9)
C(15)	8*f*	0.06865(7)	0.3640(4)	0.1898(1)	0.043(1)	0.055(1)	0.049(1)	–0.003(1)	0.025(1)	–0.001(1)
C(16)	8*f*	0.05516(7)	0.4361(5)	0.2482(2)	0.049(1)	0.076(2)	0.059(2)	0.001(1)	0.034(1)	0.000(1)
C(17)	8*f*	0.06815(8)	0.6490(5)	0.2888(2)	0.061(2)	0.083(2)	0.053(2)	0.022(1)	0.032(1)	–0.001(1)
C(18)	8*f*	0.09433(9)	0.7873(4)	0.2704(2)	0.078(2)	0.051(1)	0.053(2)	0.012(1)	0.028(1)	–0.008(1)
C(19)	8*f*	0.10843(7)	0.7152(4)	0.2125(1)	0.054(1)	0.042(1)	0.050(1)	0.002(1)	0.022(1)	0.002(1)
N(1)	8*f*	0.28806(5)	0.4847(3)	0.0504(1)	0.036(1)	0.060(1)	0.051(1)	–0.0063(8)	0.0233(9)	–0.0083(9)
N(2)	8*f*	0.22665(5)	0.4025(3)	0.0624(1)	0.039(1)	0.058(1)	0.060(1)	–0.0125(8)	0.0278(9)	–0.0168(9)
N(3)	8*f*	0.16657(5)	0.3826(3)	0.0801(1)	0.042(1)	0.064(1)	0.058(1)	–0.0093(9)	0.029(1)	–0.013(1)
N(4)	8*f*	0.14968(5)	0.4795(3)	0.1304(1)	0.039(1)	0.056(1)	0.051(1)	–0.0035(8)	0.0252(9)	–0.0060(9)
S(1)	8*f*	0.22463(2)	0.7192(1)	0.16588(4)	0.0463(4)	0.0652(4)	0.0528(4)	–0.0071(3)	0.0283(3)	–0.0140(3)

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