**Synthesis and Crystal Structure of N-Salicylidene-2-hydroxy-5-bromobenzylamine**

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The title compound, N-salicylidene-2-hydroxy-5-bromobenzylamine, was synthesized and the crystal structure was determined by the single-crystal X-ray diffraction method at 90 K. It crystallizes in the monoclinic space group *P*2₁/c with *a* = 11.3923(17) Å, *b* = 12.7998(19) Å, *c* = 8.6342(13) Å, β = 97.097(3)°, *V* = 1249.4(3) Å³, *D*ₐ = 1.628 g/cm³, and *Z* = 4. The *R*₁ ([*I* > 2σ(*I*)] and *wR*₂ (all data) values are 0.0284 and 0.0693, respectively, for all 2852 independent reflections. The molecule is bent with a dihedral angle between the two aromatic rings of 66.05(6)°.

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**Table 1 Crystal and experimental data**

| Chemical formula: C₁₄H₁₂BrNO₂ | Formula weight = 306.16 |
| Crystal system: monoclinic | *T* = 90 K |
| Space group: *P*2₁/c | *a* = 11.3923(17) Å |
| β = 97.097(3)° | *b* = 12.7998(19) Å |
| *c* = 8.6342(13) Å | *V* = 1249.4(3) Å³ |
| *D*ₐ = 1.628 g/cm³ | *Z* = 4 |
| Crystal size = 0.67 × 0.28 × 0.26 mm³ | *

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A preliminary examination was made, and data were collected on a Bruker CCD X-ray diffractometer (SMART APEX) using graphite-monochromated Mo-Kα radiation. Crystal data and details concerning data collection are given in Table 1. The structures were solved by direct methods and refined by full-matrix least-squares methods. All of the hydrogen atoms were located from subsequent difference Fourier maps and refined. The final atomic coordinates and equivalent isotropic displacement parameters for non-H atoms are listed in Table 2.

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**Fig. 1 Chemical structure.**

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The crystal structure of the present ligand is isomorphous to that of N-salicylidene-2-hydroxy-5-chlorobenzylamine. The molecular structure drawn by ORTEP is shown in Fig. 2. Selected bond distances and angles are given in Table 2. The bond lengths are almost similar to those of N-salicylidene-2-hydroxy-5-chlorobenzylamine, except for the C1–Br1 distance. The N1–C7 and N1–C8 distances are 1.473(3) Å and 1.296(3) Å, respectively, which can be considered to have the single-bond and double-bond character, respectively. The C7, N1, C8, and C9 moiety is essentially flat (r.m.s. deviation from the mean plane is 0.0194 Å), which is consistent with the sp² hybrid character of the N atom. The d-Fourier map shows that a hydrogen atom is close to the N1 atom with a distance of 0.83(2) Å, rather than the O2 atom, like in the case for the 5-chloro derivative. A similar H atom shift was observed for N-salicylidene-2-hydroxy-5-chlorobenzylamine and (E)-2-(2-oxobenzylideneamino)-5-methylphenol. The torsion angles around C7, C3-C7-N1-C8, C2-C3-C7-N1, and C4-C3-C7-N1 (Table 3) show that this molecule twists at the C7 atom, giving the dihedral angle of the aromatic rings containing C3 and C9 of 66.05(6)°. This structural feature is in harmony with the meridional coordination fashion of this ligand in metal complexes. In the crystal, the molecules are connected by O–H···O hydrogen bonds, forming a dimer structure (Fig. 3). The hydrogen-bonding parameters are summarized in Table 4. As a whole, the molecular and crystal structures are very similar to those of the 5-chloro derivative.

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References