Crystal structure of 2-chloro-*N′*-(2-methoxybenzylidene)benzohydrazide, $C_{15}H_{13}ClN_2O_2$

Yu-Mei Hao*

Baicheng Normal University, Department of Chemistry, Baicheng 137000, P. R. China

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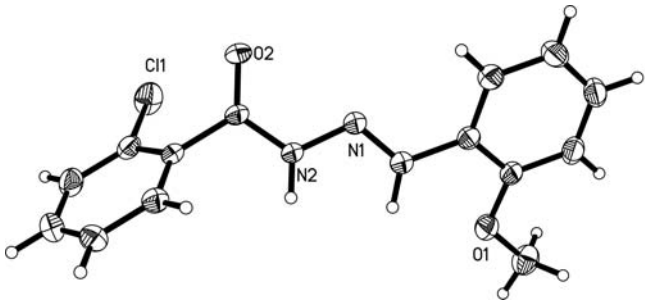

Abstract

$C_{15}H_{13}ClN_2O_2$, triclinic, $P\bar{1}$ (no. 2), a = 4.956(1) Å, b = 11.540(2) Å, c = 12.782(3) Å, α = 107.587(2)°, β = 95.724(2)°, γ = 93.646(2)°, V = 689.9 Å^3, Z = 2, $R_{gt}(F)$ = 0.045, $wR_{ref}(F^2)$ = 0.117, T = 298 K.

Source of material

2-Methoxybenzaldehyde (0.1 mmol, 13.6 mg) and 2-chlorobenzohydrazide (0.1 mmol, 17.0 mg) were refluxed in a 30 ml methanol for 30 min to give a clear colorless solution. Colorless block-shaped single crystals of the compound were formed by slow evaporation of the solvent over several days at room temperature.

Experimental details

H2 was located from a difference Fourier map and refined isotropically with the d(N—H) restrained to 0.90(1) Å, and U_{iso}(H) restrained to 0.08 Å^2. Other H atoms were constrained to ideal geometries, with d(C—H) = 0.93 - 0.96 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(C15).

Discussion

Schiff bases derived from the condensation reaction of substituted aldehydes with benzohydrazides are a kind of important compounds in biological [1-3] and coordination chemistry [4-6]. As a continuation of work on the structural investigation of such compounds [7-10], the title compound is synthesized.

The dihedral angle between the two substituted benzene rings is 89.3(2)°. All the bond lengths are within normal values and are comparable with those observed in the compounds cited above. The molecule of the compound adopts *E* configuration in respect of the C7=N1 bond. In the crystal structure, the molecules are linked through intermolecular N–H···O hydrogen bonds, forming chains along [100].

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.22 × 0.23 × 0.27 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.79 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, ω
$2\theta_{max}$:	54°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5636, 2938
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2108
$N(param)_{refined}$:	185
Programs:	SHELXS-97, SHELXL-97 [11]

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

Atom	Site	x	y	z	U_{iso}
H(3)	2*i*	1.2938	0.6666	0.8212	0.064
H(4)	2*i*	1.0220	0.6532	0.9536	0.074
H(5)	2*i*	0.6984	0.4897	0.9196	0.072
H(6)	2*i*	0.6575	0.3340	0.7542	0.059
H(7)	2*i*	1.0718	0.2960	0.5390	0.048
H(11)	2*i*	0.2988	–0.0901	0.0206	0.065
H(12)	2*i*	0.5940	–0.2380	0.0155	0.071
H(13)	2*i*	0.8377	–0.2442	0.1761	0.066
H(14)	2*i*	0.7877	–0.1040	0.3430	0.054
H(15A)	2*i*	1.3886	0.6827	0.6547	0.094
H(15B)	2*i*	1.5696	0.6009	0.5743	0.094
H(15C)	2*i*	1.6172	0.6170	0.7012	0.094
H(2)	2*i*	0.875(3)	0.130(2)	0.423(2)	0.080

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}
Cl(1)	2*i*	0.1528(1)	0.10504(5)	0.18460(5)	0.0609(4)	0.0619(4)	0.0776(4)	0.0165(3)	–0.0147(3)	0.0205(3)
N(1)	2*i*	0.7114(3)	0.2327(1)	0.5484(1)	0.0325(8)	0.0428(8)	0.0403(9)	0.0044(7)	0.0040(7)	0.0067(7)
N(2)	2*i*	0.7138(3)	0.1424(1)	0.4482(1)	0.0258(8)	0.0412(8)	0.0405(9)	0.0025(6)	0.0044(6)	0.0048(7)
O(1)	2*i*	1.2923(3)	0.5069(1)	0.6234(1)	0.0495(9)	0.0527(8)	0.0510(9)	–0.0099(7)	0.0052(7)	0.0074(7)
O(2)	2*i*	0.2582(3)	0.0956(2)	0.4266(1)	0.0244(7)	0.088(1)	0.063(1)	0.0041(7)	0.0081(7)	–0.0065(8)
C(1)	2*i*	0.9525(4)	0.4044(2)	0.6865(2)	0.033(1)	0.045(1)	0.039(1)	0.0077(8)	0.0001(8)	0.0118(8)

* e-mail: jyxygzb@163.com

Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(2)	2*i*	1.1427(4)	0.5060(2)	0.7073(2)	0.035(1)	0.047(1)	0.042(1)	0.0063(8)	–0.0006(8)	0.0103(9)
C(3)	2*i*	1.1670(4)	0.5991(2)	0.8074(2)	0.046(1)	0.052(1)	0.051(1)	0.003(1)	–0.007(1)	0.003(1)
C(4)	2*i*	1.0030(5)	0.5914(2)	0.8861(2)	0.057(1)	0.070(2)	0.043(1)	0.015(1)	–0.002(1)	–0.004(1)
C(5)	2*i*	0.8110(5)	0.4933(2)	0.8664(2)	0.053(1)	0.083(2)	0.042(1)	0.016(1)	0.010(1)	0.014(1)
C(6)	2*i*	0.7869(4)	0.4005(2)	0.7673(2)	0.042(1)	0.059(1)	0.045(1)	0.0056(9)	0.0040(9)	0.015(1)
C(7)	2*i*	0.9284(4)	0.3056(2)	0.5816(2)	0.035(1)	0.042(1)	0.042(1)	0.0028(8)	0.0057(8)	0.0085(8)
C(8)	2*i*	0.4791(3)	0.0794(2)	0.3925(2)	0.0253(9)	0.043(1)	0.045(1)	0.0042(7)	0.0041(8)	0.0100(8)
C(9)	2*i*	0.5115(3)	–0.0109(2)	0.2840(2)	0.0260(9)	0.0386(9)	0.042(1)	–0.0017(7)	0.0038(8)	0.0092(8)
C(10)	2*i*	0.3678(4)	–0.0088(2)	0.1854(2)	0.032(1)	0.044(1)	0.050(1)	–0.0014(8)	–0.0017(8)	0.0126(9)
C(11)	2*i*	0.3972(4)	–0.0929(2)	0.0855(2)	0.052(1)	0.061(1)	0.041(1)	–0.004(1)	–0.004(1)	0.010(1)
C(12)	2*i*	0.5733(5)	–0.1809(2)	0.0826(2)	0.060(1)	0.056(1)	0.049(1)	0.002(1)	0.009(1)	–0.002(1)
C(13)	2*i*	0.7184(4)	–0.1847(2)	0.1785(2)	0.049(1)	0.047(1)	0.064(2)	0.0120(9)	0.012(1)	0.007(1)
C(14)	2*i*	0.6883(4)	–0.1006(2)	0.2785(2)	0.038(1)	0.049(1)	0.049(1)	0.0058(9)	0.0044(9)	0.0150(9)
C(15)	2*i*	1.4823(5)	0.6103(2)	0.6398(2)	0.064(2)	0.056(1)	0.068(2)	–0.011(1)	0.001(1)	0.024(1)

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