Crystal structure of *N′*-(2-thienylmethylene)-furan-2-carbohydrazide, $C_{10}H_8N_2O_2S$

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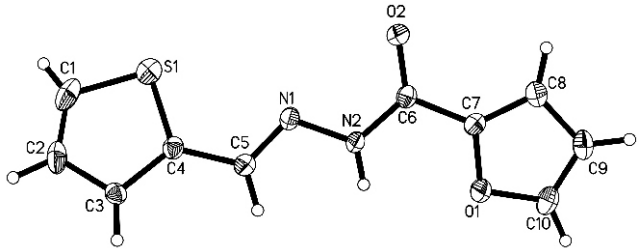

Abstract

$C_{10}H_8N_2O_2S$, orthorhombic, *Pbca* (no. 61), a = 11.9394(5) Å, b = 7.6572(3) Å, c = 22.4747(9) Å, V = 2054.7 Å^3, Z = 8, $R_{gt}(F)$ = 0.060, $wR_{ref}(F^2)$ = 0.188, T = 293 K.

Source of material

Thienyl-2-carbaldehyde (1 mmol, 0.112 g) was dissolved in anhydrous methanol (10 ml), the mixture was stirred for several minutes at room temperature, furan-2-carbohydrazide (1 mmol 0.126 g) in methanol (5 ml) was added dropwise and stirred at room temperature for 3 h, then stirred for 4 h at 350 K and evaporated to dryness. The product was separated and recrystallized from methanol, colourless single crystals were obtained after 3 d.

Experimental details

All H atoms were positioned geometrically and refined as riding with d(C—H) = 0.93 Å (aromatic), d(N—H) = 0.86 Å, and U_{iso}(H) = 1.2 U_{eq}(C).

Discussion

The chemistry of Schiff bases has been widely investigated because of their potentials in proteins and enzymes [1,2]. As part of an investigation of physical and chemical properties, we report the crystal structure of the title compound.

The title molecule adopts an (*E*) conformation with respect to the C=N double bond with the torsion angle of -176.6(3)°. The molecule is not planar, the dihedral angle between the furan ring and the thiophene ring is 29.4(2)°. In the crystal structure, classical N–H···O hydrogen bonding is observed which helps to stabilize the molecular packing.

Table 1. Data collection and handling.

Crystal:	colourless block, size 0.23 × 0.25 × 0.27 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.94 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD area detector, ω
$2\theta_{max}$:	52.74°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5163, 2097
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1600
$N(param)_{refined}$:	140
Program:	SHELXTL [3]

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

Atom	Site	x	y	z	U_{iso}
H(2A)	8*c*	0.2674	0.3879	0.9238	0.040
H(5A)	8*c*	0.3782	0.3731	0.8479	0.041
H(3A)	8*c*	0.5261	0.3304	0.7529	0.038
H(8A)	8*c*	0.0197	0.1766	1.0542	0.055
H(9A)	8*c*	0.0283	0.4322	1.1249	0.068
H(2B)	8*c*	0.5203	0.1857	0.6560	0.062
H(10A)	8*c*	0.1552	0.6418	1.0825	0.071
H(1A)	8*c*	0.3440	0.0290	0.6440	0.071

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}
S(1)	8*c*	0.28080(8)	0.0898(1)	0.73136(4)	0.0559(6)	0.0563(6)	0.0490(6)	–0.0081(4)	0.0035(4)	–0.0117(4)
N(1)	8*c*	0.2567(2)	0.2140(3)	0.8597(1)	0.040(1)	0.034(1)	0.028(1)	–0.000(1)	0.004(1)	–0.005(1)
O(2)	8*c*	0.1110(2)	0.0792(3)	0.93900(9)	0.043(1)	0.033(1)	0.034(1)	–0.0061(9)	0.002(1)	–0.0036(9)
N(2)	8*c*	0.2337(2)	0.2933(3)	0.9136(1)	0.044(1)	0.029(1)	0.028(1)	–0.005(1)	0.007(1)	–0.007(1)
C(6)	8*c*	0.1571(2)	0.2190(4)	0.9498(1)	0.032(2)	0.031(1)	0.027(2)	0.005(1)	–0.001(1)	–0.001(1)
C(5)	8*c*	0.3377(2)	0.2819(4)	0.8310(1)	0.035(2)	0.033(2)	0.035(2)	–0.001(1)	0.002(1)	–0.004(1)
C(4)	8*c*	0.3678(3)	0.2184(4)	0.7720(1)	0.038(2)	0.028(1)	0.033(2)	0.003(1)	0.003(1)	–0.000(1)
O(1)	8*c*	0.1784(2)	0.4752(3)	1.0128(1)	0.061(2)	0.042(1)	0.044(1)	–0.012(1)	0.019(1)	–0.016(1)
C(3)	8*c*	0.4678(2)	0.2603(4)	0.7394(1)	0.032(1)	0.027(1)	0.037(1)	0.000(1)	0.005(1)	0.003(1)
C(7)	8*c*	0.1308(2)	0.3156(4)	1.0042(1)	0.037(2)	0.032(2)	0.030(2)	0.000(1)	–0.002(1)	–0.003(1)

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Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(8)	8*c*	0.0621(3)	0.2775(5)	1.0497(1)	0.054(2)	0.047(2)	0.036(2)	–0.006(2)	0.011(2)	–0.001(2)
C(1)	8*c*	0.3703(4)	0.0869(5)	0.6734(2)	0.086(3)	0.051(2)	0.033(2)	0.013(2)	–0.003(2)	–0.011(2)
C(9)	8*c*	0.0669(4)	0.4206(5)	1.0892(2)	0.065(2)	0.065(2)	0.040(2)	–0.006(2)	0.022(2)	–0.010(2)
C(2)	8*c*	0.4627(3)	0.1775(5)	0.6837(2)	0.068(2)	0.052(2)	0.036(2)	0.012(2)	0.021(2)	0.001(1)
C(10)	8*c*	0.1368(4)	0.5348(5)	1.0655(2)	0.071(3)	0.058(2)	0.048(2)	–0.005(2)	0.019(2)	–0.026(2)

References

1. Kahwa, I. A.; Selbin, I.; Hsieh, T. C. Y.; Laine, R. A.: Synthesis of homodinuclear macrocyclic complexes of lanthanides and phenolic schiff bases. Inorg. Chim. Acta, **118** (1986) 179-185.
2. Santos, M. L. P.; Bagatin, I. A.; Pereira, E. M.; Ferreira, A. M. D. C.: Redox behaviour and reactivity of some di-Schiff base copper(II) complexes towards reduced oxygen species. J. Chem. Soc. Dalton Trans. (2001) 838-844.
3. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.