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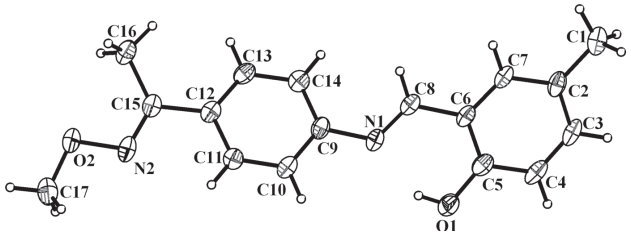
Crystal structure of (*E*)-1-(4-(((*E*)-2-hydroxy-5-methylbenzylidene)amino)phenyl)ethan-1-one *O*-methyl oxime, $C_{17}H_{18}N_2O_2$



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Abstract

$C_{17}H_{18}N_2O_2$, monoclinic, $P2_1/c$ (no. 14), $a = 33.536(6)$ Å, $b = 7.0566(10)$ Å, $c = 6.1491(10)$ Å, $\beta = 91.048(5)°$, $Z = 4$, $V = 1455.0(4)$ Å^3, $R_{gt}(F) = 0.0672$, $wR_{ref}(F^2) = 0.1823$, $T = 296(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared by modification of the reported method [1, 2]. 2-Hydroxy-5-methyl-benzaldehyde (136.2 mg, 1 mmol) dissolved in ethanol solution (3 mL) was added to 1-(4-aminophenyl)-ethanone *O*-methyl-oxime (164.2 mg, 1 mmol) dissolved in ethanol solution (3 mL). After the solution had been stirred at 328 K for 11 h, the mixture was filtered at room temperature. The product was dried under vacuum and a yellow solid was obtained (yield 79.6%, m.p. 398–405 K). The crystals were obtained by slow evaporation from a chloroform/ethanol (2:1) solution in a quiet environment at room temperature. Elemental analysis

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Table 1: Data collection and handling.

Crystal:	clear light yellow
Size:	0.27 × 0.25 × 0.22 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.085 mm^{-1}
Diffractometer, scan mode:	APEX-II CCD, φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5570, 2560, 0.054
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2040
$N(param)_{refined}$:	194
Programs:	Bruker [15], SHELX [16]

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

Atom	*x*	*Y*	*z*	U_{iso}*/U_{eq}
C1	0.95780(9)	0.5644(4)	0.6769(5)	0.0308(7)
H1A	0.9494	0.5951	0.5310	0.046*
H1B	0.9738	0.4517	0.6755	0.046*
H1C	0.9732	0.6673	0.7368	0.046*
C2	0.92159(8)	0.5315(4)	0.8142(5)	0.0241(7)
C3	0.92576(8)	0.4614(4)	1.0274(5)	0.0260(7)
H3	0.9512	0.4379	1.0836	0.031*
C4	0.89317(9)	0.4263(4)	1.1564(5)	0.0255(7)
H4	0.8969	0.3808	1.2971	0.031*
C5	0.85451(8)	0.4594(4)	1.0748(4)	0.0224(6)
C6	0.84919(8)	0.5251(4)	0.8590(4)	0.0200(6)
C7	0.88313(8)	0.5626(4)	0.7346(4)	0.0210(6)
H7	0.8797	0.6099	0.5944	0.025*
C8	0.80954(8)	0.5434(4)	0.7598(4)	0.0199(6)
H8	0.8069	0.5775	0.6142	0.024*
C9	0.73938(8)	0.5115(4)	0.7737(4)	0.0202(6)
C10	0.70825(8)	0.5849(4)	0.8945(4)	0.0214(6)
H10	0.7134	0.6359	1.0316	0.026*
C11	0.66963(8)	0.5824(4)	0.8115(4)	0.0208(6)
H11	0.6492	0.6352	0.8920	0.025*
C12	0.66069(8)	0.5012(4)	0.6072(4)	0.0199(6)
C13	0.69205(8)	0.4245(4)	0.4899(4)	0.0219(6)
H13	0.6867	0.3688	0.3554	0.026*
C14	0.73118(8)	0.4297(4)	0.5701(4)	0.0220(6)
H14	0.7517	0.3792	0.4889	0.026*
C15	0.61809(8)	0.4948(4)	0.5283(4)	0.0208(6)
C16	0.60732(9)	0.4619(4)	0.2926(5)	0.0284(7)
H16A	0.5893	0.3566	0.2806	0.043*
H16B	0.6310	0.4346	0.2133	0.043*
H16C	0.5948	0.5733	0.2336	0.043*

Table 2 (continued)

Atom	*x*	*Y*	*z*	U_{iso}*/U_{eq}
C17	0.52729(9)	0.5371(5)	0.7733(5)	0.0380(8)
H17A	0.5307	0.4310	0.8695	0.057*
H17B	0.5001	0.5426	0.7223	0.057*
H17C	0.5338	0.6519	0.8497	0.057*
N1	0.77815(6)	0.5128(3)	0.8721(4)	0.0209(5)
N2	0.59276(7)	0.5218(3)	0.6784(4)	0.0267(6)
O1	0.82324(6)	0.4246(3)	1.2059(3)	0.0278(5)
H1	0.8023	0.4460	1.1392	0.042*
O2	0.55292(6)	0.5162(3)	0.5928(3)	0.0311(5)

supports the composition of the title compound. Anal. Calcd. for $C_{17}H_{18}N_2O_2$: C, 72.32%; H, 6.43%; N, 9.92%; Found: C, 72.29%; H, 6.47%; N, 9.87%.

Experimental details

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

Comment

Oxime-type compounds are also considered a very important class of organic ligands [3–5]. And its complexes generally involve an oximato N-metal bonding, which, based on the known geometrical configuration of the ligands, has been accepted as their most stable form [6–8]. So far, a large number of transition metal complexes have been synthesized [9–11] and their supramolecular effects have been studied [12–14].

The current work reports the synthesis of title compound, which is built up by the $C_{17}H_{18}N_2O_2$ molecules. And all bond lengths are in normal ranges [1–4]. There is a strong intramolecular O1—H1···N1 hydrogen bond (d(N1···H1) = 1.878 Å, d(O1—H1) = 0.820 Å, d(O1···N1) = 2.603 Å) (*cf*. the figure).

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