Crystal structure of dimethyl (12*R**,13*R**)-3,11-dioxo-2,12-epoxycyclotri-dec-1-ene-1,13-dicarboxylate, $C_{17}H_{22}O_7(CO)_2(CH_2)_7(COOCH_3)_2$

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Source of material: The title compound was prepared from 3,4-heptamethylenefuran and dimethyl acetylene dicarboxylate as described in ref. 1.

$C_{17}H_{22}O_7$, monoclinic, $C1c1$ (No. 9), $a=12.703(3)$ Å, $b=21.322(7)$ Å, $c=8.758(2)$ Å, $\beta=132.22(1)^\circ$, $V=1756.7$ Å³, $Z=4$, $R(F)=0.040$, $R_w(F)=0.036$.

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

Crystal:	colorless prism, size 0.4 x 0.8 x 0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ :	1.00 cm ⁻¹
Diffractionmeter:	Siemens P4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	2116
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	216
Program:	SHELXTL-plus

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

Atom	Site	x	y	z	U_{iso}
H(4A)	4a	0.2670(5)	0.3466(2)	-0.0763(6)	0.08
H(4B)	4a	0.1175(5)	0.3737(2)	-0.2655(6)	0.08
H(5A)	4a	0.1678(4)	0.4679(2)	-0.1235(7)	0.08
H(5B)	4a	0.2871(4)	0.4419(2)	0.1005(7)	0.08
H(6A)	4a	0.3735(4)	0.5019(2)	-0.0286(7)	0.08
H(6B)	4a	0.3246(4)	0.4463(2)	-0.1810(7)	0.08
H(7A)	4a	0.4833(4)	0.3811(2)	0.1096(6)	0.08
H(7B)	4a	0.5586(4)	0.4324(2)	0.0836(6)	0.08
H(8A)	4a	0.5123(4)	0.4521(1)	0.3499(6)	0.08
H(8B)	4a	0.6177(4)	0.4893(1)	0.3476(6)	0.08
H(9A)	4a	0.7587(4)	0.3973(1)	0.4745(6)	0.08
H(9B)	4a	0.7554(4)	0.4301(1)	0.6315(6)	0.08
H(10A)	4a	0.7312(4)	0.3213(1)	0.6349(6)	0.08
H(10B)	4a	0.5934(4)	0.3232(1)	0.4001(6)	0.08
H(12A)	4a	0.4881(4)	0.2673(1)	0.5643(5)	0.08
H(13A)	4a	0.3915(4)	0.3510(1)	0.6553(5)	0.08
H(16A)	4a	-0.1439(5)	0.4732(2)	-0.0230(7)	0.08
H(16B)	4a	-0.0565(5)	0.4752(2)	0.2145(7)	0.08
H(16C)	4a	-0.1537(5)	0.4174(2)	0.0836(7)	0.08
H(19A)	4a	0.3633(5)	0.2196(2)	0.9804(7)	0.08
H(19B)	4a	0.3563(5)	0.1767(2)	0.8282(7)	0.08
H(19C)	4a	0.2195(5)	0.2116(2)	0.7519(7)	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)	4a	0.3525	0.30676(8)	0.2745	0.044(1)	0.055(1)	0.042(1)	0.002(1)	0.0280(9)	-0.0046(9)
C(1)	4a	0.2200(4)	0.3506(1)	0.3320(5)	0.043(2)	0.053(1)	0.043(2)	-0.002(1)	0.030(1)	0.001(1)

Table 3. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(2)	4a	0.2307(3)	0.3365(1)	0.1956(5)	0.041(1)	0.041(1)	0.043(1)	-0.004(1)	0.028(1)	-0.001(1)
C(3)	4a	0.1285(4)	0.3452(1)	-0.0355(5)	0.046(2)	0.049(2)	0.042(2)	-0.003(1)	0.028(2)	-0.005(1)
O(3)	4a	0.0075(3)	0.3277(1)	-0.1398(4)	0.050(1)	0.096(2)	0.048(1)	-0.012(1)	0.025(1)	-0.002(1)
C(4)	4a	0.1900(5)	0.3727(2)	-0.1177(6)	0.073(2)	0.095(3)	0.041(2)	-0.021(2)	0.038(2)	-0.005(2)
C(5)	4a	0.2459(4)	0.4391(2)	-0.0397(7)	0.063(2)	0.063(2)	0.080(3)	0.006(2)	0.043(2)	0.023(2)
C(6)	4a	0.3591(4)	0.4573(2)	-0.0478(7)	0.080(3)	0.087(3)	0.075(2)	-0.010(2)	0.048(2)	0.025(2)
C(7)	4a	0.5000(4)	0.4252(2)	0.1145(6)	0.071(2)	0.092(3)	0.080(3)	-0.003(2)	0.059(2)	0.013(2)
C(8)	4a	0.5795(4)	0.4487(1)	0.3332(6)	0.068(2)	0.053(2)	0.081(3)	-0.008(2)	0.046(2)	0.007(2)
C(9)	4a	0.7002(4)	0.4074(1)	0.5040(6)	0.052(2)	0.068(2)	0.075(2)	-0.010(2)	0.040(2)	0.000(2)
C(10)	4a	0.6493(4)	0.3457(1)	0.5281(6)	0.046(2)	0.055(2)	0.074(2)	0.004(1)	0.039(2)	0.006(2)
C(11)	4a	0.5610(3)	0.3553(1)	0.5827(5)	0.041(2)	0.044(1)	0.049(2)	0.003(1)	0.024(1)	0.004(1)
O(11)	4a	0.5771(3)	0.3987(1)	0.6846(5)	0.066(1)	0.062(1)	0.082(2)	-0.016(1)	0.047(1)	-0.021(1)
C(12)	4a	0.4433(4)	0.3067(1)	0.4983(5)	0.046(2)	0.042(1)	0.043(2)	0.001(1)	0.026(1)	0.004(1)
C(13)	4a	0.3475(4)	0.3235(1)	0.5395(5)	0.052(2)	0.052(1)	0.040(1)	-0.004(1)	0.031(1)	-0.000(1)
C(14)	4a	0.1056(4)	0.3826(2)	0.3039(6)	0.046(2)	0.087(2)	0.048(2)	-0.003(2)	0.029(2)	-0.010(2)
O(14)	4a	0.0899(4)	0.3785(2)	0.4229(5)	0.089(2)	0.213(4)	0.082(2)	0.037(2)	0.072(2)	0.017(2)
O(15)	4a	0.0257(3)	0.4179(1)	0.1395(5)	0.067(2)	0.082(2)	0.080(2)	0.024(1)	0.050(2)	0.007(1)
C(16)	4a	-0.0920(5)	0.4485(2)	0.1004(7)	0.059(3)	0.129(4)	0.100(4)	0.027(3)	0.037(3)	-0.018(3)
C(17)	4a	0.3046(4)	0.2665(2)	0.5900(6)	0.072(2)	0.064(2)	0.053(2)	-0.009(2)	0.044(2)	0.001(2)
O(17)	4a	0.2337(5)	0.2250(1)	0.4730(5)	0.179(3)	0.098(2)	0.083(2)	-0.076(2)	0.086(2)	-0.025(2)
O(18)	4a	0.3564(4)	0.2678(1)	0.7792(4)	0.091(2)	0.078(1)	0.060(1)	0.005(1)	0.056(1)	0.017(1)
C(19)	4a	0.3209(5)	0.2144(2)	0.8401(7)	0.151(5)	0.097(3)	0.112(4)	0.019(3)	0.110(4)	0.036(3)

References

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2. Sheldrick, G. M.: Program Package SHELXTL-plus. Release 4.1. Siemens Analytical X-Ray Instruments Inc., Madison (WI 53719), USA 1990.