Crystal structure of (*P*)-4,4'-di-*tert*-butyl-2,2',3,3'-tetramethoxy-6,6'-dimethylbiphenyl, {C₂₆H₃₈O₄(CH₃)₂[C(CH₃)₃]}₂

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Abstract

C₂₆H₃₈O₄, orthorhombic, *P*2₁2₁2₁ (No. 19), *a* = 8.360(1) Å, *b* = 11.746(1) Å, *c* = 26.024(3) Å, *V* = 2555.5 Å³, *Z* = 4, *R*_{gt}(*F*) = 0.067, *wR*(*F*) = 0.058, *T* = 293 K.

Source of material

The title compound, a synthetic precursor to a structurally simplified analog of the nerve-growth stimulating mastigophorenes from liverworts [1] was prepared in enantiomerically pure form [2], using the 'lactone method' [3].

Table 1. Data collection and handling.

Crystal:	colourless plate, size 0.4 × 0.55 × 0.15 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71073 Å)
μ:	0.70 cm ⁻¹
Diffractionmeter, scan mode:	Siemens P4, ω
2θ _{max} :	55°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	7823, 5714
Criterion for <i>F</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>F</i> _{obs} > 3 σ(<i>F</i> _{obs}), 3676
<i>N</i> (<i>param</i>) _{refined} :	271
Program:	SHELXTL-plus [4]

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(1A)	4a	1.0270(6)	0.3512(3)	0.1820(1)	0.08
H(1B)	4a	1.0448(6)	0.4053(3)	0.1272(1)	0.08
H(1C)	4a	1.1939(6)	0.3517(3)	0.1546(1)	0.08
H(3)	4a	1.1823(4)	0.2537(3)	0.0615(1)	0.08
H(12)	4a	0.9302(4)	0.1432(3)	0.3247(1)	0.08
H(14A)	4a	1.1503(4)	0.0864(3)	0.2100(1)	0.08
H(14B)	4a	1.1140(4)	0.0213(3)	0.2613(1)	0.08
H(14C)	4a	1.1893(4)	0.1434(3)	0.2630(1)	0.08
H(16A)	4a	1.3394(6)	0.1806(4)	0.0030(1)	0.08
H(16B)	4a	1.1905(6)	0.2407(4)	-0.0216(1)	0.08
H(16C)	4a	1.2926(6)	0.1552(4)	-0.0542(1)	0.08
H(17A)	4a	1.3185(7)	-0.0297(4)	0.0233(1)	0.08
H(17B)	4a	1.2810(7)	-0.0490(4)	-0.0351(1)	0.08
H(17C)	4a	1.1634(7)	-0.0953(4)	0.0069(1)	0.08
H(18A)	4a	0.9358(5)	0.0075(4)	-0.0347(1)	0.08
H(18B)	4a	1.0536(5)	0.0534(4)	-0.0768(1)	0.08
H(18C)	4a	0.9515(5)	0.1389(4)	-0.0442(1)	0.08
H(19A)	4a	0.7287(6)	-0.1542(5)	0.0245(2)	0.08
H(19B)	4a	0.7213(6)	-0.0217(5)	0.0176(2)	0.08
H(19C)	4a	0.6883(6)	-0.0762(5)	0.0716(2)	0.08
H(20A)	4a	0.7903(6)	-0.1674(4)	0.1844(2)	0.08
H(20B)	4a	0.9462(6)	-0.0969(4)	0.1947(2)	0.08
H(20C)	4a	0.9237(6)	-0.1604(4)	0.1422(2)	0.08
H(22A)	4a	0.8565(5)	0.2349(3)	0.3950(1)	0.08
H(22B)	4a	0.7734(5)	0.1154(3)	0.3928(1)	0.08
H(22C)	4a	0.7049(5)	0.2107(3)	0.4287(1)	0.08
H(23A)	4a	0.5542(5)	0.3949(3)	0.3341(1)	0.08
H(23B)	4a	0.7220(5)	0.4063(3)	0.3605(1)	0.08
H(23C)	4a	0.5703(5)	0.3791(3)	0.3937(1)	0.08
H(24A)	4a	0.4222(5)	0.1993(3)	0.3280(1)	0.08
H(24B)	4a	0.4388(5)	0.1881(3)	0.3878(1)	0.08
H(24C)	4a	0.5073(5)	0.0927(3)	0.3519(1)	0.08
H(25A)	4a	0.3826(5)	0.4439(3)	0.2372(1)	0.08
H(25B)	4a	0.5165(5)	0.4119(3)	0.1976(1)	0.08
H(25C)	4a	0.5627(5)	0.4659(3)	0.2507(1)	0.08
H(26A)	4a	0.4622(5)	0.2096(4)	0.1153(1)	0.08
H(26B)	4a	0.4322(5)	0.1863(4)	0.1739(1)	0.08
H(26C)	4a	0.5502(5)	0.1086(4)	0.1428(1)	0.08

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Table 3. 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
C(1)	4a	1.0806(6)	0.3453(3)	0.1495(1)	0.106(3)	0.081(3)	0.065(2)	−0.036(3)	0.003(2)	−0.015(2)
C(2)	4a	1.0446(4)	0.2310(3)	0.1252(1)	0.054(2)	0.057(2)	0.043(2)	−0.006(2)	−0.000(2)	0.001(2)
C(3)	4a	1.1075(4)	0.2022(3)	0.0771(1)	0.052(2)	0.066(2)	0.044(2)	−0.015(2)	0.004(2)	0.007(2)
C(4)	4a	1.0695(4)	0.1033(3)	0.0508(1)	0.052(2)	0.063(2)	0.037(2)	−0.003(2)	0.008(2)	0.003(2)
C(5)	4a	0.9621(4)	0.0293(3)	0.0749(1)	0.059(2)	0.051(2)	0.049(2)	−0.008(2)	0.009(2)	−0.008(2)
O(5)	4a	0.9168(4)	−0.0720(2)	0.05089(9)	0.097(2)	0.071(2)	0.073(2)	−0.025(2)	0.036(2)	−0.024(1)
C(6)	4a	0.9020(4)	0.0534(3)	0.1238(1)	0.046(2)	0.052(2)	0.049(2)	−0.004(2)	0.010(2)	−0.001(2)
O(6)	4a	0.7977(3)	−0.0211(2)	0.14772(8)	0.064(2)	0.058(2)	0.062(1)	−0.005(1)	0.023(1)	−0.000(1)
C(7)	4a	0.9398(4)	0.1552(3)	0.1491(1)	0.040(2)	0.058(2)	0.041(2)	0.006(2)	−0.001(2)	0.006(2)
C(8)	4a	0.8694(4)	0.1776(3)	0.2016(1)	0.047(2)	0.054(2)	0.038(2)	−0.003(2)	0.002(2)	−0.002(2)
C(9)	4a	0.7190(4)	0.2286(3)	0.2057(1)	0.048(2)	0.044(2)	0.036(2)	0.001(2)	−0.003(2)	0.004(1)
O(9)	4a	0.6416(3)	0.2575(2)	0.16042(7)	0.056(1)	0.064(2)	0.047(1)	−0.004(1)	−0.006(1)	0.013(1)
C(10)	4a	0.6498(4)	0.2525(3)	0.2532(1)	0.045(2)	0.042(2)	0.046(2)	0.003(2)	0.002(2)	0.005(2)
O(10)	4a	0.4995(3)	0.3032(2)	0.25502(7)	0.051(1)	0.052(1)	0.060(1)	0.007(1)	0.006(1)	0.007(1)
C(11)	4a	0.7263(4)	0.2185(3)	0.2987(1)	0.055(2)	0.046(2)	0.039(2)	0.005(2)	0.003(2)	−0.006(2)
C(12)	4a	0.8755(4)	0.1661(3)	0.2939(1)	0.052(2)	0.062(2)	0.042(2)	0.006(2)	−0.004(2)	0.002(2)
C(13)	4a	0.9515(4)	0.1474(3)	0.2466(1)	0.049(2)	0.062(2)	0.045(2)	0.010(2)	−0.006(2)	−0.013(2)
C(14)	4a	1.1162(4)	0.0947(3)	0.2450(1)	0.062(2)	0.094(3)	0.053(2)	0.027(2)	−0.010(2)	−0.004(2)
C(15)	4a	1.1407(5)	0.0773(3)	−0.0027(1)	0.066(3)	0.075(3)	0.043(2)	0.001(2)	0.017(2)	0.003(2)
C(16)	4a	1.2518(6)	0.1716(4)	−0.0205(1)	0.117(4)	0.158(5)	0.059(2)	−0.065(4)	0.040(3)	−0.023(3)
C(17)	4a	1.2350(7)	−0.0345(4)	−0.0019(1)	0.123(4)	0.160(5)	0.072(3)	0.049(5)	0.047(3)	0.019(3)
C(18)	4a	1.0083(5)	0.0678(4)	−0.0435(1)	0.098(3)	0.095(3)	0.047(2)	−0.003(3)	0.000(2)	−0.014(2)
C(19)	4a	0.7500(6)	−0.0823(5)	0.0406(2)	0.121(5)	0.154(5)	0.080(3)	−0.075(4)	0.030(3)	−0.044(3)
C(20)	4a	0.8700(6)	−0.1194(4)	0.1690(2)	0.098(4)	0.085(3)	0.090(3)	−0.014(3)	0.025(3)	0.020(3)
C(21)	4a	0.6482(4)	0.2386(3)	0.3525(1)	0.070(2)	0.057(2)	0.037(2)	0.005(2)	0.010(2)	0.004(2)
C(22)	4a	0.7558(5)	0.1957(3)	0.3964(1)	0.098(3)	0.084(3)	0.038(2)	0.006(3)	0.010(2)	0.001(2)
C(23)	4a	0.6216(5)	0.3668(3)	0.3612(1)	0.082(3)	0.064(3)	0.060(2)	0.003(2)	0.016(2)	−0.015(2)
C(24)	4a	0.4896(5)	0.1731(3)	0.3554(1)	0.087(3)	0.070(3)	0.060(2)	−0.001(3)	0.028(2)	−0.002(2)
C(25)	4a	0.4897(5)	0.4157(3)	0.2334(1)	0.063(2)	0.053(2)	0.082(2)	0.014(2)	−0.004(2)	0.010(2)
C(26)	4a	0.5105(5)	0.1848(4)	0.1469(1)	0.068(3)	0.091(3)	0.061(2)	−0.007(3)	−0.017(2)	0.009(2)

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