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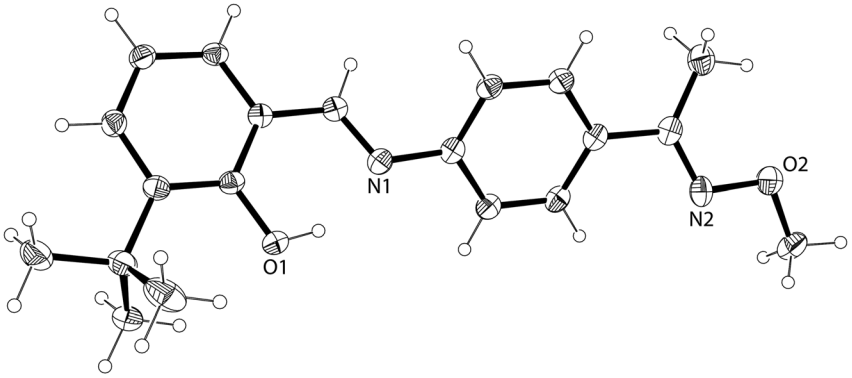
Synthesis and crystal structure of (*E*)-1-(4-(((*E*)-3-(*tert*-butyl)-2-hydroxybenzylidene)amino)phenyl) ethan-1-one *O*-methyl oxime, $C_{20}H_{24}N_2O_2$



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Abstract

$C_{20}H_{24}N_2O_2$, monoclinic, $P2_1/c$ (no. 14), a = 14.5088(4) Å, b = 17.4849(6) Å, c = 7.1398(2) Å, β = 97.933(1)°, Z = 4, V = 1793.93(9) Å^3, $R_{gt}(F)$ = 0.0561, $wR_{ref}(F^2)$ = 0.1596, T = 173 K.

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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:	Yellow block
Size:	0.17 × 0.16 × 0.12 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.08 mm^{-1}
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω
θ_{max}, completeness:	26.7°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	22,136, 3804, 0.060
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2931
$N(param)_{refined}$:	223
Programs:	Bruker [1], SHELX [2], Olex2 [3]

Source of material

All chemicals were used without further purification. 1-(4–Aminophenyl)ethan-1-one *O*-methyl oxime was prepared by a reported method [4]. 3-*tert*–Butyl-2-hydroxy-benzaldehyde (178.26 mg, 1 mmol) dissolved in ethanol (5 mL) was added to 1-(4-aminophenyl)ethan-1-one *O*-methyl oxime (164.20 mg, 1 mmol) dissolved in ethanol (5 mL) at 338 K. The mixture was kept stirring for 5 h, then cooled to room temperature and filtered. The filtrate was allowed to stand for 10 days in a quiet environment. Several clear light yellow crystals were obtained.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

The synthesis and crystal structure of Schiff bases and their derivatives have attracted much attention because they have shown great application value in various fields [5, 6].

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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}
O1	0.74657 (10)	0.40657 (9)	0.41679 (18)	0.0454 (4)
H1	0.697049	0.403520	0.464968	0.068*
O2	0.22386 (11)	0.39697 (10)	1.1559 (2)	0.0568 (4)
N1	0.57176 (11)	0.38314 (9)	0.4357 (2)	0.0372 (4)
N2	0.29675 (12)	0.40468 (10)	1.0486 (2)	0.0455 (4)
C1	0.64164 (12)	0.35625 (10)	0.1582 (2)	0.0325 (4)
C2	0.73235 (13)	0.37831 (10)	0.2389 (2)	0.0341 (4)
C3	0.80811 (13)	0.37129 (10)	0.1365 (3)	0.0361 (4)
C4	0.78927 (14)	0.34173 (11)	−0.0450 (3)	0.0397 (4)
H4	0.839429	0.336261	−0.116556	0.048*
C5	0.70087 (14)	0.31965 (11)	−0.1278 (3)	0.0394 (4)
H5	0.691262	0.299846	−0.252918	0.047*
C6	0.62780 (13)	0.32693 (10)	−0.0260 (2)	0.0351 (4)
H6	0.567140	0.311925	−0.081123	0.042*
C7	0.90697 (14)	0.39582 (12)	0.2225 (3)	0.0447 (5)
C8	0.97701 (16)	0.38147 (17)	0.0841 (4)	0.0671 (7)
H8A	0.980077	0.326557	0.058200	0.101*
H8B	1.038589	0.399738	0.139828	0.101*
H8C	0.957158	0.408951	−0.034239	0.101*
C9	0.93871 (17)	0.35127 (16)	0.4048 (4)	0.0708 (8)
H9A	0.895691	0.361136	0.496432	0.106*
H9B	1.001466	0.367753	0.457863	0.106*
H9C	0.939287	0.296427	0.376640	0.106*
C10	0.90749 (16)	0.48186 (13)	0.2625 (3)	0.0517 (5)
H10A	0.887671	0.509639	0.144589	0.078*
H10B	0.970507	0.497936	0.314869	0.078*
H10C	0.864627	0.493076	0.353633	0.078*
C11	0.56341 (13)	0.35987 (10)	0.2632 (3)	0.0350 (4)
H11	0.503809	0.344552	0.202850	0.042*
C12	0.49559 (13)	0.37883 (11)	0.5395 (2)	0.0360 (4)
C13	0.43126 (13)	0.31923 (11)	0.5175 (3)	0.0382 (4)
H13	0.435680	0.280902	0.424799	0.046*
C14	0.36091 (13)	0.31561 (11)	0.6300 (3)	0.0385 (4)
H14	0.317534	0.274644	0.613635	0.046*
C15	0.35271 (13)	0.37112 (11)	0.7668 (2)	0.0366 (4)
C16	0.41728 (14)	0.43105 (11)	0.7868 (3)	0.0388 (4)
H16	0.411939	0.470133	0.877078	0.047*
C17	0.48842 (14)	0.43432 (11)	0.6777 (3)	0.0387 (4)
H17	0.532832	0.474479	0.696513	0.046*
C18	0.27859 (14)	0.36598 (12)	0.8893 (3)	0.0411 (4)
C19	0.19332 (15)	0.31972 (14)	0.8270 (3)	0.0534 (6)
H19A	0.209726	0.265342	0.827611	0.080*
H19B	0.166720	0.335030	0.698833	0.080*
H19C	0.147561	0.328437	0.913669	0.080*
C20	0.23956 (17)	0.45378 (15)	1.3014 (3)	0.0563 (6)
H20A	0.233895	0.504812	1.244175	0.084*
H20B	0.302157	0.447435	1.371120	0.084*
H20C	0.193350	0.447962	1.388361	0.084*

For example, Schiff base compounds can form complexes with transition metals, which can be used in the research of fluorescent materials [7, 8], ion recognition [9] and so on. We will continue to investigated the synthesis and characterization of transition metal complexes of the title compounds [10, 11].

The single crystal structure of the title compound is shown in Figure 1 (*cf.* the figure). It is only built up by the $C_{20}H_{24}N_2O_2$ molecules. Comparison with reported similar structures, showed that all bond lengths and bond angles are within the normal ranges [4]. In the title compound, there is a strong intramolecular O1—H1···N1 hydrogen bond interaction (d(N1···H1)=1.836 Å, d(O1—H1)=0.840 Å and d(O1···N1)=2.591 Å).

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

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