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Synthesis and crystal structure of 1-{4-[(2-bromo-6-hydroxy-benzylidene)amino]phenyl}ethanone, $C_{15}H_{12}BrNO_2$

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Table 1: Data collection and handling.

Crystal:	Orange block
Size:	0.17 × 0.15 × 0.14 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	3.11 mm ⁻¹
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω
$\theta_{\max}$, completeness:	26.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	24608, 2593, 0.049
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2288
$N(\text{param})_{\text{refined}}$:	174
Programs:	Bruker [1], SHELX [2], Olex2 [3]

Abstract

$C_{15}H_{12}BrNO_2$, monoclinic, $P2_1/c$ (no. 14), $a = 8.0970(3)$ Å, $b = 12.7315(4)$ Å, $c = 12.8542(4)$ Å, $\beta = 93.785(1)^\circ$, $Z = 4$, $V = 1322.21(8)$ Å³, $R_{\text{gt}}(F) = 0.0210$, $wR_{\text{ref}}(F^2) = 0.0570$, $T = 173(2)$ K.

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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

All solvents and reagents were of analytical grade. The synthesis is similar to methods reported earlier [4–6]. An ethanol solution (5 mL) of 2-bromo-6-hydroxy-benzaldehyde (201.05 mg, 1 mmol) was added dropwise to a stirring ethanol solution (5 mL) of

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.82593(2)	0.95481(2)	0.08527(2)	0.03478(8)
O1	0.62308(17)	0.56026(9)	0.06731(10)	0.0314(3)
H1	0.577341	0.584163	0.011712	0.047*
O2	0.15838(18)	0.68675(11)	−0.52281(10)	0.0382(3)
N1	0.55229(18)	0.69284(11)	−0.07795(10)	0.0246(3)
C1	0.7123(2)	0.63642(13)	0.11662(13)	0.0246(4)
C2	0.8001(2)	0.61139(15)	0.21062(14)	0.0309(4)
H2	0.796031	0.542084	0.237720	0.037*
C3	0.8927(2)	0.68739(16)	0.26394(14)	0.0326(4)
H3	0.952612	0.669828	0.327582	0.039*
C4	0.8995(2)	0.78922(15)	0.22595(14)	0.0309(4)
H4	0.962500	0.841342	0.263605	0.037*
C5	0.8138(2)	0.81384(14)	0.13310(13)	0.0251(4)
C6	0.7197(2)	0.73897(13)	0.07469(12)	0.0225(3)
C7	0.6365(2)	0.76292(13)	−0.02606(13)	0.0238(4)
H7	0.644513	0.831659	−0.054027	0.029*
C8	0.4680(2)	0.71653(13)	−0.17516(12)	0.0234(4)
C9	0.4060(2)	0.81582(14)	−0.20102(13)	0.0266(4)
H9	0.424527	0.872686	−0.153837	0.032*
C10	0.3175(2)	0.83162(14)	−0.29519(13)	0.0267(4)
H10	0.275808	0.899605	−0.312454	0.032*
C11	0.2886(2)	0.74903(14)	−0.36536(12)	0.0238(4)
C12	0.3525(2)	0.65021(14)	−0.33948(13)	0.0274(4)
H12	0.335122	0.593601	−0.387096	0.033*
C13	0.4409(2)	0.63362(14)	−0.24527(13)	0.0269(4)
H13	0.483310	0.565752	−0.228215	0.032*

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C14	0.1855(2)	0.76170(15)	−0.46556(13)	0.0273(4)
C15	0.1170(3)	0.86800(16)	−0.49427(15)	0.0357(4)
H15A	0.207631	0.915070	−0.510291	0.054 [*]
H15B	0.059597	0.896639	−0.435766	0.054 [*]
H15C	0.038865	0.861769	−0.555529	0.054 [*]

1-(4-amino-phenyl)ethanone (135.16 mg, 1 mmol) at 328 K. After 10 h, the mixture was filtered. The filtrate was recrystallized, and several clear light orange crystals were obtained. **Anal. Calcd.** for C₁₅H₁₂BrNO₂: C, 56.62%; H, 3.80%; N, 4.40%. Found: C, 56.93%; H, 3.89%; N, 4.25%.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Schiff bases attract great attention due to their easy preparation, diversity and structural variability [7, 8]. They play a significant role in development of the chelate ligands in the field of coordination chemistry [9, 10]. Schiff bases and their metal complexes are widely studied due to various physical properties [11–13], supramolecular aspects [14–16], luminescence [17] and so on.

The single crystal structure of the title compound was determined by X-ray crystallography. In the title compound structure, there is a strong intramolecular O1–H1···N1 hydrogen bond interaction (*d*(N1···H1) = 1.804 Å, *d*(O1–H1) = 0.840 Å and *d*(O1···N1) = 2.554 Å) in the title structure (cf. the figure). All geometric parameters are in the typical ranges [4–8].

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