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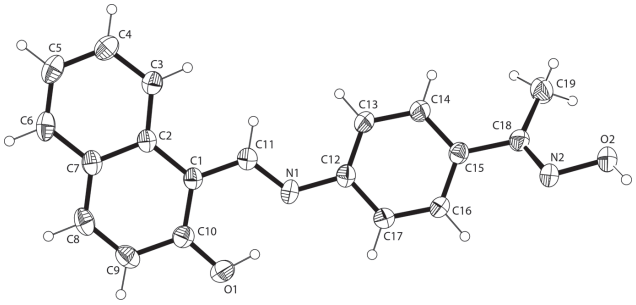
Crystal structure of (*E*)-1-(4-{[(*E*)-2-Hydroxy-1-naphthalenylmethylene] amino}phenyl)ethanone oxime, $C_{19}H_{16}N_2O_2$



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Abstract

$C_{19}H_{16}N_2O_2$, monoclinic $P2_1/c$ (no. 14), $a = 14.1712(6)$ Å, $b = 7.3611(3)$ Å, $c = 14.4212(8)$ Å, $\beta = 90.665(5)°$, $Z = 4$, $V = 1504.24(12)$ Å^3, $R_{gt}(F) = 0.0633$, $wR_{ref}(F^2) = 0.1648$, $T = 291$ 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.

Table 1: Data collection and handling.

Crystal:	Plate, clear light yellow
Size:	0.31 × 0.24 × 0.04 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.09 mm^{-1}
Diffractometer, scan mode:	SuperNova, φ and ω-scans
$2\theta_{max}$, completeness:	52°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6222, 2948, 0.031
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1820
$N(param)_{refined}$:	214
Programs:	CrysAlis^{PRO} [1], SHELX [2], OLEX2 [3]

Source of material

The title compound was prepared by modification of the reported method [4–7]. To an ethanol solution (5 mL) of 4-amino acetophenone oxime (148.2 mg, 1 mmol) was added an ethanol solution (5 mL) of 2-hydroxy-1-naphthaldehyde (175.2 mg, 1 mmol). After the solution had been stirred at 328 K for 12 h, the mixture was filtered and washed at room temperature. The isolated compound was dried under reduced pressure and recrystallized from DMF/EtOH. A light yellow solid of title compound was obtained (yield 80.7%). The single crystals were obtained by slow evaporation from a mixture of dichloromethane / methanol solution at room temperature. Elemental analysis – Anal. calcd for $C_{19}H_{16}N_2O_2$: C, 74.98%; H, 5.30%; N, 9.20%; Found: C, 75.03%; H, 5.24%; N, 9.17%.

Experimental details

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

Discussion

Oxime-type chelating agents have drawn much attention in the last decades, because they have been playing an important role in the development of coordination chemistry [8, 9]. On the other hand, many Schiff base complexes have been structurally characterized, but only a relatively small number of oxime-type complexes have been characterized and they usually have the interesting supramolecular architectures [10–12]. So, recently, particular attention has been paid to the synthesis and application of oxime-type compounds and their complexes [13, 14].

The single crystal structure of the title compound which is only built up by the $C_{19}H_{16}N_2O_2$ molecules. All bond lengths are in normal ranges. The dihedral angle of benzene ring and naphthalene ring system is 16.3°. In the compound, there is a strong intramolecular O1–H1···N1 hydrogen bond (d(N1···H1) = 1.747(3) Å, d(O1—H1) = 0.89(8) Å, d(O1···N1) = 2.542(3) Å) and there is second medium strong intermolecular O2–H2···O1 hydrogen bond interaction

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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	0.19438(15)	0.0855(3)	0.29259(16)	0.0616(6)
O2	0.71122(13)	0.2373(3)	0.72693(15)	0.0608(6)
H2	0.7430	0.1443	0.7290	0.091*
N1	0.25067(14)	0.2353(3)	0.44207(17)	0.0481(6)
N2	0.63437(15)	0.2119(3)	0.66561(17)	0.0507(6)
C1	0.08726(17)	0.1865(3)	0.40788(19)	0.0405(6)
C2	−0.01007(17)	0.1980(3)	0.43766(19)	0.0390(6)
C3	−0.03809(18)	0.2803(3)	0.5202(2)	0.0469(7)
H3	0.0075	0.3316	0.5590	0.056*
C4	−0.1315(2)	0.2873(4)	0.5458(2)	0.0557(8)
H4	−0.1476	0.3427	0.6014	0.067*
C5	−0.2010(2)	0.2135(4)	0.4903(3)	0.0620(9)
H5	−0.2639	0.2195	0.5079	0.074*
C6	−0.17679(19)	0.1312(4)	0.4090(2)	0.0581(9)
H6	−0.2237	0.0810	0.3714	0.070*
C7	−0.08213(18)	0.1211(3)	0.3812(2)	0.0456(7)
C8	−0.0567(2)	0.0344(4)	0.2968(2)	0.0575(8)
H8	−0.1040	−0.0165	0.2599	0.069*
C9	0.0335(2)	0.0235(4)	0.2683(2)	0.0552(8)
H9	0.0468	−0.0346	0.2127	0.066*
C10	0.10914(19)	0.0996(3)	0.3221(2)	0.0469(7)
C11	0.16100(17)	0.2477(3)	0.4654(2)	0.0428(7)
H11	0.1462	0.2991	0.5223	0.051*
C12	0.32929(18)	0.2764(3)	0.5004(2)	0.0458(7)
C13	0.32492(18)	0.3748(4)	0.5820(2)	0.0522(8)
H13	0.2676	0.4227	0.6012	0.063*
C14	0.40541(18)	0.4020(4)	0.6350(2)	0.0519(8)
H14	0.4017	0.4697	0.6893	0.062*
C15	0.49197(17)	0.3303(3)	0.6088(2)	0.0435(7)
C16	0.49600(18)	0.2371(4)	0.5252(2)	0.0502(7)
H16	0.5535	0.1923	0.5048	0.060*
C17	0.41613(18)	0.2102(4)	0.4721(2)	0.0520(8)
H17	0.4202	0.1468	0.4165	0.062*
C18	0.57628(18)	0.3445(4)	0.6708(2)	0.0468(7)
C19	0.5882(2)	0.5002(4)	0.7354(3)	0.0719(10)
H19A	0.5795	0.4595	0.7980	0.108*
H19B	0.5424	0.5921	0.7207	0.108*
H19C	0.6505	0.5497	0.7293	0.108*
H1	0.235(5)	0.124(15)	0.336(5)	0.39(6)*

(d(O2—H2) = 0.82 Å, d(O1···H2) = 1.937(8) Å, d(O1···O2) = 2.743(3) Å).

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