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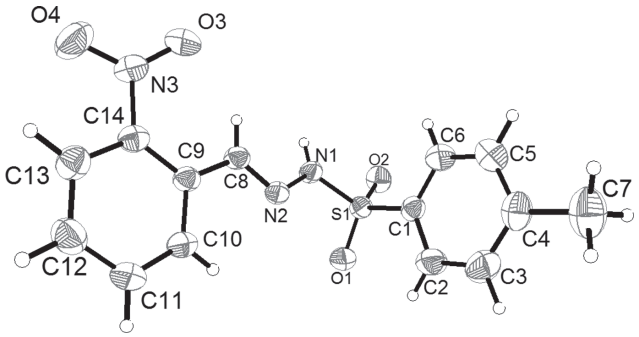
The crystal structure (*E*)-4-methyl-N′-(2-nitrobenzylidene)benzenesulfonohydrazide, $C_{14}H_{13}N_3O_4S$



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Abstract

$C_{14}H_{13}N_3O_4S$, triclinic, $P\bar{1}$ (no. 2), $a = 5.6735(11)$ Å, $b = 10.509(2)$ Å, $c = 12.180(2)$ Å, $\alpha = 93.76(3)°$, $\beta = 95.11(3)°$, $\gamma = 98.13(3)°$, $V = 713.8(2)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0446$, $wR_{ref}(F^2) = 0.1179$, $T = 293(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

The title compound was synthesized according to the literature [4]. 0.186 g (1 mmol) 4-toluenesulfonyl hydrazide was dissolved in 15 mL ethanol solution. An amount of 0.151 g (1 mmol) of 2-nitrobenzaldehyde was added to the above mentioned solution. This mixture was refluxed at 80 °C for 4 h and filtered. The resulting solution was evaporated at room temperature. Light yellow crystals of the title compound were obtained after a week.

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Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.19 × 0.18 × 0.17 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	2.5 cm^{-1}
Diffractometer, scan mode:	Bruker CCD, φ and ω
$2\theta_{max}$, completeness:	50°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5557, 2512, 0.025
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2311
$N(param)_{refined}$:	200
Programs:	Bruker programs [1], SHELX [2], DIAMOND [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
S1	0.70829(8)	0.42320(4)	0.22390(3)	0.03462(18)
O1	0.8788(2)	0.34382(13)	0.19220(11)	0.0453(4)
O3	−0.2013(3)	0.36571(14)	−0.09461(13)	0.0531(4)
O2	0.7823(3)	0.55675(13)	0.25716(12)	0.0471(4)
O4	−0.3181(3)	0.27957(17)	−0.25834(15)	0.0714(5)
N2	0.4140(3)	0.30581(13)	0.06373(12)	0.0338(3)
N1	0.5105(3)	0.42405(14)	0.11722(12)	0.0364(4)
H1	0.4689	0.4947	0.0957	0.044*
C9	0.1351(3)	0.18814(16)	−0.07501(14)	0.0318(4)
N3	−0.2066(3)	0.28007(15)	−0.16797(14)	0.0404(4)
C8	0.2397(3)	0.30833(16)	−0.00892(14)	0.0332(4)
H8	0.1793	0.3848	−0.0201	0.040*
C1	0.5522(3)	0.35074(17)	0.32779(14)	0.0349(4)
C14	−0.0730(3)	0.17280(17)	−0.14840(15)	0.0337(4)
C3	0.4878(5)	0.1826(2)	0.44779(19)	0.0562(6)
H3	0.5292	0.1069	0.4743	0.067*
C6	0.3710(4)	0.4081(2)	0.37138(17)	0.0460(5)
H6	0.3323	0.4849	0.3461	0.055*
C10	0.2514(3)	0.07967(18)	−0.06853(16)	0.0404(4)
H10	0.3944	0.0863	−0.0234	0.049*
C13	−0.1632(3)	0.05667(19)	−0.20792(16)	0.0413(4)
H13	−0.3020	0.0500	−0.2560	0.050*
C11	0.1622(4)	−0.03612(18)	−0.12640(17)	0.0450(5)
H11	0.2433	−0.1065	−0.1188	0.054*
C4	0.3038(4)	0.2364(2)	0.49166(16)	0.0467(5)
C12	−0.0475(4)	−0.04888(19)	−0.19584(17)	0.0448(5)
H12	−0.1095	−0.1278	−0.2339	0.054*

Table 2 (continued)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C7	0.1694(5)	0.1744(2)	0.5799(2)	0.0645(7)
H7A	0.1729	0.0832	0.5735	0.097*
H7B	0.0064	0.1902	0.5712	0.097*
H7C	0.2429	0.2102	0.6514	0.097*
C5	0.2493(4)	0.3506(2)	0.45212(18)	0.0507(5)
H5	0.1279	0.3892	0.4809	0.061*
C2	0.6117(4)	0.2378(2)	0.36596(18)	0.0486(5)
H2	0.7332	0.1993	0.3372	0.058*

Experimental details

H atoms were added using riding models. Their U_{iso} values were set to $1.2U_{eq}$ of the parent atoms.

Comment

Schiff base compounds have been one of the focuses of chemists for many years. These compounds may show excellent properties, such as antitumor and antibacterial activity [5, 6], catalytic property [7, 8], as fluorescent sensor [9] and so on. As part of our interest in synthesis, structure and property of Schiff base compounds, in this paper, a new Schiff base compound is reported.

The asymmetric unit contains one molecule. The dihedral angle between two benzene rings (ring 1: C1—C2—C3—C4—C5, ring 2: C9—C10—C11—C12—C13—C14) is 86.2°, which shows that the title compound molecule is not planar. The bond length of C8—N2 is 1.272(2) Å, which shows that this bond is a double bond. The molecules form 1D chains by π-π stacking.

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