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1-Benzyloxy-4-chlorobenzene

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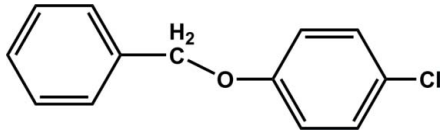
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.051; wR factor = 0.115; data-to-parameter ratio = 18.4.

In the title compound, $C_{13}H_{11}ClO$, the two benzene rings are close to coplanar, making a dihedral angle of 3.4 (1)° The crystal structure is stabilized by weak C—H$\cdots\pi$ interactions involving both benzene rings.

Related literature

For the chemistry and crystal structures of halogenated aromatic ether derivatives, see: Liu *et al.* (2006); Shen *et al.* (2003).



Experimental

Crystal data

$C_{13}H_{11}ClO$
M_r = 218.67
Orthorhombic, $Pna2_1$
a = 11.485 (2) Å
b = 13.033 (3) Å
c = 7.3333 (15) Å
V = 1097.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 298 K
0.4 × 0.35 × 0.2 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.881, T_{max} = 0.940
10943 measured reflections
2523 independent reflections
2189 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.115
S = 1.16
2523 reflections
137 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Absolute structure: Flack (1983), 1161 Friedel pairs
Flack parameter: −0.08 (9)

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C1—H1$\cdots Cg2^{i}$	0.93	2.81	3.570 (3)	140
C10—H10$\cdots Cg1^{i}$	0.93	2.88	3.624 (3)	138

Symmetry code: (i) $-x+1, -y+1, z-\frac{1}{2}$. $Cg1$ and $Cg2$ are the centroids of the C1–C6 and C8–C13 rings, respectively.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2976).

References

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
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supporting information

Acta Cryst. (2010). E**66**, o50 [doi:10.1107/S160053680905096X]

1-Benzyloxy-4-chlorobenzene

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S1. Comment

Halogenated aromatic ether derivatives have found wide range of applications in industry and coordination chemistry as ligands. They are also used in medicine as drugs, such as antibiotics. Recently, a series of halogenated aromatic ether compounds have been reported (Liu *et al.*, 2006; Shen *et al.*, 2003). As an extension of these work on the structural characterization, we report here the crystal structure of the title compound, 1-(benzyloxy)-4-chlorobenzene.

The crystal data show that in the title compound (Fig.1), the two benzene rings are essentially coplanar and twisted from each other by a dihedral angle of 3.4 (1)°. All bond lengths are within the normal range. The crystal structure is stabilized by weak C—H···π interactions.

S2. Experimental

The commercial 1-(benzyloxy)-4-chlorobenzene (3 mmol, 648 mg) was dissolved in chloroform (20 ml). The solvent was slowly evaporated in air affording colourless block-shaped crystals of the title compound suitable for X-ray analysis.

S3. Refinement

All H atoms were fixed geometrically and treated as riding with C–H = 0.93 Å (aromatic) or 0.97 Å (methylene) and U_{iso}(H) =1.2U_{eq}(C).

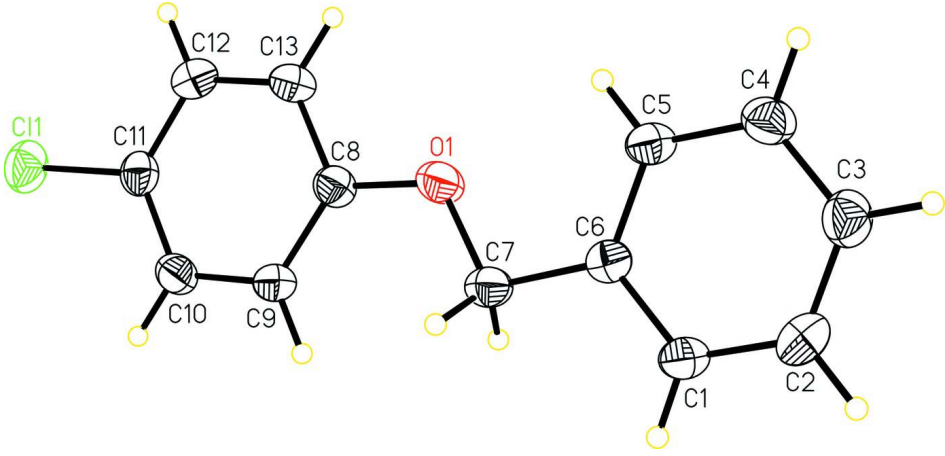

Figure 1

A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

1-Benzyloxy-4-chlorobenzene

Crystal data

$C_{13}H_{11}ClO$
$M_r = 218.67$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 11.485$ (2) Å
$b = 13.033$ (3) Å
$c = 7.3333$ (15) Å
$V = 1097.7$ (4) Å^3
$Z = 4$
$F(000) = 456$
$D_x = 1.323$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2189 reflections
$\theta = 3.1$–$27.5°$
$\mu = 0.32$ mm^{-1}
$T = 298$ K
Bock, colourless
0.4 × 0.35 × 0.2 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.881$, $T_{max} = 0.940$
10943 measured reflections
2523 independent reflections
2189 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -14 \rightarrow 14$
$k = -16 \rightarrow 16$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.115$
$S = 1.16$
2523 reflections
137 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 0.0118P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.073 (6)
Absolute structure: Flack (1983), 1161 Friedel pairs
Absolute structure parameter: −0.08 (9)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.76032 (5)	0.10633 (4)	0.35041 (15)	0.0662 (2)

C11	0.72273 (17)	0.23611 (14)	0.3557 (3)	0.0450 (4)
C6	0.53613 (16)	0.69777 (14)	0.3347 (3)	0.0400 (4)
C5	0.62546 (18)	0.74952 (15)	0.4233 (3)	0.0472 (5)
H5	0.6896	0.7134	0.4663	0.057*
C12	0.79431 (18)	0.30526 (17)	0.4443 (3)	0.0477 (5)
H12	0.8636	0.2833	0.4969	0.057*
O1	0.63588 (13)	0.54166 (11)	0.3941 (3)	0.0610 (5)
C8	0.65937 (17)	0.43950 (15)	0.3727 (3)	0.0443 (4)
C4	0.6193 (2)	0.85449 (18)	0.4478 (4)	0.0555 (6)
H4	0.6791	0.8885	0.5085	0.067*
C10	0.62149 (18)	0.26770 (16)	0.2733 (3)	0.0483 (5)
H10	0.5747	0.2206	0.2125	0.058*
C13	0.76238 (17)	0.40660 (17)	0.4542 (3)	0.0468 (5)
H13	0.8096	0.4533	0.5153	0.056*
C9	0.58956 (18)	0.37006 (16)	0.2814 (3)	0.0471 (5)
H9	0.5213	0.3920	0.2254	0.056*
C7	0.53952 (18)	0.58411 (16)	0.3009 (3)	0.0480 (5)
H7A	0.4681	0.5527	0.3441	0.058*
H7B	0.5464	0.5708	0.1712	0.058*
C2	0.4370 (2)	0.85864 (19)	0.2956 (4)	0.0603 (6)
H2	0.3736	0.8953	0.2514	0.072*
C1	0.44145 (19)	0.75356 (17)	0.2727 (3)	0.0502 (5)
H1	0.3803	0.7199	0.2151	0.060*
C3	0.5254 (2)	0.90919 (16)	0.3831 (4)	0.0587 (6)
H3	0.5221	0.9799	0.3987	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0683 (4)	0.0468 (3)	0.0835 (4)	0.0071 (2)	0.0070 (4)	−0.0037 (4)
C11	0.0476 (10)	0.0429 (9)	0.0443 (10)	0.0007 (8)	0.0080 (10)	−0.0011 (12)
C6	0.0392 (9)	0.0465 (10)	0.0344 (9)	−0.0003 (7)	0.0012 (8)	0.0031 (8)
C5	0.0399 (10)	0.0505 (12)	0.0514 (13)	−0.0016 (8)	−0.0072 (8)	0.0054 (10)
C12	0.0396 (10)	0.0555 (13)	0.0479 (11)	0.0008 (9)	−0.0008 (10)	0.0078 (10)
O1	0.0647 (9)	0.0431 (7)	0.0752 (11)	0.0053 (6)	−0.0318 (8)	−0.0081 (8)
C8	0.0474 (10)	0.0428 (9)	0.0426 (10)	−0.0012 (8)	−0.0041 (9)	−0.0006 (10)
C4	0.0502 (12)	0.0533 (12)	0.0631 (14)	−0.0104 (10)	−0.0051 (11)	−0.0005 (11)
C10	0.0460 (11)	0.0518 (11)	0.0471 (10)	−0.0068 (9)	−0.0001 (10)	−0.0095 (10)
C13	0.0452 (11)	0.0484 (12)	0.0469 (12)	−0.0071 (8)	−0.0093 (10)	0.0001 (9)
C9	0.0399 (10)	0.0547 (11)	0.0466 (11)	0.0026 (8)	−0.0082 (9)	−0.0061 (10)
C7	0.0440 (10)	0.0511 (11)	0.0488 (13)	−0.0004 (8)	−0.0100 (9)	−0.0008 (9)
C2	0.0518 (12)	0.0606 (13)	0.0686 (16)	0.0148 (11)	−0.0061 (11)	0.0069 (12)
C1	0.0395 (10)	0.0578 (13)	0.0535 (11)	0.0006 (8)	−0.0077 (10)	−0.0018 (10)
C3	0.0615 (14)	0.0442 (10)	0.0705 (17)	0.0003 (9)	0.0027 (13)	0.0021 (12)

Geometric parameters (Å, º)

Cl1—C11	1.7460 (19)	C4—C3	1.377 (3)
C11—C10	1.374 (3)	C4—H4	0.93
C11—C12	1.382 (3)	C10—C9	1.385 (3)
C6—C1	1.385 (3)	C10—H10	0.93
C6—C5	1.389 (3)	C13—H13	0.93
C6—C7	1.502 (3)	C9—H9	0.93
C5—C4	1.382 (3)	C7—H7A	0.97
C5—H5	0.93	C7—H7B	0.97
C12—C13	1.373 (3)	C2—C3	1.370 (3)
C12—H12	0.93	C2—C1	1.381 (3)
O1—C8	1.367 (2)	C2—H2	0.93
O1—C7	1.413 (2)	C1—H1	0.93
C8—C9	1.382 (3)	C3—H3	0.93
C8—C13	1.393 (3)		
C10—C11—C12	120.99 (19)	C12—C13—C8	120.0 (2)
C10—C11—Cl1	119.34 (16)	C12—C13—H13	120.0
C12—C11—Cl1	119.67 (17)	C8—C13—H13	120.0
C1—C6—C5	118.59 (18)	C8—C9—C10	119.85 (19)
C1—C6—C7	118.95 (17)	C8—C9—H9	120.1
C5—C6—C7	122.45 (17)	C10—C9—H9	120.1
C4—C5—C6	120.25 (19)	O1—C7—C6	109.07 (15)
C4—C5—H5	119.9	O1—C7—H7A	109.9
C6—C5—H5	119.9	C6—C7—H7A	109.9
C13—C12—C11	119.55 (19)	O1—C7—H7B	109.9
C13—C12—H12	120.2	C6—C7—H7B	109.9
C11—C12—H12	120.2	H7A—C7—H7B	108.3
C8—O1—C7	118.71 (15)	C3—C2—C1	120.4 (2)
O1—C8—C9	125.35 (17)	C3—C2—H2	119.8
O1—C8—C13	114.72 (17)	C1—C2—H2	119.8
C9—C8—C13	119.93 (19)	C2—C1—C6	120.7 (2)
C3—C4—C5	120.5 (2)	C2—C1—H1	119.7
C3—C4—H4	119.7	C6—C1—H1	119.7
C5—C4—H4	119.7	C2—C3—C4	119.5 (2)
C11—C10—C9	119.62 (19)	C2—C3—H3	120.2
C11—C10—H10	120.2	C4—C3—H3	120.2
C9—C10—H10	120.2		
C1—C6—C5—C4	−0.2 (3)	O1—C8—C9—C10	−178.3 (2)
C7—C6—C5—C4	178.7 (2)	C13—C8—C9—C10	0.9 (3)
C10—C11—C12—C13	1.6 (3)	C11—C10—C9—C8	−0.3 (3)
Cl1—C11—C12—C13	−177.57 (17)	C8—O1—C7—C6	−176.12 (18)
C7—O1—C8—C9	−7.0 (3)	C1—C6—C7—O1	−173.0 (2)
C7—O1—C8—C13	173.7 (2)	C5—C6—C7—O1	8.0 (3)
C6—C5—C4—C3	−0.7 (4)	C3—C2—C1—C6	−1.2 (4)
C12—C11—C10—C9	−1.0 (3)	C5—C6—C1—C2	1.2 (3)

Cl1—C11—C10—C9	178.22 (17)	C7—C6—C1—C2	−177.8 (2)
C11—C12—C13—C8	−1.0 (3)	C1—C2—C3—C4	0.2 (4)
O1—C8—C13—C12	179.0 (2)	C5—C4—C3—C2	0.7 (4)
C9—C8—C13—C12	−0.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···*Cg*2^{i}	0.93	2.81	3.570 (3)	140
C10—H10···*Cg*1^{i}	0.93	2.88	3.624 (3)	138

Symmetry code: (i) −*x*+1, −*y*+1, *z*−1/2.