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Crystal structure of (*E*)-4-bromo-*N'*-(3-chloro-2-hydroxybenzylidene)benzohydrazide, $C_{14}H_{10}BrClN_2O_2$

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	U_{iso}^*/U_{eq}
Br1	0.452101 (8)	0.37299 (7)	0.37825 (5)	0.05116 (10)
C1	0.77455 (9)	0.2614 (5)	0.2959 (3)	0.0323 (5)
C2	0.80327 (9)	0.4113 (5)	0.2085 (3)	0.0344 (6)
H2A	0.7938	0.5528	0.1399	0.041*
C3	0.84509 (9)	0.3579 (6)	0.2199 (3)	0.0375 (6)
H3	0.8641	0.4590	0.1581	0.045*
C4	0.85917 (9)	0.1562 (6)	0.3219 (3)	0.0357 (6)
H4	0.8879	0.1186	0.3305	0.043*
C5	0.83119 (8)	0.0094 (5)	0.4114 (3)	0.0324 (5)
C6	0.78870 (8)	0.0523 (5)	0.3986 (3)	0.0310 (5)
C7	0.73095 (9)	0.3248 (5)	0.2820 (3)	0.0348 (6)
H7	0.7220	0.4832	0.2234	0.042*
C8	0.63575 (7)	0.0391 (5)	0.3868 (4)	0.0326 (5)
C9	0.59170 (7)	0.1319 (5)	0.3837 (4)	0.0326 (4)
C10	0.57672 (9)	0.3278 (6)	0.2802 (3)	0.0384 (6)
H10	0.5950	0.4132	0.2097	0.046*
C11	0.53526 (9)	0.4003 (6)	0.2786 (4)	0.0419 (6)
H11	0.5250	0.5347	0.2076	0.050*
C12	0.50908 (8)	0.2746 (5)	0.3814 (4)	0.0376 (5)
C13	0.52331 (10)	0.0784 (6)	0.4854 (4)	0.0441 (7)
H13	0.5049	−0.0050	0.5562	0.053*
C14	0.56461 (10)	0.0046 (6)	0.4853 (3)	0.0408 (6)
H14	0.5746	−0.1336	0.5549	0.049*
Cl1	0.84879 (2)	−0.23586 (15)	0.54354 (8)	0.03891 (15)
N1	0.70466 (7)	0.1655 (4)	0.3493 (2)	0.0329 (5)
N2	0.66363 (7)	0.2374 (4)	0.3396 (3)	0.0325 (5)
H2	0.6557	0.4048	0.3044	0.039*
O1	0.76313 (6)	−0.1055 (4)	0.4846 (2)	0.0365 (4)
H1	0.7386	−0.0615	0.4653	0.055*
O2	0.64574 (6)	−0.2015 (4)	0.4268 (2)	0.0386 (4)

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Abstract

$C_{14}H_{10}BrClN_2O_2$, orthorhombic, $Pca2_1$ (no. 29), $a = 32.4137(12)$ Å, $b = 4.6683(2)$ Å, $c = 8.8873(3)$ Å, $V = 1344.80(9)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0239$, $wR_{ref}(F^2) = 0.0611$, $T = 150(2)$ K.

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Table 1: Data collection and handling.

Crystal:	Colourless plate
Size:	$0.20 \times 0.20 \times 0.18$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	3.26 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	26.4° , >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	17,170, 2726, 0.037
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 2518
$N(param)_{refined}$:	182
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

3-Chloro-2-hydroxybenzaldehyde (0.156 g, 1.0 mmol) and 4-bromobenzohydrazide (0.215 g, 1 mmol) were added to a stirring 30 methanol solution and refluxed for 12 h. The mixture was filtered and kept undisturbed at room

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temperature. The colorless square shaped crystals of title compound were afforded after one week.

Experimental details

The structure was solved with the Olex2 program [2] as an interface together with the SHELXT and SHELXL programs (Flack-Parameter: 0.00(1)) [3, 4]. All H atoms were placed in geometrically idealized positions and refined using a riding model, with O–H = 0.84 (phenolic hydroxyl), 0.95 Å (benzene), and with $U_{iso}(H) = 1.2 U_{eq}(C)$ for H atoms on phenolic hydroxyl and benzene.

Comment

Hydrazones characterized by the $-NHN=CH-$ group represent an important class of compounds in the field of medical science and ion recognition [5, 6]. As a part of our current research interest in exploring the relationship between molecular structure and physicochemical properties of halogenated Schiff-base compounds [7, 8], in this work, we report a new bromide hydrazone.

X-ray diffraction analysis reveals that the asymmetric unit contains a planar hydrazone molecule, as shown in the figure, the five non-hydrogen conjugated atoms $[C(=O)N=N=C]$ constitute the central chromophore. The dihedral angles formed between the central plane and the least-squares planes through the flanking chloro-phenol and bromo-phenyl rings are $15.45(15)^\circ$ and $19.7(15)^\circ$, respectively. The central chromophore and chloro-phenol ring generates an intramolecular hydroxy-O–H $\cdots$ N hydrogen bond [O1–H1 $\cdots$ N1: O1–H1 = 0.838(19) Å, H1 $\cdots$ N1 = 1.843(2) Å, O1 $\cdots$ N1 = 2.58(3) Å with angle at H1 = $145.18(13)^\circ$].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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