Yi Jin, Tao Fu, Bo-Yang Ma, Ping Wei, Ji-Xing Zhao and Li Zhao*

Synthesis and crystal structure of 1-{4-[(3-bromo-2-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:	0.19 × 0.17 × 0.14 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	3.02 mm ⁻¹
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω
$\theta_{\max}$, completeness:	26.7°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	16513, 2878, 0.053
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2268
$N(\text{param})_{\text{refined}}$:	177
Programs:	Bruker [1], SHELX [2], Olex2 [3]

Abstract

$C_{15}H_{12}BrNO_2$, monoclinic, $P2_1/c$ (no. 14), $a = 11.7848(3)$ Å, $b = 10.0857(3)$ Å, $c = 12.2695(4)$ Å, $\beta = 111.2020(10)^\circ$, $Z = 4$, $V = 1359.61(7)$ Å³, $R_{\text{gt}}(F) = 0.0306$, $wR_{\text{ref}}(F^2) = 0.0745$, $T = 173(2)$ 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

Synthesis of the title compound was prepared by a method reported earlier [4–6]. 3-Bromo-2-hydroxy-benzaldehyde (201.02 mg, 1 mmol) dissolved in EtOH solution (5 mL) was added to 1-(4-amino-phenyl)ethanone (135.16 mg, 1 mmol) dissolved in EtOH solution (5 mL). The solution had been stirred at 328 K for 10 h. The filtrate was recrystallized and several clear light orange crystals were obtained. **Anal. Calcd.**

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.67409(2)	0.99765(3)	0.31965(2)	0.04061(10)
O1	0.49403(15)	0.79837(16)	0.34311(14)	0.0313(4)
H1	0.442(2)	0.752(2)	0.356(3)	0.048(8)*
O2	−0.10570(16)	0.32640(19)	0.3465(2)	0.0528(5)
N1	0.37801(17)	0.66521(18)	0.45082(17)	0.0271(4)
C1	0.56172(19)	0.8472(2)	0.4488(2)	0.0261(5)
C2	0.6513(2)	0.9415(2)	0.4576(2)	0.0285(5)
C3	0.7228(2)	0.9937(2)	0.5644(2)	0.0331(5)
H3	0.782949	1.058198	0.568244	0.040*
C4	0.7074(2)	0.9527(3)	0.6659(2)	0.0343(5)
H4	0.756546	0.988796	0.739310	0.041*
C5	0.6200(2)	0.8590(2)	0.6594(2)	0.0311(5)
H5	0.609738	0.830376	0.729038	0.037*
C6	0.5461(2)	0.8053(2)	0.5520(2)	0.0256(5)
C7	0.45130(19)	0.7117(2)	0.5481(2)	0.0265(5)
H7	0.443319	0.684266	0.619058	0.032*
C8	0.2853(2)	0.5751(2)	0.4493(2)	0.0258(5)
C9	0.3046(2)	0.4722(2)	0.5298(2)	0.0295(5)
H9	0.382069	0.461217	0.589869	0.035*
C10	0.2106(2)	0.3859(2)	0.5221(2)	0.0305(5)
H10	0.223952	0.316030	0.577273	0.037*
C11	0.0963(2)	0.4005(2)	0.4341(2)	0.0297(5)
C12	0.0792(2)	0.5030(2)	0.3535(2)	0.0349(5)
H12	0.001914	0.513855	0.293061	0.042*
C13	0.1724(2)	0.5889(2)	0.3600(2)	0.0320(5)
H13	0.159641	0.657280	0.303574	0.038*
C14	−0.0070(2)	0.3094(2)	0.4230(3)	0.0371(6)

*Corresponding author: Li Zhao, School of Chemical and Biological Engineering, Lanzhou Jiaotong University, Lanzhou 730070, P.R. China, e-mail: zhaoli_72@163.com. <https://orcid.org/0000-0002-9898-9552>

Yi Jin, Tao Fu, Bo-Yang Ma and Ping Wei: School of Chemical and Biological Engineering, Lanzhou Jiaotong University, Lanzhou 730070, P.R. China

Ji-Xing Zhao: Shihezi University, Analysis and Testing Center, Xinjiang 832003, P.R. China

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C15	0.0122(2)	0.1955(3)	0.5062(3)	0.0544(8)
H15A	−0.063379	0.144533	0.486341	0.082 [*]
H15B	0.035579	0.229468	0.586179	0.082 [*]
H15C	0.076944	0.138170	0.500507	0.082 [*]

for C₁₅H₁₂BrNO₂: C, 56.62%; H, 3.80%; N, 4.40%. Found: C, 56.85%; H, 3.97%; N, 4.12%.

Experimental details

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

Comment

Schiff base compounds and their complexes have been the centre of attraction for many researcher in recent years [7, 8]. The Schiff base can be used as a more or less flexible ligand [9, 10]. It is usually coordinated by the O atom of the substituted phenol group and the N atom of the azomethine group to the transition metal [11–13]. We have designed and prepared another Schiff base compound, and we predict that it has useful properties and applications, for example for copper(II) complexes [14–16].

The single crystal structure of the title compound was determined by X-ray crystallography. All geometric parameters are in the typical ranges. There is a strong intramolecular O1–H1···N1 hydrogen bond interaction (*d*(N1···H1) = 1.823 Å, *d*(O1–H1) = 0.836(10) Å and *d*(O1···N1) = 2.594 Å) in the title structure (cf. the figure).

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