Crystal structure of (1*S**,2*R**,9*R**,10*S**)-2,10-diacetoxi-13-oxa-bicyclo[7.3.1]tridec-5-ene, C₁₆H₂₄O₅

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Abstract

C₁₆H₂₄O₅, monoclinic, *P*12₁/*c*1 (No. 14), *a* = 14.941(2) Å, *b* = 11.213(2) Å, *c* = 9.888(2) Å, β = 101.4(1)°, *V* = 1623.9 Å³, *Z* = 4, *R*_g(*F*) = 0.051, *R*_w(*F*²) = 0.113, *T* = 293 K.

Source of material

The compound was prepared using literature procedures [1–3].

Discussion

The molecular structure of this compound possesses a ten-membered ring trans-fused with a six-membered ring, and two acetoxi-group. In the cyclodecane part of the molecule, there is only C=C double bond, namely C5=C6; all the other C–C bond lengths have values in the simple bond range, with C4–C5 and C6–C7 being Csp²–Csp³ bonds, while the rest are Csp³–Csp³ and Csp³–O. The six-membered ring exhibits a slightly distorted chair conformation. All distances and angles are normal.

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.15 x 0.16 x 0.12 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	0.89 cm ⁻¹
Diffractometer, scan mode:	Siemens R3m/V, ω
2θ _{max} :	62°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	5496, 5220
Criterion for <i>F</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>F</i> _{obs} > 3 σ(<i>F</i> _{obs}), 1365
<i>N</i> (<i>param</i>) _{refined} :	190
Programs:	SHELXS-86 [4], SHELXL-93 [5]

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)	4e	0.2117(2)	0.5265(2)	−0.2805(3)	0.062
H(2)	4e	0.1820(2)	0.5567(2)	−0.0084(2)	0.060
H(3A)	4e	0.0319(2)	0.4990(2)	−0.1006(3)	0.069
H(3B)	4e	0.0546(2)	0.4879(2)	−0.2477(3)	0.069
H(4A)	4e	0.0644(2)	0.6944(2)	−0.2644(2)	0.062
H(4B)	4e	−0.0316(2)	0.6579(2)	−0.2373(2)	0.062
H(5)	4e	0.0176(1)	0.7215(2)	−0.0037(2)	0.061
H(6)	4e	0.0913(2)	0.8874(2)	0.0200(2)	0.062
H(7A)	4e	0.1300(1)	0.9842(2)	−0.1677(2)	0.062
H(7B)	4e	0.1233(1)	0.8640(2)	−0.2500(2)	0.062
H(8A)	4e	0.2769(1)	0.9106(2)	−0.1888(3)	0.062
H(8B)	4e	0.2698(1)	0.9307(2)	−0.0343(3)	0.062
H(9)	4e	0.2478(1)	0.7281(2)	−0.0044(2)	0.053
H(10)	4e	0.3979(1)	0.7448(2)	−0.1424(3)	0.064
H(11A)	4e	0.3644(2)	0.5758(2)	0.0567(3)	0.084
H(11B)	4e	0.4507(2)	0.5738(2)	−0.0120(3)	0.084
H(12A)	4e	0.3356(2)	0.4371(2)	−0.1200(3)	0.085
H(12B)	4e	0.3630(2)	0.5281(2)	−0.2252(3)	0.085
H(14A)	4e	0.2019(2)	0.1840(2)	−0.0576(3)	0.126
H(14B)	4e	0.1758(2)	0.1729(2)	0.0878(3)	0.126
H(14C)	4e	0.2781(2)	0.1896(2)	0.0762(3)	0.126
H(16A)	4e	0.5030(2)	0.9080(3)	0.2392(3)	0.134
H(16B)	4e	0.5700(2)	0.9682(3)	0.1562(3)	0.134
H(16C)	4e	0.5983(2)	0.8499(3)	0.2379(3)	0.134

Table 3. 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(13)	4e	0.22940(9)	0.6867(1)	−0.2040(2)	0.0435(9)	0.0451(9)	0.0496(9)	−0.0010(7)	0.0040(7)	0.0003(8)
O(2)	4e	0.1810(1)	0.3891(1)	−0.0839(2)	0.106(1)	0.0330(9)	0.060(1)	−0.0055(9)	0.007(1)	−0.0023(9)
O(3)	4e	0.2180(2)	0.3997(2)	0.1434(2)	0.173(2)	0.068(1)	0.063(1)	0.023(1)	0.002(1)	0.003(1)
O(4)	4e	0.4199(1)	0.7964(1)	0.0556(2)	0.0342(9)	0.069(1)	0.066(1)	−0.0073(8)	0.0012(8)	−0.0035(9)
O(5)	4e	0.5476(1)	0.7917(3)	−0.0263(3)	0.056(1)	0.208(3)	0.125(2)	−0.037(2)	0.034(1)	−0.060(2)
C(1)	4e	0.2341(2)	0.5598(2)	−0.1884(3)	0.057(2)	0.041(1)	0.055(2)	0.001(1)	0.010(1)	−0.004(1)
C(2)	4e	0.1679(2)	0.5179(2)	−0.0990(2)	0.064(2)	0.031(1)	0.052(1)	−0.004(1)	0.005(1)	−0.002(1)
C(3)	4e	0.0674(2)	0.5338(2)	−0.1629(3)	0.056(2)	0.058(2)	0.060(2)	−0.016(1)	0.014(1)	−0.006(1)
C(4)	4e	0.0329(2)	0.6613(2)	−0.1961(2)	0.042(1)	0.058(2)	0.052(2)	−0.009(1)	0.001(1)	−0.004(1)
C(5)	4e	0.0453(1)	0.7437(2)	−0.0762(2)	0.045(1)	0.058(2)	0.050(1)	−0.001(1)	0.013(1)	−0.002(1)
C(6)	4e	0.0914(2)	0.8453(2)	−0.0610(2)	0.044(1)	0.054(2)	0.054(2)	0.009(1)	0.005(1)	−0.005(1)
C(7)	4e	0.1436(1)	0.8996(2)	−0.1597(2)	0.044(1)	0.042(1)	0.065(2)	0.005(1)	0.003(1)	0.010(1)
C(8)	4e	0.2475(1)	0.8828(2)	−0.1156(3)	0.044(1)	0.042(1)	0.069(2)	−0.003(1)	0.008(1)	0.008(1)
C(9)	4e	0.2724(1)	0.7539(2)	−0.0844(2)	0.035(1)	0.040(1)	0.056(1)	0.002(1)	0.002(1)	0.002(1)
C(10)	4e	0.3737(1)	0.7257(2)	−0.0598(3)	0.037(1)	0.058(2)	0.062(2)	−0.001(1)	0.005(1)	−0.002(1)
C(11)	4e	0.3864(2)	0.5939(2)	−0.0270(3)	0.044(1)	0.062(2)	0.099(2)	0.017(1)	0.002(1)	0.002(2)
C(12)	4e	0.3336(2)	0.5205(2)	−0.1465(3)	0.062(2)	0.052(2)	0.098(2)	0.010(1)	0.012(2)	−0.009(2)
C(13)	4e	0.2051(2)	0.3420(2)	0.0414(3)	0.056(2)	0.048(2)	0.067(2)	−0.002(1)	0.005(1)	0.006(2)
C(14)	4e	0.2162(2)	0.2105(2)	0.0365(3)	0.095(2)	0.046(2)	0.111(3)	−0.001(1)	0.019(2)	0.017(2)
C(15)	4e	0.5073(2)	0.8230(3)	0.0607(3)	0.043(2)	0.092(2)	0.081(2)	−0.009(2)	0.012(2)	−0.002(2)
C(16)	4e	0.5483(2)	0.8935(3)	0.1844(3)	0.059(2)	0.118(3)	0.087(2)	−0.036(2)	0.003(2)	−0.005(2)

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