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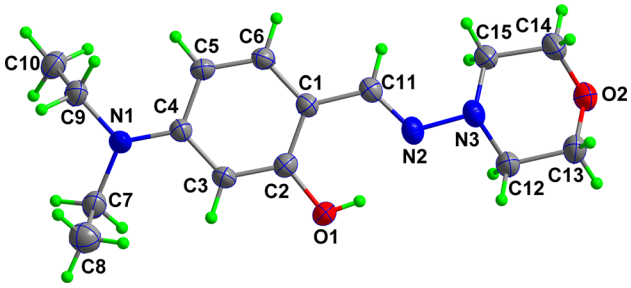
Crystal structure of (*E*)-5-(diethylamino)-2-((morpholinoimino)methyl)phenol, $C_{15}H_{23}N_3O_2$



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Abstract

$C_{15}H_{23}N_3O_2$, monoclinic, $P2_1$ (no. 4), a = 7.5122(15) Å, b = 7.8955(16) Å, c = 12.875(3) Å, β = 92.919(3)°, V = 762.7(3) Å^3, Z = 2, $R_{gt}(F)$ = 0.0545, w$R_{ref}(F^2)$ = 0.1802, T = 293(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

4–Diethylamino-2-hydroxy-benzaldehyde (0.1931 g, 1 mmol) and 4-aminomorpholine (0.1021 g, 1 mmol) were dissolved in an ethanol solution (10 ml). The mixture was refluxed for 1 h in presence of two drops of acetic acid. The resulting solution was left in air for a few days, yielding colorless block crystals.

Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [1]. The

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.12 × 0.12 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.08 mm^{-1}
Diffractometer, scan mode:	Bruker D8, φ and ω
θ_{max}, completeness:	28.1°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4703, 3319, 0.018
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2463
$N(param)_{refined}$:	185
Programs:	SHELX [1], Bruker [2]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4758 (5)	0.1333 (5)	0.1856 (3)	0.0453 (8)
C2	0.3116 (5)	0.0472 (5)	0.1789 (3)	0.0501 (9)
C3	0.2083 (5)	0.0426 (6)	0.0870 (3)	0.0531 (10)
H3	0.1009	−0.0162	0.0848	0.064*
C4	0.2614 (5)	0.1242 (5)	−0.0034 (3)	0.0474 (9)
C5	0.4260 (4)	0.2141 (5)	0.0038 (3)	0.0487 (8)
H5	0.4651	0.2718	−0.0538	0.058*
C6	0.5262 (5)	0.2157 (5)	0.0952 (3)	0.0490 (9)
H6	0.6336	0.2744	0.0976	0.059*
C7	0.0148 (5)	−0.0115 (7)	−0.1131 (3)	0.0658 (12)
H7A	0.0155	−0.0518	−0.1843	0.079*
H7B	0.0366	−0.1075	−0.0672	0.079*
C8	−0.1588 (7)	0.0624 (8)	−0.0943 (5)	0.0838 (15)
H8A	−0.1610	0.0976	−0.0230	0.126*
H8B	−0.2504	−0.0204	−0.1086	0.126*
H8C	−0.1792	0.1586	−0.1389	0.126*
C9	0.2036 (5)	0.2222 (6)	−0.1839 (3)	0.0612 (11)
H9A	0.2528	0.3294	−0.1594	0.073*
H9B	0.0946	0.2459	−0.2250	0.073*
C10	0.3351 (6)	0.1378 (7)	−0.2526 (3)	0.0708 (13)
H10A	0.4431	0.1130	−0.2124	0.106*
H10B	0.3610	0.2123	−0.3087	0.106*
H10C	0.2846	0.0345	−0.2802	0.106*
C11	0.5924 (5)	0.1384 (5)	0.2789 (3)	0.0491 (9)
H11	0.7024	0.1918	0.2764	0.059*
C12	0.6280 (5)	−0.0560 (7)	0.5228 (3)	0.0641 (12)
H12A	0.6564	−0.1619	0.4892	0.077*
H12B	0.5025	−0.0577	0.5372	0.077*
C13	0.7389 (6)	−0.0388 (8)	0.6235 (3)	0.0725 (13)
H13A	0.7043	0.0633	0.6592	0.087*

Table 2: (continued)

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
H13B	0.7164	−0.1347	0.6680	0.087*
C14	0.9553 (7)	0.1102 (9)	0.5422 (4)	0.0823 (16)
H14A	1.0818	0.1160	0.5305	0.099*
H14B	0.9229	0.2126	0.5783	0.099*
C15	0.8515 (6)	0.1024 (7)	0.4378 (3)	0.0677 (13)
H15A	0.8714	0.2052	0.3988	0.081*
H15B	0.8925	0.0072	0.3979	0.081*
N1	0.1610 (4)	0.1191 (6)	−0.0943 (3)	0.0659 (11)
N2	0.5485 (4)	0.0714 (4)	0.3649 (2)	0.0529 (8)
N3	0.6628 (4)	0.0838 (5)	0.4542 (2)	0.0541 (8)
O1	0.2486 (4)	−0.0338 (5)	0.2630 (2)	0.0697 (9)
H1	0.3118	−0.0108	0.3149	0.105*
O2	0.9225 (4)	−0.0313 (5)	0.6053 (2)	0.0697 (9)

hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Comment

Schiff bases derived from 4-aminomorpholine have been paid much attention due to their excellent biological activities [3]. In particular, those with an OH group in ortho position to the imino group are of great interest in photochromism field, primarily because of their tautomerism between enol-imine and keto-amine form [4]. Herein, we reported the crystal structure of the title compound, which is produced through condensation between 4-aminomorpholine and 4-diethylamino-2-hydroxybenzaldehyde.

The title molecule is shown in the figure. The bond distances of C2—O1 and C11–N2 are 1.363(5) and 1.285(5) Å, which are consistent with a single bond and a double bond, respectively. This is a common phenomenon in some reported analogues [5]. In the crystal, nonclassical intermolecular hydrogen bond C15—H15A···O2^{i} (symmetry code i: 2–*x*, 0.5+*y*, 1–*z*) links the molecules into zig–zag chains along *b* axis, which are further connected with each other into a one-dimensional network by C8—H8b···Cg^{ii} (where Cg represents the centroid of benzene ring of C1–C6, symmetry code ii: –*x*, 0.5+*y*, –*z*). In addition, a strong intramolecular O1—H1···N2 hydrogen bond is also present with the D–A distance of 2.681 (4) Å.

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

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