Crystal structure of 1-(3′,5′-dimethoxyphenyl)-2-methyloximopropanol, $C_6H_3(OCH_3)_2CH(OH)C(NOCH_3)(CH_3)$

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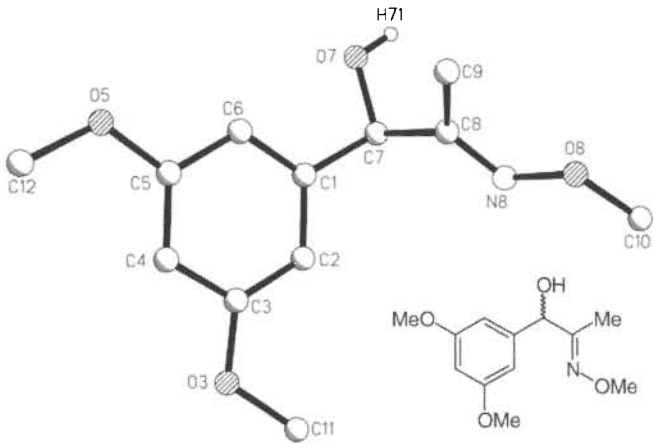

Abstract

$C_{12}H_{17}NO_4$, monoclinic, $P12_1/c1$ (No. 14), $a = 9.380(1)$ Å, $b = 17.631(1)$ Å, $c = 8.248(1)$ Å, $\beta = 113.05(1)°$, $V = 1255.2$ Å^3, $Z = 4$, $R_{gt}(F) = 0.052$, $wR(F) = 0.054$, $T = 293$ K.

Source of material

The racemic title compound was synthesized by reduction of the corresponding ketone (as prepared from the *N*-hydroxy derivative [1] using $NaBH_4$ in THF according to [2]).

Table 1. Data collection and handling.

Crystal:	colourless lath, size 0.2 × 0.45 × 1.2 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.00 cm^{-1}
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	3187, 2886
Criterion for F_{obs}, $N(hkl)_{unique}$:	$F_{obs} > 3\ \sigma(F_{obs})$, 2220
$N(param)_{refined}$:	158
Program:	SHELXTL-plus [3]

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

Atom	Site	x	y	z	U_{iso}
H(2)	4*e*	0.4689(2)	0.6820(1)	0.5425(3)	0.08
H(4)	4*e*	0.7799(2)	0.5151(1)	0.5720(3)	0.08
H(6)	4*e*	0.4533(2)	0.5775(1)	0.0949(2)	0.08
H(7)	4*e*	0.3208(2)	0.7353(1)	0.2499(2)	0.08
H(71)	4*e*	0.221(3)	0.720(2)	–0.044(4)	0.088(9)
H(9A)	4*e*	0.1534(2)	0.5657(1)	0.0433(3)	0.08
H(9B)	4*e*	–0.0132(2)	0.5941(1)	0.0145(3)	0.08
H(9C)	4*e*	0.0812(2)	0.5446(1)	0.1796(3)	0.08
H(10A)	4*e*	–0.2000(3)	0.6838(2)	0.3773(4)	0.08
H(10B)	4*e*	–0.1308(3)	0.7537(2)	0.3156(4)	0.08
H(10C)	4*e*	–0.0360(3)	0.7150(2)	0.4972(4)	0.08
H(11A)	4*e*	0.7006(3)	0.6391(2)	0.9839(3)	0.08
H(11B)	4*e*	0.5388(3)	0.6151(2)	0.8424(3)	0.08
H(11C)	4*e*	0.6135(3)	0.6923(2)	0.8231(3)	0.08
H(12A)	4*e*	0.8246(3)	0.4082(2)	0.2427(3)	0.08
H(12B)	4*e*	0.7777(3)	0.4102(2)	0.4054(3)	0.08
H(12C)	4*e*	0.8919(3)	0.4712(2)	0.3867(3)	0.08

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}
C(1)	4*e*	0.4429(2)	0.6364(1)	0.3027(2)	0.0381(9)	0.0375(9)	0.040(1)	–0.0029(8)	0.0149(8)	0.0021(8)
C(2)	4*e*	0.5089(2)	0.6451(1)	0.4856(3)	0.042(1)	0.047(1)	0.039(1)	–0.0021(8)	0.0156(8)	–0.0032(8)
C(3)	4*e*	0.6327(2)	0.5994(1)	0.5836(2)	0.043(1)	0.055(1)	0.035(1)	–0.0056(9)	0.0106(8)	–0.0008(9)
O(3)	4*e*	0.7085(2)	0.6033(1)	0.7629(2)	0.0574(9)	0.089(1)	0.0337(7)	0.0115(8)	0.0058(6)	–0.0061(8)
C(4)	4*e*	0.6933(2)	0.5462(1)	0.5028(3)	0.0392(9)	0.048(1)	0.042(1)	0.0020(9)	0.0094(8)	0.0029(9)
C(5)	4*e*	0.6261(2)	0.5389(1)	0.3214(3)	0.042(1)	0.044(1)	0.042(1)	–0.0011(8)	0.0162(8)	–0.0011(8)
O(5)	4*e*	0.6753(2)	0.48834(9)	0.2284(2)	0.0554(9)	0.0609(9)	0.0472(8)	0.0169(7)	0.0141(7)	–0.0048(7)
C(6)	4*e*	0.5003(2)	0.5836(1)	0.2206(2)	0.0411(9)	0.045(1)	0.0340(9)	–0.0009(8)	0.0116(8)	0.0009(8)
C(7)	4*e*	0.3046(2)	0.6857(1)	0.1979(2)	0.046(1)	0.0355(9)	0.038(1)	0.0032(8)	0.0168(8)	0.0021(8)
O(7)	4*e*	0.2915(2)	0.69027(8)	0.0212(2)	0.068(1)	0.0556(9)	0.0415(8)	0.0195(8)	0.0255(7)	0.0150(7)

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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(8)	4*e*	0.1565(2)	0.6535(1)	0.2040(2)	0.0409(9)	0.0335(9)	0.0326(9)	0.0019(7)	0.0061(8)	0.0028(7)
N(8)	4*e*	0.0992(2)	0.69138(9)	0.2952(2)	0.0381(8)	0.0437(9)	0.0443(9)	–0.0054(7)	0.0139(7)	–0.0024(7)
O(8)	4*e*	–0.0384(2)	0.65765(9)	0.2936(2)	0.0445(8)	0.0559(9)	0.072(1)	–0.0128(7)	0.0275(7)	–0.0126(8)
C(9)	4*e*	0.0883(2)	0.5832(1)	0.1011(3)	0.053(1)	0.045(1)	0.053(1)	–0.0046(9)	0.011(1)	–0.011(1)
C(10)	4*e*	–0.1066(3)	0.7063(2)	0.3778(4)	0.068(2)	0.076(2)	0.119(2)	–0.016(1)	0.058(2)	–0.027(2)
C(11)	4*e*	0.6344(3)	0.6405(2)	0.8609(3)	0.055(1)	0.098(2)	0.039(1)	–0.012(1)	0.018(1)	–0.013(1)
C(12)	4*e*	0.8026(3)	0.4406(2)	0.3235(3)	0.058(1)	0.079(2)	0.063(1)	0.025(1)	0.014(1)	–0.007(1)

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