Crystal structure of 4-(1',3'-dioxolane-2'-yl)-3-methyl-1,2,5-oxadiazole-2-oxide, C₆H₈N₂O₄

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Table 1. Parameters used for the X-ray data collection

Crystal:	colorless prism, size 0.2 x 0.2 x 0.6 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.30 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	1790
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	110
Program:	SHELXTL-plus

Source of material: The title compound was isolated as a by-product in the Michael addition of nitrous acid to crotonaldehyde, followed by acetalization with ethyleneglycol (see ref. 1). The title compound (mp 371–372 K) was then obtained by recrystallization from methylene chloride (see ref. 2).

C₆H₈N₂O₄, triclinic, $P\bar{1}$ (No. 2), $a = 7.210(2)$ Å, $b = 8.296(2)$ Å, $c = 7.038(2)$ Å, $\alpha = 104.30(2)^\circ$, $\beta = 81.65(2)^\circ$, $\gamma = 108.20(2)^\circ$, $V = 386.5$ Å³, $Z = 2$, $R(F) = 0.055$, $R_w(F) = 0.051$.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1A)	2i	0.1502(4)	0.6946(4)	−0.0558(5)	0.08
H(3A)	2i	0.3036(5)	0.8837(4)	0.4379(5)	0.08
H(3B)	2i	0.0986(5)	0.8901(4)	0.3961(5)	0.08
H(4A)	2i	−0.0090(5)	0.6054(4)	0.3030(5)	0.08
H(4B)	2i	0.1628(5)	0.6035(4)	0.4150(5)	0.08
H(11A)	2i	0.6159(5)	0.8099(5)	0.2338(5)	0.08
H(11B)	2i	0.8085(5)	0.9262(5)	0.1450(5)	0.08
H(11C)	2i	0.7866(5)	0.7305(5)	0.1360(5)	0.08

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(1)	2i	0.2585(4)	0.7175(4)	0.0216(5)	0.055(2)	0.058(2)	0.051(2)	0.019(1)	−0.004(1)	0.011(2)
O(2)	2i	0.2811(3)	0.8750(3)	0.1591(3)	0.092(2)	0.047(1)	0.065(2)	0.026(1)	0.022(1)	0.018(1)
C(3)	2i	0.2036(5)	0.8395(4)	0.3465(5)	0.079(2)	0.066(2)	0.053(2)	0.019(2)	0.005(2)	0.012(2)
C(4)	2i	0.1303(5)	0.6448(4)	0.3119(5)	0.069(2)	0.062(2)	0.058(2)	0.014(2)	0.007(2)	0.019(2)
O(5)	2i	0.2299(3)	0.5878(3)	0.1277(3)	0.074(1)	0.043(1)	0.066(1)	0.016(1)	0.014(1)	0.017(1)
C(6)	2i	0.4403(4)	0.7241(4)	−0.1136(4)	0.058(2)	0.045(2)	0.041(2)	0.016(1)	−0.003(1)	0.009(1)
N(7)	2i	0.4295(4)	0.6936(4)	−0.3024(4)	0.077(2)	0.083(2)	0.050(2)	0.024(2)	−0.005(1)	0.011(2)
O(8)	2i	0.6186(4)	0.7116(3)	−0.3846(3)	0.091(2)	0.089(2)	0.043(1)	0.029(1)	0.008(1)	0.011(1)
N(9)	2i	0.7445(4)	0.7561(3)	−0.2270(4)	0.066(2)	0.046(1)	0.056(2)	0.019(1)	0.007(1)	0.014(1)
O(9)	2i	0.9227(3)	0.7809(3)	−0.2718(4)	0.065(2)	0.075(2)	0.085(2)	0.023(1)	0.026(1)	0.024(1)

Table 3. (Continued)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(10)	2i	0.6334(4)	0.7633(4)	−0.0620(4)	0.058(2)	0.041(2)	0.045(2)	0.016(1)	0.005(1)	0.014(1)
C(11)	2i	0.7185(5)	0.8116(5)	0.1300(5)	0.059(2)	0.098(3)	0.059(2)	0.023(2)	−0.008(2)	0.014(2)

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