Crystal structure of (±)-[(2*R*,3*S*)-3-(hydroxymethyl)oxiran-2-yl](phenyl)-methanone, $C_{10}H_{10}O_3$

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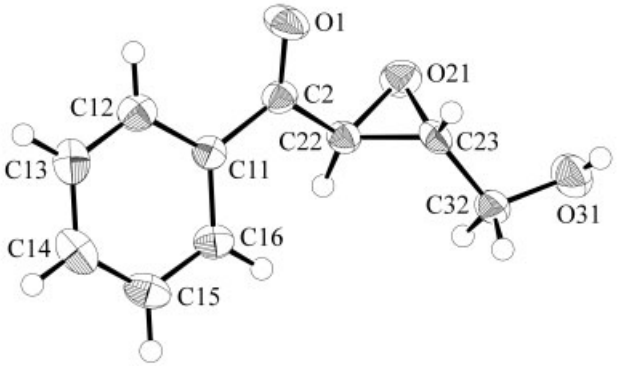

Abstract
$C_{10}H_{10}O_3$, orthorhombic, $Pca2_1$ (No. 29), a = 20.165(4) Å, b = 5.667(1) Å, c = 7.583(2) Å, V = 866.6 Å^3, Z = 4, $R_{gt}(F)$ = 0.072, $wR_{ref}(F^2)$ = 0.177, T = 223 K.

Source of material
The title compound was prepared according to [1] and recrystallised from a CH_2Cl_2/hexane/heptane solution of the compound (mp 333 K – 335 K).

Experimental details
The H atoms were placed in their geometrically calculated positions and included in the final refinement in the riding model approximation.

Discussion
The structure determination confirms the *trans*-disposition of the carbon-bound substituents of the epoxide ring. Hydrogen bonding interactions, primarily involving the hydroxy and carbonyl group propogated by a screw axis, link the molecules into helical chains. The parameters associated with the hydrogen bonding: d(O31–H···O1^i) = 2.12 Å, d(O31···O1^i) = 2.826(5) Å and angle ∠O31–H–O1^i = 142° for symmetry operation i: 1–x, –y, –1/2+z. The rather large deviation from linearity for the hydrogen bond may be explained by the presence of a weaker interaction, at least in terms of the O···H separation, between O31-H and the epoxide-oxygen atom so that d(O31–H···O21^i) = 2.60 Å, d(O3···O21^i) = 3.323(5) Å for angle ∠O31–H–O1^i of 147°. These interactions serve to reinforce the previously mentioned hydrogen-bonding interactions.

Table 1. Data collection and handling.

Crystal:	colourless block, size 0.05 × 0.31 × 0.55 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.01 cm^{-1}
Diffractometer, scan mode:	Bruker AXS SMART CCD, ω
$2\theta_{max}$:	60°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	6493, 1348
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1041
$N(param)_{refined}$:	119
Programs:	teXsan [2], SIR92 [3], SHELXL-97 [4], ORTEPII [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(31)	4*a*	0.5608	0.2928	0.4791	0.077
H(12)	4*a*	0.2402	–0.2684	0.8504	0.042
H(13)	4*a*	0.1286	–0.1803	0.8150	0.048
H(14)	4*a*	0.0964	0.1813	0.6925	0.050
H(15)	4*a*	0.1763	0.4544	0.6108	0.046
H(16)	4*a*	0.2886	0.3681	0.6475	0.039
H(22)	4*a*	0.3830	0.3270	0.8083	0.035
H(23)	4*a*	0.4498	0.0353	0.5482	0.035
H(32a)	4*a*	0.4626	0.4370	0.4603	0.041
H(32b)	4*a*	0.4695	0.5188	0.6592	0.041

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	4*a*	0.3640(1)	–0.2300(4)	0.7886(6)	0.038(1)	0.023(1)	0.078(2)	0.004(1)	–0.003(2)	–0.003(2)
O(21)	4*a*	0.4634(1)	0.1010(5)	0.8163(4)	0.037(1)	0.044(1)	0.039(2)	–0.001(1)	–0.009(1)	0.009(1)
O(31)	4*a*	0.5506(1)	0.3827(5)	0.5611(6)	0.034(2)	0.048(2)	0.072(2)	0.001(1)	0.000(2)	0.002(2)
C(2)	4*a*	0.3467(2)	–0.0271(6)	0.7700(5)	0.035(2)	0.023(2)	0.032(2)	–0.001(1)	0.001(2)	–0.001(2)
C(11)	4*a*	0.2758(2)	0.0404(6)	0.7493(5)	0.032(2)	0.024(1)	0.026(2)	–0.001(1)	0.001(1)	–0.006(1)

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Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(12)	4*a*	0.2275(2)	–0.1230(6)	0.8013(6)	0.043(2)	0.027(2)	0.034(2)	–0.001(1)	0.001(2)	–0.006(2)
C(13)	4*a*	0.1610(2)	–0.0703(7)	0.7804(6)	0.037(2)	0.042(2)	0.040(2)	–0.007(2)	0.004(2)	–0.011(2)
C(14)	4*a*	0.1417(2)	0.1465(8)	0.7077(7)	0.034(2)	0.047(2)	0.046(2)	0.004(2)	–0.007(2)	–0.020(2)
C(15)	4*a*	0.1892(2)	0.3084(6)	0.6587(6)	0.048(2)	0.031(2)	0.037(2)	0.009(2)	–0.011(2)	–0.010(2)
C(16)	4*a*	0.2564(2)	0.2565(6)	0.6801(6)	0.040(2)	0.022(1)	0.035(2)	–0.002(1)	–0.003(2)	–0.006(2)
C(22)	4*a*	0.3980(2)	0.1697(6)	0.7679(5)	0.027(2)	0.024(1)	0.035(2)	0.000(1)	–0.000(2)	–0.002(2)
C(23)	4*a*	0.4510(2)	0.1654(6)	0.6353(5)	0.020(2)	0.031(2)	0.037(2)	0.004(1)	–0.002(1)	–0.002(2)
C(32)	4*a*	0.4813(2)	0.3942(6)	0.5753(6)	0.026(2)	0.033(2)	0.045(2)	0.002(1)	–0.002(2)	0.004(2)

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