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# CRYSTAL STRUCTURE OF N-(*p*-METHYLBENZYLIDENE)-*p*-BROMOANILINE

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The asymmetric unit of the title compound $C_{14}H_{12}BrN$ (systematic name (*E*)-*N*-(4-bromophenyl)-1-(*p*-tolyl)methanimine) contains one half-molecule: a crystallographic center of inversion is located at the midpoint of the bridging N=C bond. The central HC=N unit makes dihedral angles of 15.7(3)° and 15.2(4)° with bromobenzene and methylbenzene ring systems, respectively. The C and N atoms of the HC=N central unit are disordered over two sites in a 50:50 ratio. The Br atom of the 4-bromoaniline ring and the methyl atom of the 4-methylbenzilidene ring systems are also 50 % disordered. In the crystal, molecules are linked by C—H···π interactions forming slabs parallel to the *bc* plane. The atomic coordinates are not available for the previously reported crystal structure of the title compound: CSD refcode MBZCLE. The reported *R* factor of 0.103 for the analysis in the space group $P2_1/a$ is much higher than in the present analysis, which gives 0.033 in the space group $P2_1/c$.

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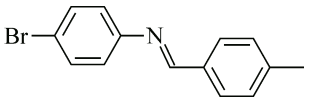
**K e y w o r d s:** synthesis, crystal structure, benzylidene, aniline, hydrogen bonding.

Schiff base ligands exhibit many pharmaceutical activities, such as antifungal and antibacterial, radical scavenging effect, enzyme activity inhibition [ 1—4 ]. As a continuation of our work on the synthesis and structural characterization of Schiff base compounds [ 5—8 ], herein we report the crystal structure of the title compound.

**Experimental. Synthesis and crystallization.** The title compound was synthesized from 4-methylbenzaldehyde and 4-bromoaniline by the condensation method. The reaction mixture was refluxed in ethanol for about 8 h and the resulting solution was slowly evaporated at room temperature. After 15 days, colorless block-like crystals of the title compound, suitable for the X-ray crystallographic analysis, were obtained.




**X-ray crystallography.** For the crystal structure determination the single crystal of the $C_{14}H_{12}BrN$ compound was used for data collection on a Bruker Kappa APEX II CCD diffractometer [ 9 ] using Mo$K_\alpha$ radiation ($\lambda = 0.71073$ Å), and a multiscan absorption correction was applied using SADABS [ 9 ]. The lattice parameters were determined by the least_squares technique using SAINT Plus [ 9 ].

Table 1

*Hydrogen bond geometry* (Å, deg.)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| C2—H2···Cg1$^{i}$ | 0.93 | 2.82 | 3.530(2) | 134 |
| C5—H5···Cg1$^{ii}$ | 0.93 | 2.87 | 3.600(2) | 136 |

Cg1 is the centroid of the C1—C6 benzene ring; symmetry codes: $^{i}$ $x$, $-y+1/2$, $z+1/2$; $^{ii}$ $x$, $-y-1/2$, $z-1/2$.

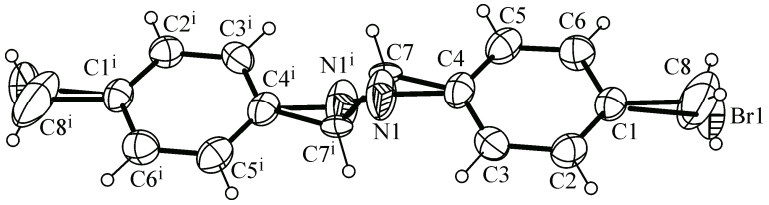



*Fig. 1.* Molecular structure of the title compound with atom labeling.
Displacement ellipsoids are drawn at the 50 % probability level

The structure was solved by direct methods using SHELXS97 [10] and refined using full-matrix least squares procedures (SHELXL97) [ 10 ]. All non-hydrogen atoms were refined anisotropically and all hydrogen atoms bound to carbon were placed in the calculated positions, and their thermal parameters were refined isotropically with $U_{iso}(H) = 1.2—1.5\ U_{eq}(C)$. Molecular plots and packing diagrams were produced using Mercury [ 11 ] along with the other material for publication produced using the WinGX publication routines [ 12 ]. Intermolecular C—H···π interactions are given in Table 1.

Crystallographic characteristics of $C_{14}H_{12}BrN$: $FW = 274.16$, $a = 13.8666(17)$ Å, $b = 7.4071(9)$ Å, $c = 5.9609(8)$ Å, $\beta = 99.718(5)°$, $V = 603.47(13)$ Å$^3$, $P2_1/c$, $Z = 2$, $d_{calc} = 1.509$ g/cm$^3$, $\mu = 3.337$ mm$^{-1}$, $2.98° < \theta < 25.99°$, 1057 $I_{hkl}$ were measured, out of which 1057 were independent ($R_{int} = 0.0000$), 736 $I_{hkl}$ with $I > 2\sigma_I$, 92 refined parameters; GOOF = 1.01; $R_1 = 0.0325$, $wR_2 = 0.0745$ for $I > 2\sigma_I$; $R_1 = 0.0593$, $wR_2 = 0.0846$ for all $I_{hkl}$; the residual electron density (max/min) 0.146/–0.178 e/Å$^3$.

**Results and discussion.** The title compound adopts an *E* conformation with respect to the N1=C7 bond. The asymmetric unit of the title compound (Fig. 1) contains one-half molecule. A crystallographic centre of inversion is located at the midpoint of the bridging N1=C7 bond. Both C7 and N1 atoms of this central bond are 50 % disordered. The central HC=N unit makes dihedral angles of 15.7(3)° and 15.2(4)° with the 4-bromobenzene and 4-methylbenzene ring systems, respectively. The Br1 atom of the 4-bromoaniline ring and the C8 atom of the 4-methylbenzylidene ring are also 50 % disordered. The experimental details are given in Table 1.

In the crystal, molecules are linked by C—H···π interactions forming slabs parallel to the *bc* plane (Table 1 and Fig. 2). The atomic coordinates are not available for the previously reported crystal structure of the title compound: CSD [ 13 ] refcode MBZCLE [ 14 ]. The reported *R* factor of 0.103 for

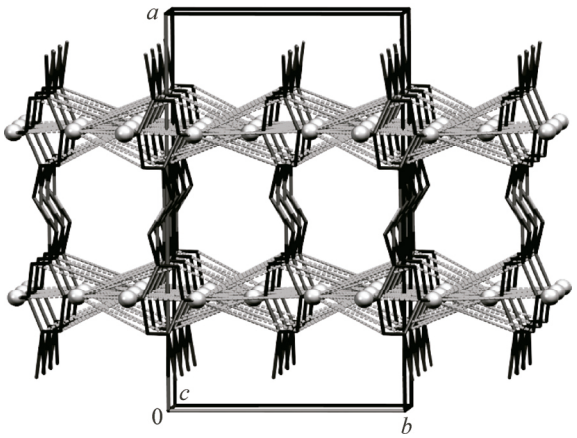



*Fig. 2.* A view along the *c* axis of the crystal packing of the title compound.
The C—H···π contacts are represented by dashed lines and the involved H atoms as grey balls (Table 1). H atoms not involved in these interactions have been omitted for clarity

the analysis in the space group $P2_1/a$, is much higher than in the present analysis which gives $R = 0.033$ in the space group $P2_1/c$.

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**Supplementary material.** CCDC-924041 for the compound discussed contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at http://www.ccdc.cam.ac.uk/const/retrieving.html or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223-336033 or e-mail: data_request@ccdc.cam.ac.uk.

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