Crystal structure of 1-[2-(benzyloxy)phenyl]ethanone, $C_{15}H_{14}O_2$

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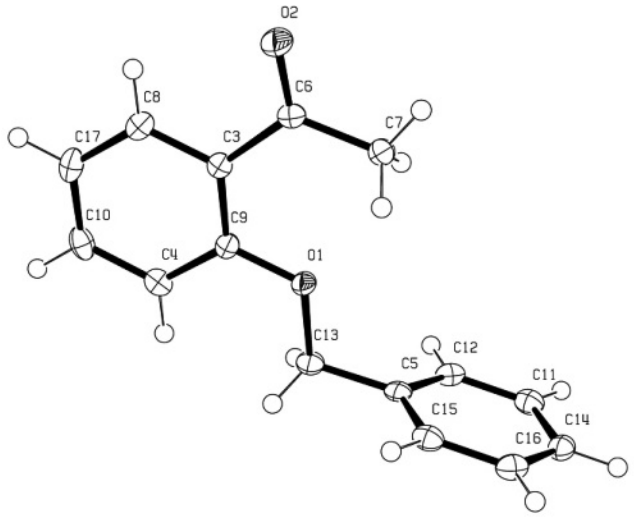

Abstract

$C_{15}H_{14}O_2$, monoclinic, $P2_1/c$ (no. 14), a = 10.664(2) Å, b = 14.406(3) Å, c = 7.686(1) Å, β = 94.260(3)°, V = 1177.6 Å^3, Z = 4, $R_{gt}(F)$ = 0.0417, $wR_{ref}(F^2)$ = 0.1036, T = 103 K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.25×0.45×0.625 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.83 cm^{-1}
Diffractometer, scan mode:	Bruker SMART APEX II, φ and ω
$2\theta_{max}$:	56.6°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	7307, 2711
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2237
$N(param)_{refined}$:	155
Programs:	SHELX [4]

Source of material

1-[2-(benzyloxy)phenyl]ethanone (2-benzyloxyacetophenone) was prepared by condensation of 2-hydroxyacetophenone with benzyl bromide in refluxing acetone in the presence of an excess of anhydrous potassium carbonate [1–3].

Experimental details

All hydrogen atoms were placed in calculated positions. The U_{iso}(H) values were fixed to 1.2U_{eq}(C_{aryl}, CH_2) and 1.5 U_{eq}(C_{methyl}).

Discussion

The title compound, $C_{15}H_{14}O_2$, has been prepared in a Williamson ether synthesis as a model for a novel class of cyclooxygenase (COX) inhibitors containing a phenyl-benzyl ether moiety. The aromatic rings are almost orthogonal to each other, with a between-the-ring-planes angle of 85.7°. The acetyl substituent is almost coplanar with the acetophenone ring, enclosing an angle of 2.0°.

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

Atom	Site	x	y	z	U_{iso}
H(4)	4*e*	0.7009	1.1451	0.1614	0.023
H(7A)	4*e*	0.7371	0.7772	–0.2130	0.029
H(7B)	4*e*	0.7100	0.8186	–0.0262	0.029
H(7C)	4*e*	0.8202	0.8613	–0.1317	0.029
H(8)	4*e*	0.4961	1.0313	–0.3516	0.023
H(10)	4*e*	0.5604	1.2390	–0.0053	0.026
H(11)	4*e*	0.9467	0.7681	0.6033	0.025
H(12)	4*e*	0.8071	0.8802	0.4853	0.023
H(13A)	4*e*	0.7761	1.0271	0.3340	0.024
H(13B)	4*e*	0.8839	1.0679	0.2202	0.024
H(14)	4*e*	1.1487	0.7572	0.5071	0.024
H(15)	4*e*	1.0718	0.9708	0.1743	0.024
H(16)	4*e*	1.2112	0.8583	0.2915	0.025
H(17)	4*e*	0.4571	1.1820	–0.2620	0.026

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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*e*	0.77116(8)	0.97520(6)	0.0910(1)	0.0203(4)	0.0170(4)	0.0164(4)	0.0021(3)	–0.0044(3)	–0.0028(3)
O(2)	4*e*	0.58631(9)	0.88016(6)	–0.3658(1)	0.0328(5)	0.0265(5)	0.0203(5)	0.0027(4)	–0.0080(4)	–0.0038(4)
C(3)	4*e*	0.6250(1)	0.99676(8)	–0.1536(2)	0.0141(6)	0.0170(6)	0.0150(6)	–0.0004(4)	0.0033(4)	0.0012(4)
C(4)	4*e*	0.6606(1)	1.12190(8)	0.0559(2)	0.0207(6)	0.0190(6)	0.0192(6)	–0.0019(5)	0.0045(5)	–0.0017(5)
C(5)	4*e*	0.9256(1)	0.93730(8)	0.3187(2)	0.0197(6)	0.0189(6)	0.0134(5)	–0.0025(5)	–0.0036(5)	–0.0056(4)
C(6)	4*e*	0.6448(1)	0.90194(8)	–0.2289(2)	0.0153(6)	0.0196(6)	0.0145(5)	–0.0025(5)	0.0022(4)	0.0000(5)
C(7)	4*e*	0.7359(1)	0.83385(8)	–0.1424(2)	0.0196(6)	0.0181(6)	0.0205(6)	0.0021(5)	–0.0010(5)	–0.0028(5)
C(8)	4*e*	0.5392(1)	1.05433(9)	–0.2479(2)	0.0159(6)	0.0243(7)	0.0169(6)	0.0007(5)	0.0025(5)	0.0031(5)
C(9)	4*e*	0.6866(1)	1.03192(8)	0.0011(2)	0.0131(5)	0.0173(6)	0.0162(6)	0.0000(4)	0.0031(4)	0.0031(4)
C(10)	4*e*	0.5763(1)	1.17748(8)	–0.0425(2)	0.0237(7)	0.0157(6)	0.0279(7)	0.0025(5)	0.0112(5)	0.0014(5)
C(11)	4*e*	0.9721(1)	0.80931(9)	0.5161(2)	0.0238(7)	0.0220(7)	0.0165(6)	–0.0046(5)	0.0015(5)	–0.0007(5)
C(12)	4*e*	0.8893(1)	0.87616(9)	0.4460(2)	0.0163(6)	0.0244(7)	0.0176(6)	–0.0025(5)	0.0008(5)	–0.0036(5)
C(13)	4*e*	0.8367(1)	1.01111(9)	0.2472(2)	0.0240(6)	0.0199(6)	0.0163(6)	–0.0002(5)	–0.0037(5)	–0.0056(5)
C(14)	4*e*	1.0919(1)	0.80280(9)	0.4589(2)	0.0205(6)	0.0210(6)	0.0183(6)	0.0013(5)	–0.0022(5)	–0.0031(5)
C(15)	4*e*	1.0461(1)	0.92979(9)	0.2616(2)	0.0232(6)	0.0221(7)	0.0160(6)	–0.0054(5)	0.0020(5)	–0.0016(5)
C(16)	4*e*	1.1291(1)	0.86291(9)	0.3312(2)	0.0177(6)	0.0265(7)	0.0195(6)	–0.0020(5)	0.0021(5)	–0.0047(5)
C(17)	4*e*	0.5151(1)	1.14393(9)	–0.1947(2)	0.0191(6)	0.0230(7)	0.0243(7)	0.0056(5)	0.0055(5)	0.0079(5)

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