Crystal structure of [1*R**,2*S**,3*R**(*S**),4*S**]- α -oxo-3-(10-oxo-9-phenyl-bicyclo[6.2.0]-dec-1(8)-en-9-ylbicyclo[2.2.1]heptane-2-acetic acid methyl ester, C₄O(C₆H₁₂)(C₆H₅)[C₇H₁₀(C₃H₃O₃)]

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Source of material: The title compound was prepared according to ref. 1.

C₂₆H₃₀O₄, triclinic, $P\bar{1}$ (No. 2), $a = 10.611(2)$ Å, $b = 10.635(2)$ Å, $c = 11.528(2)$ Å, $\alpha = 96.95(3)^\circ$, $\beta = 112.57(3)^\circ$, $\gamma = 110.79(3)^\circ$, $V = 1072.1$ Å³, $Z = 2$, $R(F) = 0.052$, $R_w(F) = 0.049$.

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

Crystal:	colorless plate, size 0.4 x 0.85 x 0.25 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.80 cm ⁻¹
Diffractometer:	Nicolet P3
Scan mode:	Wyckoff
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	3904
Criterion for F_o :	$F_o > 3 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	272
Program:	SHELXTL-plus

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

Atom	Site	x	y	z	U_{iso}
H(1)	2i	0.2676(3)	0.0268(2)	-0.3677(2)	0.08
H(2)	2i	0.4160(2)	0.2988(2)	-0.2762(2)	0.08
H(3)	2i	0.3897(2)	0.3770(2)	-0.1043(2)	0.08
H(4)	2i	0.2173(2)	0.1738(2)	-0.0566(2)	0.08
H(5A)	2i	0.4919(3)	0.2359(3)	0.0085(2)	0.08
H(5B)	2i	0.3956(3)	0.0803(3)	-0.0016(2)	0.08
H(6A)	2i	0.5214(3)	0.1595(3)	-0.1633(2)	0.08
H(6B)	2i	0.4283(3)	0.0038(3)	-0.1714(2)	0.08
H(7A)	2i	0.0768(3)	0.0435(2)	-0.2976(2)	0.08
H(7B)	2i	0.1476(3)	-0.0472(2)	-0.2227(2)	0.08
H(10A)	2i	-0.1151(2)	0.2431(3)	-0.4050(2)	0.08
H(10B)	2i	-0.1027(2)	0.1094(3)	-0.3679(2)	0.08
H(11A)	2i	-0.2584(3)	0.2279(3)	-0.2827(3)	0.08
H(11B)	2i	-0.3432(3)	0.1175(3)	-0.4223(3)	0.08
H(12A)	2i	-0.3239(3)	-0.0559(3)	-0.3364(3)	0.08
H(12B)	2i	-0.3826(3)	0.0207(3)	-0.2591(3)	0.08
H(13A)	2i	-0.2070(3)	-0.0459(3)	-0.1236(3)	0.08
H(13B)	2i	-0.0852(3)	0.0577(3)	-0.1550(3)	0.08
H(14A)	2i	-0.2129(3)	0.1423(3)	-0.0097(3)	0.08
H(14B)	2i	-0.0474(3)	0.1550(3)	0.0509(3)	0.08
H(15A)	2i	-0.0094(3)	0.3755(3)	0.0539(2)	0.08
H(15B)	2i	-0.1479(3)	0.3257(3)	-0.0858(2)	0.08
H(24A)	2i	0.1877(4)	0.4327(4)	-0.7311(3)	0.08
H(24B)	2i	0.2744(4)	0.3388(4)	-0.7219(3)	0.08
H(24C)	2i	0.3535(4)	0.4873(4)	-0.6185(3)	0.08
H(82)	2i	0.4396(2)	0.5161(2)	-0.2104(2)	0.08
H(83)	2i	0.4870(3)	0.6989(2)	-0.3063(2)	0.08
H(84)	2i	0.3084(3)	0.7859(3)	-0.3871(2)	0.08
H(85)	2i	0.0787(3)	0.6859(3)	-0.3800(2)	0.08
H(86)	2i	0.0286(3)	0.5004(2)	-0.2888(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
C(1)	2i	0.2904(3)	0.0854(2)	-0.2853(2)	0.069(2)	0.045(1)	0.047(1)	0.030(1)	0.023(1)	0.007(1)
C(2)	2i	0.3178(2)	0.2381(2)	-0.2868(2)	0.041(1)	0.043(1)	0.039(1)	0.018(1)	0.018(1)	0.010(1)
C(3)	2i	0.2989(2)	0.2948(2)	-0.1653(2)	0.037(1)	0.032(1)	0.035(1)	0.0141(9)	0.0150(9)	0.0093(9)
C(4)	2i	0.2623(2)	0.1665(2)	-0.1136(2)	0.051(1)	0.043(1)	0.047(1)	0.022(1)	0.022(1)	0.019(1)
C(5)	2i	0.4073(3)	0.1477(3)	-0.0495(2)	0.064(2)	0.052(1)	0.049(1)	0.033(1)	0.019(1)	0.019(1)
C(6)	2i	0.4286(3)	0.0946(3)	-0.1674(2)	0.072(2)	0.062(2)	0.068(2)	0.045(1)	0.030(1)	0.025(1)
C(7)	2i	0.1695(3)	0.0427(2)	-0.2390(2)	0.057(1)	0.037(1)	0.059(2)	0.016(1)	0.018(1)	0.015(1)
C(8)	2i	0.1946(2)	0.3695(2)	-0.1798(2)	0.033(1)	0.035(1)	0.032(1)	0.0124(9)	0.0124(9)	0.0084(9)
C(9)	2i	0.0251(2)	0.2856(2)	-0.2144(2)	0.037(1)	0.039(1)	0.041(1)	0.0156(9)	0.018(1)	0.016(1)
C(10)	2i	-0.1122(2)	0.1931(3)	-0.3407(2)	0.036(1)	0.060(2)	0.045(1)	0.011(1)	0.012(1)	0.015(1)
C(11)	2i	-0.2624(3)	0.1475(3)	-0.3346(3)	0.038(1)	0.076(2)	0.060(2)	0.014(1)	0.015(1)	0.008(1)
C(12)	2i	-0.2971(3)	0.0290(3)	-0.2736(3)	0.064(2)	0.061(2)	0.094(2)	0.006(1)	0.052(2)	0.005(2)
C(13)	2i	-0.1736(3)	0.0419(3)	-0.1429(3)	0.087(2)	0.056(2)	0.112(3)	0.029(2)	0.071(2)	0.042(2)
C(14)	2i	-0.1256(3)	0.1595(3)	-0.0238(3)	0.071(2)	0.080(2)	0.076(2)	0.027(2)	0.047(2)	0.041(2)
C(15)	2i	-0.0632(3)	0.3098(3)	-0.0327(2)	0.056(1)	0.061(2)	0.052(1)	0.024(1)	0.033(1)	0.016(1)
C(16)	2i	0.0415(2)	0.3351(2)	-0.0937(2)	0.042(1)	0.042(1)	0.044(1)	0.018(1)	0.022(1)	0.017(1)
C(17)	2i	0.2039(2)	0.4218(2)	-0.0423(2)	0.041(1)	0.039(1)	0.039(1)	0.021(1)	0.017(1)	0.014(1)
O(17)	2i	0.3071(2)	0.5025(2)	0.0619(1)	0.0479(9)	0.060(1)	0.0391(9)	0.0181(8)	0.0142(8)	0.0022(8)
C(21)	2i	0.2124(3)	0.2385(2)	-0.4185(2)	0.044(1)	0.042(1)	0.038(1)	0.017(1)	0.018(1)	0.006(1)
O(21)	2i	0.0763(2)	0.1847(2)	-0.4660(2)	0.043(1)	0.078(1)	0.0443(9)	0.0154(9)	0.0155(8)	0.0176(9)
C(22)	2i	0.2852(3)	0.3005(3)	-0.5021(2)	0.050(1)	0.063(2)	0.040(1)	0.023(1)	0.021(1)	0.012(1)
O(22)	2i	0.4029(2)	0.3054(2)	-0.4910(2)	0.075(1)	0.132(2)	0.079(1)	0.058(1)	0.053(1)	0.052(1)
O(23)	2i	0.2001(2)	0.3433(2)	-0.5887(2)	0.061(1)	0.109(2)	0.059(1)	0.037(1)	0.0291(9)	0.048(1)
C(24)	2i	0.2587(4)	0.4056(4)	-0.6721(3)	0.083(2)	0.154(3)	0.081(2)	0.041(2)	0.041(2)	0.074(2)
C(81)	2i	0.2277(2)	0.4875(2)	-0.2418(2)	0.038(1)	0.033(1)	0.032(1)	0.0140(9)	0.0129(9)	0.0079(9)
C(82)	2i	0.3644(2)	0.5498(2)	-0.2464(2)	0.041(1)	0.039(1)	0.047(1)	0.014(1)	0.018(1)	0.015(1)
C(83)	2i	0.3932(3)	0.6590(2)	-0.3015(2)	0.054(1)	0.044(1)	0.057(1)	0.012(1)	0.025(1)	0.019(1)
C(84)	2i	0.2879(3)	0.7093(3)	-0.3502(2)	0.067(2)	0.045(1)	0.053(1)	0.019(1)	0.021(1)	0.024(1)
C(85)	2i	0.1530(3)	0.6507(3)	-0.3460(2)	0.062(2)	0.056(2)	0.066(2)	0.034(1)	0.021(1)	0.030(1)
C(86)	2i	0.1235(3)	0.5413(2)	-0.2914(2)	0.049(1)	0.051(1)	0.058(1)	0.026(1)	0.024(1)	0.023(1)

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