Crystal structure of dimethyl (2*R**,3*R**,3*aR**,4*R**,5*S**,6*aR**)-3,5-butano-4-hydroxy-2-methoxy-1-oxa-6-oxo-perhydro-pentalene-3*a*,4-dicarboxylate, C₁₁H₁₂O₂(OH)(OCH₃)(COOCH₃)₂

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

Crystal:	colorless prism, size 0.25 x 0.3 x 0.5 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.10 cm ⁻¹
Diffractometer:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	3692
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	222
Program:	SHELXTL-plus

Source of material: The title compound was prepared as described in ref. 1.

C₁₆H₂₂O₈, monoclinic, $P12_1/n1$ (No. 14), $a = 7.882(1)$ Å, $b = 10.735(1)$ Å, $c = 19.180(1)$ Å, $\beta = 96.79(1)^\circ$, $V = 1611.5$ Å³, $Z = 4$, $R(F) = 0.070$, $R_w(F) = 0.074$.

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

Atom	Site	x	y	z	U_{iso}
H(2)	4e	0.3846(4)	0.5646(3)	0.3771(2)	0.08
H(3)	4e	0.5520(4)	0.3791(3)	0.4450(2)	0.08
H(4)	4e	0.585(5)	0.092(3)	0.448(2)	0.05(1)
H(5)	4e	0.3501(4)	0.0641(3)	0.2771(1)	0.08
H(7)	4e	0.1038(3)	0.2796(3)	0.3424(1)	0.08
H(9A)	4e	0.5419(4)	0.1082(4)	0.2153(2)	0.08
H(9B)	4e	0.6344(4)	0.0617(4)	0.2875(2)	0.08
H(10A)	4e	0.8004(5)	0.2053(4)	0.2546(2)	0.08
H(10B)	4e	0.6473(5)	0.2937(4)	0.2289(2)	0.08
H(11A)	4e	0.8343(5)	0.3634(4)	0.3277(2)	0.08
H(11B)	4e	0.7517(5)	0.2611(4)	0.3713(2)	0.08
H(12A)	4e	0.6472(5)	0.4851(3)	0.3551(2)	0.08
H(12B)	4e	0.5186(5)	0.4124(3)	0.3012(2)	0.08
H(20A)	4e	0.1007(6)	0.6141(4)	0.4933(2)	0.08
H(20B)	4e	0.0528(6)	0.5873(4)	0.4130(2)	0.08
H(20C)	4e	0.1993(6)	0.6817(4)	0.4379(2)	0.08
H(42A)	4e	-0.0978(4)	-0.0184(4)	0.3580(2)	0.08
H(42B)	4e	-0.0113(4)	-0.0016(4)	0.4354(2)	0.08
H(42C)	4e	0.0382(4)	-0.1152(4)	0.3905(2)	0.08
H(82A)	4e	0.4541(5)	0.2249(3)	0.6255(2)	0.08
H(82B)	4e	0.3031(5)	0.1429(3)	0.5902(2)	0.08
H(82C)	4e	0.2745(5)	0.2850(3)	0.6035(2)	0.08

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

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	4e	0.2143(3)	0.4402(2)	0.3362(1)	0.052(1)	0.036(1)	0.045(1)	0.008(1)	-0.005(1)	0.0053(9)
C(2)	4e	0.3386(4)	0.4867(3)	0.3906(2)	0.047(2)	0.031(2)	0.048(2)	0.001(1)	0.006(1)	-0.001(1)
O(2)	4e	0.2667(3)	0.5069(2)	0.4530(1)	0.049(1)	0.043(1)	0.045(1)	0.011(1)	0.007(1)	-0.006(1)
C(3)	4e	0.4732(4)	0.3849(3)	0.4030(2)	0.034(2)	0.033(2)	0.044(2)	-0.002(1)	0.002(1)	-0.000(1)
C(4)	4e	0.4161(3)	0.1376(2)	0.3780(1)	0.028(1)	0.031(1)	0.029(1)	0.003(1)	0.002(1)	0.000(1)
O(4)	4e	0.5820(3)	0.1089(2)	0.4082(1)	0.029(1)	0.044(1)	0.033(1)	0.0069(8)	-0.0007(8)	0.0042(9)
C(5)	4e	0.4013(4)	0.1396(3)	0.2964(1)	0.038(2)	0.039(2)	0.029(1)	0.005(1)	0.000(1)	-0.004(1)
C(6)	4e	0.2875(4)	0.2493(3)	0.2741(2)	0.042(2)	0.042(2)	0.031(1)	-0.001(1)	-0.005(1)	0.001(1)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O(6)	4e	0.2520(4)	0.2861(3)	0.2153(1)	0.082(2)	0.068(2)	0.035(1)	0.015(1)	-0.008(1)	0.006(1)
C(7)	4e	0.2184(3)	0.3073(3)	0.3389(1)	0.031(1)	0.036(1)	0.035(1)	0.005(1)	-0.001(1)	0.004(1)
C(8)	4e	0.3520(3)	0.2697(3)	0.3997(1)	0.025(1)	0.029(1)	0.030(1)	0.003(1)	0.001(1)	-0.000(1)
C(9)	4e	0.5718(4)	0.1292(4)	0.2638(2)	0.049(2)	0.068(2)	0.035(2)	0.004(2)	0.010(1)	-0.008(1)
C(10)	4e	0.6932(5)	0.2379(4)	0.2655(2)	0.047(2)	0.078(3)	0.046(2)	0.005(2)	0.015(2)	0.000(2)
C(11)	4e	0.7324(5)	0.3163(4)	0.3318(2)	0.050(2)	0.067(2)	0.069(2)	-0.004(2)	0.020(2)	0.005(2)
C(12)	4e	0.5922(5)	0.4063(3)	0.3446(2)	0.049(2)	0.050(2)	0.080(3)	-0.007(2)	0.023(2)	0.002(2)
C(20)	4e	0.1448(6)	0.6055(4)	0.4490(2)	0.076(3)	0.072(3)	0.068(2)	0.039(2)	0.008(2)	-0.009(2)
C(40)	4e	0.2925(4)	0.0397(3)	0.4020(1)	0.035(1)	0.033(1)	0.035(1)	0.001(1)	0.001(1)	-0.002(1)
O(40)	4e	0.3287(3)	-0.0303(2)	0.4500(1)	0.051(1)	0.051(1)	0.044(1)	-0.009(1)	-0.006(1)	0.017(1)
O(41)	4e	0.1398(3)	0.0446(2)	0.3642(1)	0.035(1)	0.042(1)	0.046(1)	-0.0068(9)	-0.0031(9)	0.0044(9)
C(42)	4e	0.0060(4)	-0.0289(4)	0.3891(2)	0.042(2)	0.060(2)	0.065(2)	-0.019(2)	0.005(2)	0.002(2)
C(80)	4e	0.2779(4)	0.2551(2)	0.4697(2)	0.033(1)	0.032(1)	0.033(1)	0.001(1)	0.007(1)	-0.004(1)
O(80)	4e	0.1304(3)	0.2373(2)	0.4761(1)	0.033(1)	0.059(1)	0.051(1)	-0.000(1)	0.014(1)	-0.005(1)
O(81)	4e	0.4043(3)	0.2528(2)	0.5229(1)	0.040(1)	0.052(1)	0.030(1)	-0.005(1)	0.0044(9)	0.0021(8)
C(82)	4e	0.3548(5)	0.2240(3)	0.5912(2)	0.060(2)	0.059(2)	0.034(2)	-0.008(2)	0.011(1)	0.002(1)

References

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