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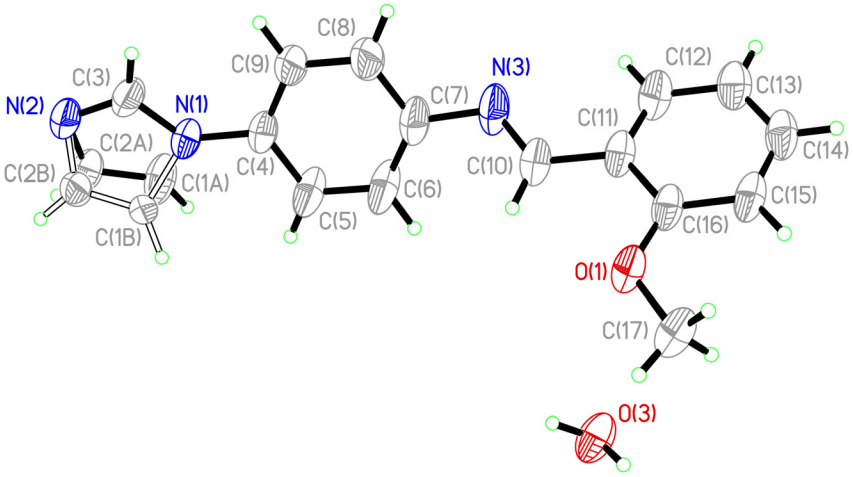
Crystal structure of (*E*)-(4-imidazol-1-yl-phenyl)-(2-methoxy-benzylidene)-amine monohydrate, $C_{17}H_{17}N_3O_2$



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Abstract

$C_{17}H_{17}N_3O_2$, monoclinic, $P2_1/c$ (no. 14), a = 10.655(5) Å, b = 5.056(5) Å, c = 28.712 Å, β = 99.034(1)°, V = 1527.6(17) Å^3, Z = 4, $R_{gt}(F)$ = 0.0520, $wR_{ref}(F^2)$ = 0.1611, T = 298(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.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.30 × 0.20 × 0.20 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	Bruker Smart Apex, ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	10,113, 2663, 0.033
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1943
$N(param)_{refined}$:	227
Programs:	Bruker [1], Olex2 [2], SHELX [3]

Source of material

All chemicals were purchased from commercial sources and used as received without further purification. The 4-imidazol-1-yl-phenylamine (2.45 mmol, 0.39 g) and 2-methoxy-benzaldehyde (6.98 mmol, 0.95 g) were dissolved in EtOH (25 mL). The mixture was refluxed for 8 h, and then the precipitate was collected by filtration and washed with EtOH. The product was recrystallized from a mixture of ethyl acetate and cyclohexane to afford colorless crystals. Yield: 0.51 g (75.5%). **m.p.**: 84.1–85.5 °C. **^{1}H NMR** ($CDCl_3$, 400 MHz, ppm): δ 8.95 (s, 1H), 8.15 (dd, J = 7.76 Hz, 1.80 Hz, 1H), 7.89 (s, 1H), 7.48 (td, J = 7.88 Hz, 1.76 Hz, 1H), 7.41 (dt, J = 8.76 Hz, 2.68 Hz, 2H), 7.34–7.30 (m, 3H), 7.23–7.15 (m, 2H), 7.08–7.05 (m, 1H), 3.92 (s, 3H).

Experimental details

All H-atoms bonded to C-atoms were placed geometrically and refined using a riding model with common isotropic displacement factors U_{iso}(H) = 1.2 or 1.5 U_{eq}(parent C-atom).

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1A[a]	0.0757 (5)	0.0162 (7)	−0.05858 (12)	0.0932 (12)
H1A[a]	0.081909	−0.074216	−0.030103	0.112*
C1B[b]	−0.0008 (8)	0.130 (2)	−0.0625 (3)	0.063 (2)
H1B[b]	−0.044410	0.136482	−0.036883	0.075*
C2A[a]	0.0112 (5)	−0.0629 (10)	−0.10036 (19)	0.0782 (13)
H2A[a]	−0.042280	−0.209061	−0.104756	0.094*
C2B[b]	−0.0379 (13)	0.020 (3)	−0.1031 (6)	0.075 (4)
H2B[b]	−0.106062	−0.096709	−0.109572	0.090*
C3	0.1129 (3)	0.2678 (7)	−0.11160 (8)	0.1042 (10)
H3	0.154129	0.394777	−0.127132	0.125*
C4	0.2051 (2)	0.4062 (4)	−0.03099 (7)	0.0722 (6)
C5	0.1788 (3)	0.4169 (5)	0.01415 (7)	0.0974 (9)
H5	0.111548	0.318975	0.022229	0.117*
C6	0.2511 (3)	0.5714 (5)	0.04774 (8)	0.1027 (10)
H6	0.232183	0.576394	0.078266	0.123*
C7	0.3503 (3)	0.7171 (5)	0.03669 (9)	0.0877 (8)
C8	0.3760 (3)	0.7033 (8)	−0.00882 (11)	0.1262 (13)
H8	0.443450	0.800059	−0.017069	0.151*
C9	0.3036 (3)	0.5488 (7)	−0.04228 (10)	0.1161 (12)
H9	0.322503	0.542272	−0.072799	0.139*
C10	0.3899 (2)	0.9940 (5)	0.10190 (8)	0.0783 (7)
H10	0.302850	0.992150	0.102344	0.094*
C11	0.4732 (2)	1.1430 (4)	0.13828 (7)	0.0740 (7)
C12	0.6036 (3)	1.1094 (6)	0.14438 (9)	0.0933 (8)
H12	0.638103	0.989457	0.125324	0.112*
C13	0.6842 (3)	1.2497 (6)	0.17814 (9)	0.0940 (8)
H13	0.771565	1.223038	0.181844	0.113*
C14	0.6342 (3)	1.4269 (5)	0.20585 (8)	0.0896 (8)
H14	0.688017	1.524333	0.228102	0.107*
C15	0.5047 (3)	1.4634 (5)	0.20128 (7)	0.0821 (7)
H15	0.471542	1.584219	0.220550	0.099*
C16	0.4233 (2)	1.3198 (4)	0.16785 (7)	0.0718 (6)
C17	0.2357 (3)	1.5125 (6)	0.19105 (9)	0.1009 (9)
H17A	0.260398	1.459579	0.223290	0.151*
H17B	0.144949	1.501676	0.182859	0.151*
H17C	0.262619	1.691276	0.187145	0.151*
N1	0.12871 (18)	0.2476 (4)	−0.06562 (6)	0.0704 (5)
N2	0.0348 (2)	0.0954 (5)	−0.13374 (7)	0.0881 (7)
N3	0.4337 (2)	0.8684 (5)	0.07002 (8)	0.0993 (8)
O1	0.29396 (17)	1.3413 (4)	0.16099 (5)	0.0878 (6)
O3	0.0365 (2)	0.9465 (4)	0.23458 (7)	0.0980 (7)
H3A	0.006 (3)	0.944 (8)	0.2040 (14)	0.145 (13)*
H3B	0.008 (4)	1.121 (9)	0.2434 (14)	0.156 (14)*

[a]Occupancy: 0.75, [b]Occupancy: 0.25.

Comment

The imidazole ring is broadly present in many natural products from a diversity of sources and is a key structural motif of essential biomolecules such as nucleic acids, purine, histamine, and histidine [4]. Imidazole-containing compounds feature relevant biological activities and show a lot of therapeutic activities [4–6]. Furthermore, due to their photophysical and chemical properties as well as their good thermal stability, the imidazole derivatives are functional materials [7–9]. The title compound was synthesized by the aldehyde-amine condensation reaction to give the Schiff base, which has wide research in biology and chemistry [10, 11].

The title molecule exhibits an *E* configuration. The bond length of C10=N3 is 1.262 Å. The diheral angle of the two aromatic rings is 50.71°. The angle of C11–C10=N3 and C7–N3=C10 are 121.54° and 119.69°, respectively. The bond length of C10–C11 is 1.468 Å, shorter than normal C–C single bonds (1.54 Å). The geometric parameters are similar to those seen in the structures of related compounds [12, 13].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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