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Crystal structure of (*E*)-2-(1-((2-aminophenyl)imino)ethyl)-4-bromophenol, C₁₄H₁₃BrN₂O

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Abstract

C₁₄H₁₃BrN₂O, monoclinic, *P*₂₁ (no. 4), *a* = 6.8679(5) Å, *b* = 7.7096(5) Å, *c* = 12.4043(7) Å, β = 101.332(2)°, *V* = 643.99(7) Å³, *Z* = 2, *R*_{gt}(*F*) = 0.0294, *wR*_{ref}(*F*²) = 0.0691, *T* = 293(2) K.

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

Source of material

Equimolar amounts of 1,2-diaminobenzene (1 mmol, 0.108 g) and 1-(5-chloro-2-hydroxyphenyl)ethanone (1 mmol, 0.171 g) were added to ethanol (10 mL), then the mixture was refluxed for 2 h. After concentration, the precipitate was dissolved in dichloromethane and evaporated slowly at room temperature to obtain colorless prismatic crystals.

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Table 1: Data collection and handling.

Crystal:	Block, colorless
Size:	0.31 × 0.17 × 0.15 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	3.18 mm ^{−1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω-scans
θ _{max} , completeness:	27.5°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	10038, 2903, 0.025
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 2431
<i>N</i> (<i>param</i>) _{refined} :	166
Programs:	Bruker programs [1], SHELX [2], OLEX2 [3]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
Br1	0.09369(5)	0.39222(8)	−0.08673(2)	0.06741(17)
O1	0.8082(3)	0.4051(5)	0.27947(17)	0.0494(6)
H1	0.778062	0.436423	0.337194	0.074*
N2	0.5881(3)	0.5073(3)	0.40602(19)	0.0325(6)
N1	0.9213(4)	0.6491(5)	0.5362(3)	0.0561(8)
H1A	1.030924	0.636232	0.583621	0.067*
H1B	0.926563	0.585053	0.479492	0.067*
C1	0.7640(4)	0.5997(4)	0.5841(3)	0.0350(7)
C2	0.7748(6)	0.6146(5)	0.6968(3)	0.0439(9)
H2	0.889116	0.659868	0.740538	0.053*
C3	0.6215(6)	0.5645(4)	0.7446(3)	0.0497(9)
H3	0.632727	0.575101	0.820234	0.060*
C4	0.4488(6)	0.4978(5)	0.6812(3)	0.0477(9)
H4	0.344383	0.463595	0.714098	0.057*
C5	0.4331(5)	0.4824(5)	0.5687(3)	0.0406(7)
H5	0.317842	0.436982	0.525970	0.049*
C6	0.5883(4)	0.5344(4)	0.5190(2)	0.0313(6)
C7	0.4406(4)	0.5346(4)	0.3260(2)	0.0305(6)
C8	0.2501(5)	0.6221(4)	0.3379(3)	0.0377(8)
H8A	0.146465	0.537107	0.332208	0.057*
H8B	0.214519	0.706952	0.280757	0.057*
H8C	0.267888	0.678086	0.408264	0.057*
C9	0.4641(4)	0.4769(4)	0.2161(2)	0.0302(6)
C10	0.3016(4)	0.4722(4)	0.1282(2)	0.0347(7)
H10	0.179321	0.514699	0.137643	0.042*
C11	0.3205(4)	0.4060(5)	0.0288(2)	0.0410(7)
C12	0.5006(6)	0.3478(5)	0.0105(3)	0.0496(9)
H12	0.512338	0.306103	−0.058335	0.060*
C13	0.6621(5)	0.3521(5)	0.0947(3)	0.0504(10)
H13	0.784404	0.314048	0.082478	0.060*
C14	0.6471(4)	0.4121(5)	0.1979(2)	0.0377(7)

Experimental details

The H atoms were positioned geometrically with $d(C-H) = 0.93-0.98 \text{ \AA}$ and refined as riding with $U_{iso}(H) = 1.2 U_{eq}(\text{carrier})$ or $1.5 U_{eq}(\text{methyl})$. Solving, refining and finishing of the crystal structure were finished by SHELX [2] and OLEX2 [3].

Discussion

Schiff bases are a class of important synthetic intermediates and they are being used as ligands to form coordination complexes with metal ions. Their complexes can be used for catalysis [4]. Mono-imine is also key intermediate for the synthesis of unsymmetrical tetradentate Schiff base ligand [5].

There is one title molecule in the asymmetric unit. The geometric parameters are similar to those reported in the literature [6]. The angle between the planes of the two benzene rings (C1–C2–C3–C4–C5–C6 and C9–C10–C11–C12–C13–C14) is 39.3° . The intramolecular O–H $\cdots$ N hydrogen bond is present (*cf.* the figure). The packing of crystal structure is dominated by van der Waals forces.

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