Crystal structure of 1-(2′-benzoyl-4′,6′-dimethylphenyl)-2-methylnaphthaline, $[C_{10}H_6CH_3][C_6H_2(OCH_2C_6H_5)(CH_3)_2]$

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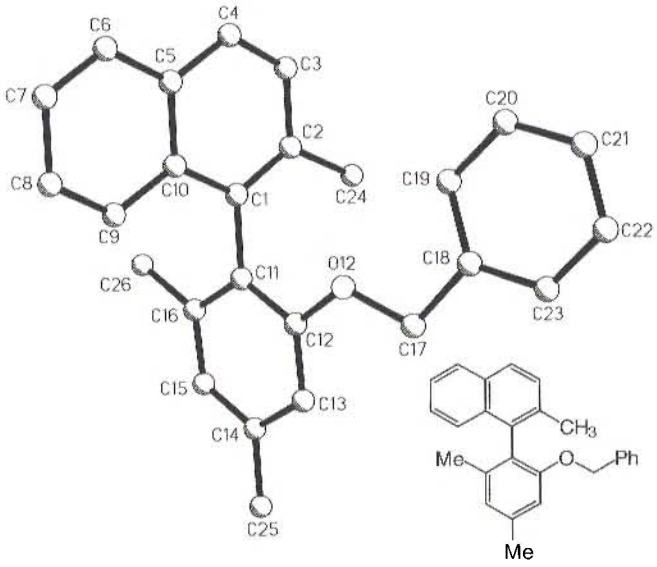

Abstract

$C_{26}H_{24}O$, monoclinic, $P12_1/c1$ (No. 14), $a = 19.319(1)$ Å, $b = 12.149(1)$ Å, $c = 8.909(1)$ Å, $\beta = 102.85(1)°$, $V = 2038.6$ Å^3, $Z = 4$, $R_{gt}(F) = 0.094$, $R(F) = 0.094$, $T = 293$ K.

Source of material

The title compound was an unexpected product in the attempted phosphinylation of 1-(2′-benzyloxy-4′,6′-dimethylphenyl)-2-bromomethylnaphthaline [1] with $KPPh_2$ (36% yield).

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.65 × 0.75 × 0.5 mm
Wavelength:	Mo K_α radiation (0.71073 A)
μ:	0.70 cm^{-1}
Diffractometer, scan mode:	Bruker AXS P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5155, 4628
Criterion for F_{obs}, $N(hkl)_{gt}$:	$F_{obs} > 3\ \sigma(F_{obs})$, 3701
$N(param)_{refined}$:	244
Program:	SHELXTL-plus [2]

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

Atom	Site	x	y	z	U_{iso}
H(3)	4e	0.8892(2)	0.6425(3)	0.3019(4)	0.08
H(4)	4e	0.8609(2)	0.6804(3)	0.5345(5)	0.08
H(6)	4e	0.7770(3)	0.6683(3)	0.7053(5)	0.08
H(7)	4e	0.6721(3)	0.6084(4)	0.7527(5)	0.08
H(8)	4e	0.5896(2)	0.5127(3)	0.5598(5)	0.08
H(9)	4e	0.6142(2)	0.4813(3)	0.3233(4)	0.08
H(13)	4e	0.6619(2)	0.2186(3)	-0.0514(4)	0.08
H(15)	4e	0.5338(2)	0.4833(3)	-0.1608(4)	0.08
H(17A)	4e	0.7505(2)	0.1544(3)	0.1669(4)	0.08
H(17B)	4e	0.7822(2)	0.2078(3)	0.0368(4)	0.08
H(19)	4e	0.8653(2)	0.3491(4)	0.3388(5)	0.08
H(20)	4e	0.9800(2)	0.3197(5)	0.4873(6)	0.08
H(21)	4e	1.0389(2)	0.1560(4)	0.4748(6)	0.08
H(22)	4e	0.9826(2)	0.0162(4)	0.3184(6)	0.08
H(23)	4e	0.8677(2)	0.0415(3)	0.1701(5)	0.08
H(24A)	4e	0.7823(2)	0.4985(3)	-0.0166(4)	0.08
H(24B)	4e	0.8621(2)	0.4947(3)	0.0716(4)	0.08
H(24C)	4e	0.8280(2)	0.6064(3)	0.0046(4)	0.08
H(25A)	4e	0.5590(2)	0.2032(4)	-0.2471(4)	0.08
H(25B)	4e	0.5364(2)	0.3105(4)	-0.3433(4)	0.08
H(25C)	4e	0.4947(2)	0.2731(4)	-0.2199(4)	0.08
H(26A)	4e	0.6395(2)	0.6656(3)	0.1154(4)	0.08
H(26B)	4e	0.5583(2)	0.6420(3)	0.0557(4)	0.08
H(26C)	4e	0.6051(2)	0.6723(3)	-0.0612(4)	0.08

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}
C(1)	4e	0.7321(2)	0.5297(2)	0.2268(4)	0.044(2)	0.047(2)	0.058(2)	0.001(1)	-0.000(1)	0.002(1)
C(2)	4e	0.7970(2)	0.5614(3)	0.2031(4)	0.051(2)	0.061(2)	0.071(2)	-0.002(2)	0.001(2)	0.004(2)
C(3)	4e	0.8442(2)	0.6191(3)	0.3197(4)	0.054(2)	0.069(2)	0.086(3)	-0.014(2)	-0.010(2)	0.009(2)
C(4)	4e	0.8275(2)	0.6414(3)	0.4569(5)	0.078(2)	0.062(2)	0.076(3)	-0.013(2)	-0.016(2)	0.001(2)

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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(5)	4*e*	0.7626(2)	0.6093(3)	0.4855(4)	0.079(2)	0.049(2)	0.060(2)	0.000(2)	–0.003(2)	0.000(2)
C(6)	4*e*	0.7444(3)	0.6289(3)	0.6264(5)	0.111(3)	0.073(3)	0.066(3)	–0.002(2)	0.003(2)	–0.006(2)
C(7)	4*e*	0.6831(3)	0.5950(4)	0.6543(5)	0.137(4)	0.089(3)	0.066(3)	0.015(3)	0.030(3)	–0.003(2)
C(8)	4*e*	0.6337(2)	0.5380(3)	0.5395(5)	0.090(3)	0.085(3)	0.080(3)	0.010(2)	0.029(2)	0.005(2)
C(9)	4*e*	0.6485(2)	0.5182(3)	0.4014(4)	0.065(2)	0.064(2)	0.066(2)	0.004(2)	0.011(2)	0.003(2)
C(10)	4*e*	0.7135(2)	0.5514(2)	0.3684(4)	0.059(2)	0.044(2)	0.058(2)	0.005(1)	0.002(2)	0.002(1)
C(11)	4*e*	0.6811(2)	0.4656(3)	0.1047(3)	0.043(1)	0.056(2)	0.054(2)	–0.002(1)	0.006(1)	–0.000(1)
C(12)	4*e*	0.6951(2)	0.3564(3)	0.0785(4)	0.042(2)	0.060(2)	0.063(2)	–0.001(1)	0.003(1)	–0.003(2)
O(12)	4*e*	0.7553(1)	0.3147(2)	0.1745(3)	0.057(1)	0.064(2)	0.085(2)	0.011(1)	–0.012(1)	–0.010(1)
C(13)	4*e*	0.6508(2)	0.2940(3)	–0.0350(4)	0.049(2)	0.063(2)	0.077(2)	–0.003(2)	0.001(2)	–0.013(2)
C(14)	4*e*	0.5901(2)	0.3435(3)	–0.1246(4)	0.044(2)	0.077(2)	0.065(2)	–0.006(2)	0.004(1)	–0.015(2)
C(15)	4*e*	0.5758(2)	0.4507(3)	–0.0990(4)	0.042(2)	0.081(2)	0.064(2)	0.004(2)	0.001(1)	–0.001(2)
C(16)	4*e*	0.6202(2)	0.5150(3)	0.0153(4)	0.042(2)	0.065(2)	0.061(2)	0.002(1)	0.006(1)	0.000(2)
C(17)	4*e*	0.7809(2)	0.2114(3)	0.1437(4)	0.061(2)	0.059(2)	0.099(3)	0.008(2)	–0.004(2)	–0.011(2)
C(18)	4*e*	0.8551(2)	0.1974(3)	0.2411(4)	0.055(2)	0.066(2)	0.078(2)	0.008(2)	0.009(2)	0.002(2)
C(19)	4*e*	0.8887(2)	0.2799(4)	0.3334(5)	0.062(2)	0.091(3)	0.107(3)	0.015(2)	–0.008(2)	–0.024(2)
C(20)	4*e*	0.9570(2)	0.2623(5)	0.4205(6)	0.064(3)	0.132(4)	0.137(4)	0.012(3)	–0.018(3)	–0.041(4)
C(21)	4*e*	0.9915(2)	0.1661(4)	0.4146(6)	0.057(2)	0.127(4)	0.118(4)	0.024(3)	–0.003(2)	0.002(3)
C(22)	4*e*	0.9587(2)	0.0849(4)	0.3232(6)	0.072(3)	0.095(3)	0.126(4)	0.032(3)	0.019(3)	0.022(3)
C(23)	4*e*	0.8903(2)	0.0998(3)	0.2357(5)	0.073(2)	0.069(2)	0.114(3)	0.013(2)	0.014(2)	0.007(2)
C(24)	4*e*	0.8195(2)	0.5381(3)	0.0515(4)	0.060(2)	0.103(3)	0.093(3)	–0.018(2)	0.017(2)	0.001(2)
C(25)	4*e*	0.5406(2)	0.2764(4)	–0.2445(4)	0.060(2)	0.112(3)	0.082(3)	0.000(2)	–0.004(2)	–0.030(2)
C(26)	4*e*	0.6044(2)	0.6344(3)	0.0330(4)	0.058(2)	0.070(2)	0.084(3)	0.010(2)	0.002(2)	0.000(2)

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