Crystal structure of [4*S*-[3(2*R**,3*Z*,5*R**),4*R**]]-3-[2,5-bis(acetyloxy)-1-oxo-3-hexenyl]-2,2-dimethyl-4-phenyl-oxazolidine, $[C_6H_7O(OCOCH_3)_2][C_3H_3NO(CH_3)_2C_6H_5]$

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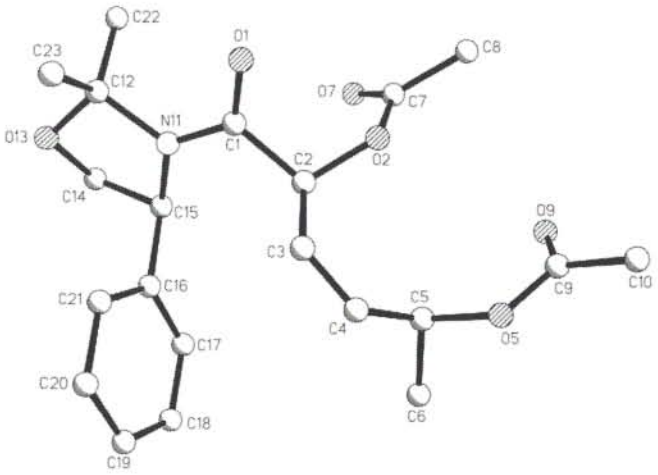

Abstract

$C_{21}H_{27}NO_6$, orthorhombic, $P2_12_12_1$ (No. 19), $a = 9.852(1)$ Å, $b = 10.258(1)$ Å, $c = 21.054(2)$ Å, $V = 2127.8$ Å^3, $Z = 4$, $R_{gt}(F) = 0.050$, $wR(F) = 0.050$, $T = 293$ K.

Source of material

The title compound was prepared according to [1].

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.45 × 0.65 × 0.75 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.90 cm^{-1}
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6682, 4883
Criterion for F_{obs}, $N(hkl)_{gt}$:	$F_{obs} > 3\ \sigma(F_{obs})$, 4212
$N(param)_{refined}$:	254
Program:	SHELXTL-plus [2]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(2)	4*a*	0.4473(2)	1.0414(2)	0.71967(8)	0.08
H(3)	4*a*	0.3318(2)	0.8012(2)	0.7329(1)	0.08
H(4)	4*a*	0.2113(2)	0.8181(2)	0.6445(1)	0.08
H(5)	4*a*	0.3818(2)	1.0313(2)	0.6092(1)	0.08
H(6A)	4*a*	0.1677(3)	1.1059(3)	0.6163(1)	0.08
H(6B)	4*a*	0.1162(3)	0.9940(3)	0.5717(1)	0.08
H(6C)	4*a*	0.2096(3)	1.1044(3)	0.5445(1)	0.08
H(8A)	4*a*	0.8594(2)	1.0431(3)	0.6255(1)	0.08
H(8B)	4*a*	0.7470(2)	0.9792(3)	0.5830(1)	0.08
H(8C)	4*a*	0.8249(2)	0.8948(3)	0.6332(1)	0.08
H(10A)	4*a*	0.5706(3)	0.8486(3)	0.4374(1)	0.08
H(10B)	4*a*	0.4154(3)	0.8184(3)	0.4300(1)	0.08
H(10C)	4*a*	0.5039(3)	0.7367(3)	0.4774(1)	0.08
H(14A)	4*a*	0.3196(2)	1.1794(2)	0.9158(1)	0.08

Table 2. Contiuned.

Atom	Site	*x*	*y*	*z*	U_{iso}
H(14B)	4*a*	0.4737(2)	1.2042(2)	0.9018(1)	0.08
H(15)	4*a*	0.4009(2)	1.1466(2)	0.80004(9)	0.08
H(17)	4*a*	0.1958(2)	1.2047(2)	0.7643(1)	0.08
H(18)	4*a*	−0.0333(3)	1.1559(3)	0.7466(1)	0.08
H(19)	4*a*	−0.1283(3)	0.9680(3)	0.7895(1)	0.08
H(20)	4*a*	0.0039(3)	0.8273(3)	0.8494(2)	0.08
H(21)	4*a*	0.2336(2)	0.8798(2)	0.8716(1)	0.08
H(22A)	4*a*	0.7301(2)	0.9435(3)	0.8865(1)	0.08
H(22B)	4*a*	0.6954(2)	0.9924(3)	0.9552(1)	0.08
H(22C)	4*a*	0.6801(2)	1.0870(3)	0.8971(1)	0.08
H(23A)	4*a*	0.5653(3)	0.7582(2)	0.8989(1)	0.08
H(23B)	4*a*	0.4132(3)	0.7865(2)	0.9158(1)	0.08
H(23C)	4*a*	0.5263(3)	0.8042(2)	0.9675(1)	0.08

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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*a*	0.5332(2)	0.9164(2)	0.78551(9)	0.040(1)	0.057(1)	0.041(1)	0.006(1)	0.0041(9)	–0.0050(9)
O(1)	4*a*	0.6217(2)	0.8329(2)	0.79012(8)	0.065(1)	0.087(1)	0.0545(9)	0.035(1)	–0.0021(8)	–0.0083(9)
C(2)	4*a*	0.4770(2)	0.9523(2)	0.71978(8)	0.046(1)	0.062(1)	0.0337(9)	0.003(1)	0.0045(8)	–0.0066(9)
O(2)	4*a*	0.5825(2)	0.9270(1)	0.67323(6)	0.0525(8)	0.0673(9)	0.0390(7)	–0.0079(7)	0.0105(6)	–0.0138(7)
C(3)	4*a*	0.3572(2)	0.8676(2)	0.7031(1)	0.051(1)	0.061(1)	0.043(1)	–0.005(1)	0.007(1)	–0.002(1)
C(4)	4*a*	0.2865(2)	0.8766(2)	0.6501(1)	0.048(1)	0.064(1)	0.048(1)	–0.006(1)	0.0016(9)	–0.010(1)
C(5)	4*a*	0.3120(2)	0.9705(2)	0.5974(1)	0.056(1)	0.063(1)	0.044(1)	0.000(1)	–0.010(1)	–0.009(1)
O(5)	4*a*	0.3480(2)	0.8892(2)	0.54210(7)	0.0574(9)	0.074(1)	0.0463(8)	–0.0054(9)	–0.0008(7)	–0.0109(8)
C(6)	4*a*	0.1908(3)	1.0512(3)	0.5809(1)	0.079(2)	0.097(2)	0.064(2)	0.021(2)	–0.013(1)	–0.014(1)
C(7)	4*a*	0.6847(2)	1.0138(2)	0.6718(1)	0.045(1)	0.066(1)	0.056(1)	–0.005(1)	–0.001(1)	–0.003(1)
O(7)	4*a*	0.6884(2)	1.1062(2)	0.7063(1)	0.0581(9)	0.077(1)	0.105(1)	–0.011(1)	0.005(1)	–0.034(1)
C(8)	4*a*	0.7880(2)	0.9795(3)	0.6243(1)	0.059(1)	0.112(2)	0.073(2)	–0.020(2)	0.021(1)	–0.017(2)
C(9)	4*a*	0.4585(3)	0.9200(3)	0.5091(1)	0.069(2)	0.075(1)	0.050(1)	–0.001(1)	–0.002(1)	0.003(1)
O(9)	4*a*	0.5258(3)	1.0148(2)	0.5198(1)	0.129(2)	0.106(2)	0.106(2)	–0.046(2)	0.045(2)	–0.029(1)
C(10)	4*a*	0.4899(3)	0.8216(3)	0.4593(1)	0.073(2)	0.094(2)	0.049(1)	0.013(2)	0.001(1)	0.000(1)
N(11)	4*a*	0.4780(2)	0.9764(2)	0.83585(7)	0.0414(8)	0.0512(8)	0.0343(7)	0.0061(8)	0.0018(7)	0.0002(7)
C(12)	4*a*	0.5254(2)	0.9520(2)	0.90235(9)	0.057(1)	0.061(1)	0.0330(9)	0.004(1)	0.0018(9)	–0.0003(9)
O(13)	4*a*	0.4343(2)	1.0301(2)	0.93827(6)	0.067(1)	0.0672(9)	0.0354(7)	0.0019(8)	0.0088(6)	–0.0015(7)
C(14)	4*a*	0.4023(2)	1.1406(2)	0.9008(1)	0.052(1)	0.051(1)	0.049(1)	–0.001(1)	0.0049(9)	–0.010(1)
C(15)	4*a*	0.3822(2)	1.0865(2)	0.83389(9)	0.0400(9)	0.0440(9)	0.0402(9)	0.0007(9)	0.0042(8)	–0.0009(8)
C(16)	4*a*	0.2355(2)	1.0477(2)	0.81988(9)	0.043(1)	0.049(1)	0.040(1)	–0.0002(9)	0.0072(8)	–0.0090(9)
C(17)	4*a*	0.1563(2)	1.1281(2)	0.7829(1)	0.050(1)	0.068(1)	0.051(1)	0.002(1)	–0.001(1)	0.006(1)
C(18)	4*a*	0.0211(3)	1.0984(3)	0.7721(1)	0.050(1)	0.107(2)	0.060(1)	0.002(2)	–0.006(1)	0.005(1)
C(19)	4*a*	–0.0342(3)	0.9872(3)	0.7966(1)	0.044(1)	0.112(2)	0.069(2)	–0.009(2)	–0.003(1)	–0.010(2)
C(20)	4*a*	0.0426(3)	0.9064(3)	0.8331(2)	0.057(1)	0.074(2)	0.092(2)	–0.022(1)	0.010(1)	–0.006(1)
C(21)	4*a*	0.1792(2)	0.9363(2)	0.8456(1)	0.049(1)	0.061(1)	0.075(2)	–0.005(1)	0.004(1)	0.005(1)
C(22)	4*a*	0.6711(2)	0.9983(3)	0.9111(1)	0.060(1)	0.105(2)	0.049(1)	0.007(1)	–0.015(1)	0.001(1)
C(23)	4*a*	0.5054(3)	0.8127(2)	0.9231(1)	0.094(2)	0.073(2)	0.055(1)	0.013(2)	–0.003(1)	0.015(1)

References

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