Crystal structure of 1-(2-hydroxy-4,6-dimethoxyphenyl)-2-propyl naphthoate, $C_{10}H_6(COOC_3H_7)[C_6H_2(OCH_3)_2OH]$

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Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.55 x 0.6 x 0.75 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.90 cm ⁻¹
Diffraction, scan mode:	Siemens P4, ω
2 θ _{max} :	55°
$N(hkl)$ _{measured} , $N(hkl)$ _{unique} :	4946, 4479
Criterion for F_{obs} , $N(hkl)_{gt}$:	$F_{obs} > 3 \sigma(F_{obs})$, 3824
$N(param)_{refined}$:	249
Program:	SHELXTL-plus [2]

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

Atom	Site	x	y	z	U_{iso}
H(3)	4e	0.4995(2)	0.0455(2)	0.9356(1)	0.08
H(4)	4e	0.5276(2)	-0.1242(2)	0.8728(1)	0.08
H(6)	4e	0.4588(2)	-0.2614(2)	0.7496(2)	0.08
H(7)	4e	0.3316(2)	-0.3042(2)	0.6109(2)	0.08
H(8)	4e	0.1785(2)	-0.1739(2)	0.5306(2)	0.08
H(9)	4e	0.1517(2)	0.0005(2)	0.5903(1)	0.08
H(13)	4e	0.328(2)	0.227(2)	0.551(2)	0.097(9)
H(14)	4e	0.1289(2)	0.3343(2)	0.5226(1)	0.08
H(16)	4e	-0.0996(2)	0.2852(2)	0.6826(1)	0.08
H(18)	4e	0.3549(2)	0.4087(2)	0.9457(2)	0.08
H(19A)	4e	0.3679(4)	0.5735(2)	0.8728(3)	0.08
H(19B)	4e	0.3295(4)	0.5086(2)	0.7834(3)	0.08
H(19C)	4e	0.4628(4)	0.4843(2)	0.8526(3)	0.08
H(20A)	4e	0.1665(3)	0.5007(3)	0.9061(2)	0.08
H(20B)	4e	0.1413(3)	0.3698(3)	0.9009(2)	0.08
H(20C)	4e	0.1275(3)	0.4394(3)	0.8152(2)	0.08
H(21A)	4e	-0.2464(2)	0.4763(2)	0.5209(2)	0.08
H(21B)	4e	-0.1727(2)	0.4595(2)	0.6202(2)	0.08
H(21C)	4e	-0.2464(2)	0.3576(2)	0.5648(2)	0.08
H(22A)	4e	-0.0464(2)	0.1189(2)	0.8689(2)	0.08
H(22B)	4e	-0.1280(2)	0.1446(2)	0.7725(2)	0.08
H(22C)	4e	-0.0509(2)	0.2421(2)	0.8317(2)	0.08

Abstract

$C_{22}H_{22}O_5$, monoclinic, $P12_1/c1$ (No. 14), $a = 10.805(1)$ Å, $b = 11.813(1)$ Å, $c = 15.982(1)$ Å, $\beta = 106.86(1)^\circ$, $V = 1952.3$ Å³, $Z = 4$, $R_g(F) = 0.065$, $R_w(F) = 0.068$, $T = 293$ K.

Source of material

The racemic title compound was prepared [1] in 77% yield by ring opening of the corresponding biaryl lactone with NaOⁱPr in ⁱPrOH for comparison with material obtained by atropenantio-meric Ti-TADDOLat-mediated lactone cleavage.

Discussion

The intermolecular hydrogen bridge O1...H13...O13 [O13–O1 = 271.3 pm] forms a chain parallel [001].

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(1)	4e	0.3508(2)	0.2038(1)	0.95898(9)	0.101(1)	0.069(1)	0.0369(8)	0.0083(9)	0.0270(8)	-0.0037(7)
C(1)	4e	0.3421(2)	0.2115(2)	0.8819(1)	0.049(1)	0.053(1)	0.0354(9)	0.0006(9)	0.0142(8)	-0.0015(8)
O(2)	4e	0.3253(2)	0.3071(1)	0.83759(9)	0.077(1)	0.0480(8)	0.0444(8)	0.0038(7)	0.0216(7)	-0.0021(6)
C(2)	4e	0.3561(2)	0.1087(2)	0.8309(1)	0.046(1)	0.046(1)	0.0339(8)	0.0006(8)	0.0166(7)	0.0037(7)
C(3)	4e	0.4476(2)	0.0284(2)	0.8772(1)	0.052(1)	0.057(1)	0.038(1)	0.0038(9)	0.0113(8)	0.0071(8)

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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(4)	4e	0.4631(2)	-0.0719(2)	0.8408(1)	0.057(1)	0.057(1)	0.052(1)	0.014(1)	0.0161(9)	0.014(1)
C(5)	4e	0.3851(2)	-0.1005(2)	0.7559(1)	0.053(1)	0.044(1)	0.056(1)	0.0057(8)	0.0264(9)	0.0051(9)
C(6)	4e	0.3971(2)	-0.2071(2)	0.7176(2)	0.067(1)	0.050(1)	0.073(2)	0.009(1)	0.031(1)	0.001(1)
C(7)	4e	0.3222(2)	-0.2322(2)	0.6362(2)	0.082(2)	0.049(1)	0.085(2)	-0.002(1)	0.037(1)	-0.018(1)
C(8)	4e	0.2308(2)	-0.1546(2)	0.5884(2)	0.074(2)	0.061(1)	0.058(1)	-0.009(1)	0.021(1)	-0.015(1)
C(9)	4e	0.2155(2)	-0.0515(2)	0.6234(1)	0.058(1)	0.053(1)	0.047(1)	-0.005(1)	0.0148(9)	-0.0050(9)
C(10)	4e	0.2933(2)	-0.0212(2)	0.7084(1)	0.047(1)	0.045(1)	0.0398(9)	-0.0006(8)	0.0191(8)	0.0007(8)
C(11)	4e	0.2800(2)	0.0868(2)	0.7462(1)	0.0435(9)	0.0435(9)	0.0340(8)	0.0028(7)	0.0168(7)	0.0046(7)
C(12)	4e	0.1833(2)	0.1688(2)	0.6949(1)	0.045(1)	0.0435(9)	0.0318(8)	0.0024(8)	0.0105(7)	0.0003(7)
C(13)	4e	0.2039(2)	0.2228(2)	0.6222(1)	0.046(1)	0.047(1)	0.0332(9)	0.0001(8)	0.0120(8)	-0.0000(7)
O(13)	4e	0.3156(1)	0.1972(1)	0.60354(9)	0.0523(8)	0.0634(9)	0.0425(8)	0.0057(6)	0.0223(6)	0.0104(6)
C(14)	4e	0.1139(2)	0.2978(2)	0.5724(1)	0.057(1)	0.052(1)	0.0371(9)	0.0049(9)	0.0108(8)	0.0072(8)
C(15)	4e	0.0023(2)	0.3197(2)	0.5952(1)	0.056(1)	0.048(1)	0.041(1)	0.0082(9)	0.0050(8)	-0.0004(8)
O(15)	4e	-0.0821(2)	0.3940(1)	0.5412(1)	0.067(1)	0.069(1)	0.0574(9)	0.0248(8)	0.0066(8)	0.0119(8)
C(16)	4e	-0.0220(2)	0.2690(2)	0.6671(1)	0.047(1)	0.062(1)	0.047(1)	0.0103(9)	0.0137(9)	-0.0047(9)
C(17)	4e	0.0708(2)	0.1930(2)	0.7166(1)	0.049(1)	0.055(1)	0.0361(9)	0.0040(9)	0.0138(8)	0.0016(8)
O(17)	4e	0.0581(1)	0.1389(2)	0.78878(9)	0.0567(9)	0.093(1)	0.0527(9)	0.0159(8)	0.0300(7)	0.0199(8)
C(18)	4e	0.3125(2)	0.4120(2)	0.8840(2)	0.083(2)	0.049(1)	0.062(1)	0.005(1)	0.029(1)	-0.009(1)
C(19)	4e	0.3736(4)	0.5027(2)	0.8447(3)	0.156(3)	0.060(2)	0.181(4)	-0.003(2)	0.099(3)	-0.015(2)
C(20)	4e	0.1750(3)	0.4322(3)	0.8758(2)	0.103(2)	0.078(2)	0.119(3)	0.006(2)	0.045(2)	-0.022(2)
C(21)	4e	-0.1962(2)	0.4243(2)	0.5636(2)	0.064(1)	0.073(2)	0.068(2)	0.025(1)	0.006(1)	-0.007(1)
C(22)	4e	-0.0504(2)	0.1630(2)	0.8178(2)	0.062(1)	0.110(2)	0.063(1)	0.003(1)	0.035(1)	0.004(1)

References

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