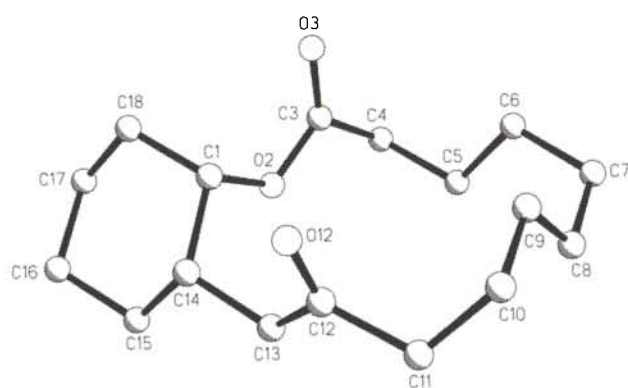


Crystal structure of (1*S*,14*S*)-(+)-2-oxabicyclo[12.4.0]octadecan-3,12-dione, (CH₂COC₈H₁₆COO)(C₆H₁₀)

K. Peters*¹, E.-M. Peters¹, B. Bollbuck^{II} and W. Tochtermann^{II}¹ Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70506 Stuttgart, Germany^{II} Universität Kiel, Institut für Organische Chemie, Olshausenstraße 40, D-24098 Kiel, Germany

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**Abstract**

C₁₇H₂₈O₃, orthorhombic, *P*2₁2₁2₁ (No. 19), *a* = 5.559(1) Å, *b* = 15.381(4) Å, *c* = 19.203(6) Å, *V* = 1641.9 Å³, *Z* = 4, *R*_{gt}(*F*) = 0.056, *wR*(*F*) = 0.050, *T* = 293 K.

Source of material

The title compound was prepared as described in [1, 2].

Table 1. Data collection and handling.

Crystal:	colourless column, size 0.4 × 0.55 × 1.2 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71073 Å)
μ:	0.80 cm ⁻¹
Diffractionmeter, scan mode:	Bruker AXS P4, ω
2θ _{max} :	55°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	5185, 3684
Criterion for <i>F</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>F</i> _{obs} > 3 σ(<i>F</i> _{obs}), 2821
<i>N</i> (<i>param</i>) _{refined} :	181
Program:	SHELXTL-plus [3]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4 <i>a</i>	1.1585(4)	0.6722(1)	0.3228(1)	0.08
H(4A)	4 <i>a</i>	0.4582(4)	0.7890(1)	0.3399(1)	0.08
H(4B)	4 <i>a</i>	0.5772(4)	0.8758(1)	0.3145(1)	0.08
H(5A)	4 <i>a</i>	0.3490(4)	0.8064(1)	0.2254(1)	0.08
H(5B)	4 <i>a</i>	0.5324(4)	0.7290(1)	0.2278(1)	0.08
H(6A)	4 <i>a</i>	0.6379(5)	0.8973(2)	0.1836(1)	0.08
H(6B)	4 <i>a</i>	0.8373(5)	0.8263(2)	0.1936(1)	0.08
H(7A)	4 <i>a</i>	0.4648(6)	0.8112(2)	0.0956(2)	0.08
H(7B)	4 <i>a</i>	0.7241(6)	0.8431(2)	0.0762(2)	0.08
H(8A)	4 <i>a</i>	0.6660(5)	0.6986(2)	0.0442(1)	0.08
H(8B)	4 <i>a</i>	0.6203(5)	0.6746(2)	0.1225(1)	0.08
H(9A)	4 <i>a</i>	1.0129(5)	0.7071(2)	0.1484(1)	0.08
H(9B)	4 <i>a</i>	1.0586(5)	0.7312(2)	0.0702(1)	0.08
H(10A)	4 <i>a</i>	0.9876(5)	0.5857(2)	0.0413(1)	0.08
H(10B)	4 <i>a</i>	1.2188(5)	0.5990(2)	0.0868(1)	0.08
H(11A)	4 <i>a</i>	0.7817(5)	0.5423(2)	0.1419(1)	0.08
H(11B)	4 <i>a</i>	0.9914(5)	0.4788(2)	0.1221(1)	0.08
H(13A)	4 <i>a</i>	0.7570(4)	0.5709(1)	0.2638(1)	0.08
H(13B)	4 <i>a</i>	0.8447(4)	0.4744(1)	0.2699(1)	0.08
H(14)	4 <i>a</i>	1.1541(4)	0.5269(1)	0.3433(1)	0.08
H(15A)	4 <i>a</i>	0.8331(5)	0.4516(2)	0.3925(2)	0.08
H(15B)	4 <i>a</i>	0.6851(5)	0.5381(2)	0.3978(2)	0.08
H(16A)	4 <i>a</i>	1.1059(7)	0.5033(3)	0.4738(2)	0.08
H(16B)	4 <i>a</i>	0.8476(7)	0.5072(3)	0.5064(2)	0.08
H(17A)	4 <i>a</i>	0.8251(7)	0.6541(2)	0.4823(1)	0.08
H(17B)	4 <i>a</i>	1.0541(7)	0.6364(2)	0.5278(1)	0.08
H(18A)	4 <i>a</i>	1.2958(5)	0.6441(2)	0.4305(1)	0.08
H(18B)	4 <i>a</i>	1.1432(5)	0.7297(2)	0.4346(1)	0.08

Table 3. 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)	4 <i>a</i>	1.0396(4)	0.6506(1)	0.3547(1)	0.051(1)	0.048(1)	0.057(1)	0.0005(9)	-0.0038(9)	-0.0028(9)
O(2)	4 <i>a</i>	0.8105(2)	0.69418(8)	0.34407(8)	0.0503(7)	0.0433(7)	0.0670(9)	-0.0033(6)	0.0013(7)	-0.0014(6)
C(3)	4 <i>a</i>	0.8175(3)	0.7794(1)	0.3288(1)	0.050(1)	0.043(1)	0.065(1)	0.001(1)	0.003(1)	-0.0080(9)
O(3)	4 <i>a</i>	0.9992(3)	0.82099(9)	0.3287(1)	0.0543(8)	0.0475(8)	0.131(2)	-0.0061(7)	-0.0046(9)	-0.0015(8)
C(4)	4 <i>a</i>	0.5770(4)	0.8137(1)	0.3095(1)	0.057(1)	0.049(1)	0.081(2)	0.000(1)	0.000(1)	-0.003(1)

* Correspondence author

(e-mail: karp@vsibml.mpi-stuttgart.mpg.de)

Table 3. Continued.

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
C(5)	4a	0.5135(4)	0.7906(1)	0.2338(1)	0.060(1)	0.057(1)	0.082(2)	-0.001(1)	-0.005(1)	0.007(1)
C(6)	4a	0.6721(5)	0.8362(2)	0.1814(1)	0.090(2)	0.052(1)	0.091(2)	-0.011(1)	-0.001(1)	0.012(1)
C(7)	4a	0.6328(6)	0.8057(2)	0.1063(2)	0.104(2)	0.080(2)	0.083(2)	-0.007(2)	-0.012(1)	0.029(2)
C(8)	4a	0.7082(5)	0.7119(2)	0.0915(1)	0.099(2)	0.086(2)	0.064(2)	-0.013(2)	-0.020(1)	0.011(1)
C(9)	4a	0.9708(5)	0.6938(2)	0.1011(1)	0.096(2)	0.082(2)	0.063(1)	-0.020(2)	-0.005(1)	0.015(1)
C(10)	4a	1.0463(5)	0.6015(2)	0.0866(1)	0.101(2)	0.101(2)	0.055(1)	-0.003(2)	0.001(1)	-0.005(1)
C(11)	4a	0.9532(5)	0.5361(2)	0.1384(1)	0.104(2)	0.059(1)	0.070(2)	-0.005(1)	-0.023(1)	-0.009(1)
C(12)	4a	1.0606(4)	0.5480(1)	0.2102(1)	0.069(1)	0.045(1)	0.064(1)	0.000(1)	-0.011(1)	-0.003(1)
O(12)	4a	1.2702(3)	0.5663(1)	0.21813(9)	0.072(1)	0.097(1)	0.068(1)	-0.0028(9)	-0.0010(8)	-0.0023(9)
C(13)	4a	0.8946(4)	0.5341(1)	0.2704(1)	0.063(1)	0.044(1)	0.076(2)	-0.0014(9)	-0.006(1)	-0.005(1)
C(14)	4a	0.9981(4)	0.5535(1)	0.3420(1)	0.061(1)	0.046(1)	0.061(1)	-0.000(1)	0.003(1)	-0.0005(9)
C(15)	4a	0.8434(5)	0.5133(2)	0.3996(2)	0.105(2)	0.060(1)	0.090(2)	-0.009(1)	0.014(2)	0.013(1)
C(16)	4a	0.9510(7)	0.5307(3)	0.4711(2)	0.154(3)	0.113(2)	0.076(2)	0.006(2)	0.026(2)	0.032(2)
C(17)	4a	0.9807(7)	0.6271(2)	0.4831(1)	0.135(3)	0.117(3)	0.057(1)	0.012(2)	0.004(2)	-0.013(2)
C(18)	4a	1.1367(5)	0.6680(2)	0.4272(1)	0.082(2)	0.078(2)	0.067(2)	0.008(1)	-0.014(1)	-0.014(1)

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