Crystal structure of 3-ethoxy-2-hydroxybenzaldehyde oxime, $C_9H_{11}NO_3$

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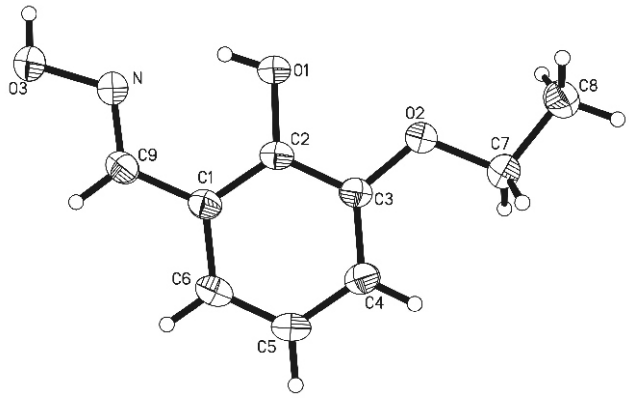

Abstract

$C_9H_{11}NO_3$, monoclinic, $P12_1/c1$ (no. 14), a = 9.259(2) Å, b = 14.679(3) Å, c = 7.036(1) Å, β = 108.40(2)°, V = 907.4 Å^3, Z = 4, $R_{gt(F)}$ = 0.044, $wR_{ref}(F^2)$ = 0.131, T = 293 K.

Source of material

The title compound was synthesized by the reaction of 3-ethoxy-2-hydroxybenzaldehyde (1 mmol, 0.166 g) with hydroxylamine hydrochloride (1.2 mmol, 0.084 g) in the presence of $NaHCO_3$ (1.2 mmol, 0.1 g) in methanol at room temperature (3 h). When evaporated to dryness, the product was extracted with dichloromethane and recrystallised from methanol. Colourless single crystals of the title compound were obtained over a period of one week.

Discussion

Oxime derivatives are often the source of iminoxy radicals when oxidized chemically [1], which have potential enzymatical application [2].

In the title crystal structure, the molecule adopts an *E* geometry with respect to the C=N double bond. The molecule is planar, atom C8 is displaced from the plane by –0.207(2) Å. An intramolecular O–H···N hydrogen bond is observed which helps to stablize the molecule structure. An intermolecular O–H···O hydrogen bond links the molecules into centrosymmetric dimers.

Table 1. Data collection and handling.

Crystal:	colourless block, size 0.18 × 0.21 × 0.22 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.00 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, ω
$2\theta_{max}$:	52.76°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3523, 1857
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1293
$N(param)_{refined}$:	119
Program:	SHELXTL [3]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1A)	4*e*	–0.0087	0.0521	0.1343	0.087
H(3A)	4*e*	–0.2705	–0.0561	–0.2128	0.099
H(9A)	4*e*	–0.3716	0.0338	0.1284	0.061
H(6A)	4*e*	–0.3435	0.1091	0.4473	0.067
H(4A)	4*e*	0.0574	0.2021	0.7935	0.065
H(5A)	4*e*	–0.2003	0.1804	0.7325	0.074
H(7A)	4*e*	0.3060	0.1630	0.8555	0.067
H(7B)	4*e*	0.2889	0.2565	0.7409	0.067
H(8A)	4*e*	0.5442	0.2118	0.8479	0.104
H(8B)	4*e*	0.4833	0.2140	0.6132	0.104
H(8C)	4*e*	0.5002	0.1208	0.7269	0.104

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	4*e*	0.0525(1)	0.07597(9)	0.2323(2)	0.0463(7)	0.081(1)	0.0525(7)	–0.0046(6)	0.0229(5)	–0.0205(7)
O(2)	4*e*	0.2190(1)	0.15052(9)	0.5607(2)	0.0459(7)	0.0719(9)	0.0515(7)	–0.0071(6)	0.0197(5)	–0.0134(6)
C(3)	4*e*	0.0678(2)	0.1433(1)	0.5400(2)	0.0459(9)	0.044(1)	0.0483(9)	0.0012(7)	0.0206(7)	–0.0008(8)
N	4*e*	–0.2111(1)	0.0125(1)	0.0176(2)	0.0439(8)	0.063(1)	0.0476(8)	–0.0021(7)	0.0120(6)	–0.0059(7)
C(2)	4*e*	–0.0201(2)	0.1016(1)	0.3640(2)	0.0459(9)	0.044(1)	0.0450(9)	0.0056(7)	0.0207(7)	0.0019(8)
C(1)	4*e*	–0.1748(2)	0.0878(1)	0.3270(2)	0.0435(9)	0.044(1)	0.0483(9)	0.0058(7)	0.0183(7)	0.0033(8)
O(3)	4*e*	–0.3157(1)	–0.0314(1)	–0.1437(2)	0.0493(7)	0.089(1)	0.0565(7)	–0.0070(7)	0.0129(6)	–0.0192(7)
C(9)	4*e*	–0.2682(2)	0.0419(1)	0.1481(2)	0.0423(9)	0.057(1)	0.055(1)	0.0031(8)	0.0180(8)	0.0036(9)
C(6)	4*e*	–0.2401(2)	0.1180(1)	0.4693(3)	0.0477(9)	0.062(1)	0.065(1)	0.0048(9)	0.0284(8)	–0.000(1)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(4)	4*e*	–0.0003(2)	0.1732(1)	0.6767(3)	0.058(1)	0.056(1)	0.053(1)	–0.0003(9)	0.0230(8)	–0.0085(9)
C(5)	4*e*	–0.1546(2)	0.1602(1)	0.6400(3)	0.060(1)	0.073(1)	0.062(1)	0.006(1)	0.0338(9)	–0.010(1)
C(7)	4*e*	0.3158(2)	0.1929(1)	0.7373(3)	0.055(1)	0.060(1)	0.052(1)	–0.0071(9)	0.0174(8)	–0.0081(9)
C(8)	4*e*	0.4752(2)	0.1841(2)	0.7307(3)	0.052(1)	0.091(2)	0.064(1)	–0.005(1)	0.0169(9)	–0.004(1)

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