Crystal structure of (5*S*,4*R*)-5-(2-oxo-2-phenylethyl)-4-(phenylsulfanyl)-2(3*H*)-dihydrofuranone, C₁₈H₁₆O₃S

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

Crystal:	yellowish, block shaped, size 0.38 x 0.50 x 0.60 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	2.2 cm ⁻¹
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	ω
$T_{\text{measurement}}$:	150 K
$2\theta_{\text{max}}$:	55°
$N(hkl)_{\text{unique}}$:	2102
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	263
Programs:	SHELXS-86, SHELXL-93

Source of material: See ref. 1.

The structure determination established the trans positioning of the two substituents on the lactone ring. The lactone ring has an envelope puckering with C3 out of the plane determined by the other four ring members. All O atoms show C–H...O hydrogen bond type of interactions to neighbouring molecules.

C₁₈H₁₆O₃S, orthorhombic, $P2_12_12_1$ (No. 19), $a = 5.2694(4)$ Å, $b = 10.2982(5)$ Å, $c = 28.761(2)$ Å, $V = 1560.7$ Å³, $Z = 4$, $R(F) = 0.033$, $R_w(F^2) = 0.083$.

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

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(1)	4a	1.104(5)	0.848(2)	0.0566(8)	0.014(6)
H(2)	4a	0.697(5)	0.926(2)	0.1123(8)	0.020(6)
H(3)	4a	0.779(6)	1.042(3)	0.0181(9)	0.032(7)
H(4)	4a	0.923(5)	0.938(2)	-0.0096(8)	0.023(6)
H(5)	4a	1.084(6)	0.544(3)	0.164(1)	0.045(8)
H(6)	4a	1.190(9)	0.383(3)	0.220(1)	0.07(1)
H(7)	4a	1.033(5)	0.770(3)	0.1372(9)	0.025(7)
H(8)	4a	0.898(6)	0.674(3)	0.1031(9)	0.035(8)
H(9)	4a	0.475(7)	0.658(3)	0.242(1)	0.041(8)
H(10)	4a	0.586(7)	0.503(3)	0.299(1)	0.06(1)
H(11)	4a	0.810(7)	1.119(3)	0.1584(9)	0.046(8)
H(12)	4a	0.929(7)	0.360(3)	0.284(1)	0.05(1)
H(13)	4a	1.057(7)	1.262(3)	0.036(1)	0.050(9)
H(14)	4a	0.771(8)	1.430(3)	0.041(1)	0.06(1)
H(15)	4a	0.525(8)	1.284(4)	0.163(1)	0.07(1)
H(16)	4a	0.493(8)	1.443(4)	0.104(1)	0.07(1)

Table 3. Final 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
S(1)	4a	1.1750(1)	1.04116(5)	0.08987(2)	0.0213(2)	0.0225(2)	0.0289(3)	-0.0016(2)	-0.0063(2)	-0.0023(2)
O(1)	4a	0.4505(3)	0.8489(2)	-0.00993(5)	0.0236(8)	0.0278(8)	0.0173(7)	-0.0005(7)	-0.0044(7)	-0.0023(6)
O(2)	4a	0.5764(3)	0.8142(1)	0.06277(5)	0.0182(7)	0.0234(7)	0.0131(6)	-0.0015(6)	-0.0012(6)	0.0016(6)
O(3)	4a	0.4809(3)	0.7626(2)	0.16492(6)	0.0289(9)	0.038(1)	0.0262(8)	0.0073(8)	0.0065(8)	0.0080(8)
C(1)	4a	0.6028(4)	0.8686(2)	0.02026(7)	0.021(1)	0.021(1)	0.0144(9)	0.0025(9)	0.0012(8)	-0.0015(8)
C(2)	4a	0.8344(5)	0.9541(2)	0.01881(7)	0.025(1)	0.028(1)	0.0154(9)	-0.005(1)	-0.0018(9)	0.0032(9)
C(3)	4a	0.9804(4)	0.9166(2)	0.06248(7)	0.021(1)	0.0192(9)	0.0168(9)	-0.0020(9)	0.0006(9)	-0.0003(8)
C(4)	4a	0.7763(4)	0.8594(2)	0.09411(7)	0.019(1)	0.0206(9)	0.0139(9)	0.0001(8)	-0.0008(8)	-0.0031(8)
C(5)	4a	0.8693(4)	0.7465(2)	0.12302(7)	0.020(1)	0.022(1)	0.0162(9)	0.0009(9)	-0.0008(9)	0.0002(8)
C(6)	4a	0.6874(5)	0.7105(2)	0.16182(7)	0.025(1)	0.0221(9)	0.0135(9)	-0.002(1)	-0.0003(9)	-0.0016(8)
C(7)	4a	0.7691(5)	0.6119(2)	0.19686(7)	0.027(1)	0.024(1)	0.017(1)	-0.002(1)	-0.0033(9)	0.0020(8)

Table 3. (Continued)

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(8)	4a	0.9799(5)	0.5338(3)	0.19048(9)	0.033(1)	0.044(2)	0.032(1)	0.008(1)	0.005(1)	0.016(1)
C(9)	4a	1.0399(7)	0.4392(3)	0.2235(1)	0.043(2)	0.049(2)	0.056(2)	0.012(2)	0.001(2)	0.025(2)
C(10)	4a	0.8935(6)	0.4262(3)	0.2625(1)	0.048(2)	0.050(2)	0.038(2)	0.004(2)	−0.007(1)	0.025(1)
C(11)	4a	0.6886(7)	0.5053(3)	0.2699(1)	0.055(2)	0.062(2)	0.026(1)	0.004(2)	0.006(2)	0.021(1)
C(12)	4a	0.6243(6)	0.5980(3)	0.23707(9)	0.040(2)	0.040(1)	0.027(1)	0.005(1)	0.006(1)	0.009(1)
C(13)	4a	0.9569(5)	1.1718(2)	0.09544(8)	0.024(1)	0.020(1)	0.029(1)	−0.0016(9)	−0.007(1)	−0.0039(9)
C(14)	4a	0.8008(6)	1.1828(2)	0.13388(9)	0.044(2)	0.029(1)	0.031(1)	−0.001(1)	0.003(1)	−0.008(1)
C(15)	4a	0.6275(7)	1.2837(3)	0.1370(1)	0.057(2)	0.042(2)	0.054(2)	0.005(2)	0.011(2)	−0.016(1)
C(16)	4a	0.6153(6)	1.3762(3)	0.1021(1)	0.043(2)	0.030(1)	0.081(2)	0.009(1)	−0.010(2)	−0.013(2)
C(17)	4a	0.7752(7)	1.3681(3)	0.0645(1)	0.046(2)	0.029(1)	0.060(2)	0.003(1)	−0.014(2)	0.008(1)
C(18)	4a	0.9466(6)	1.2670(2)	0.0611(1)	0.035(1)	0.027(1)	0.038(1)	−0.002(1)	−0.005(1)	0.006(1)

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References

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