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2-Benzyl-4-chloro-1-(4-nitrobenzyloxy)benzene

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The crystal structure of the title compound, $C_{20}H_{16}ClNO_3$, is stabilized by π–π stacking interactions.

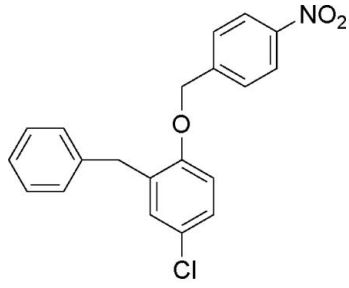
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.053
wR factor = 0.153
Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

In our studies on the benzylation of phenols, we have prepared chloro derivatives of benzylphenols. The title compound, (I) (Fig. 1), is one of these compounds and its crystal structure is reported here. The dihedral angle between the C1–C6 and C8–C13 benzene ring mean planes is 75.93 (15)°, and that between the C8–C13 and C15–C20 mean planes is 2.62 (14)°



(I)

In the crystal structure, π–π interactions exist between the C8–C13 (centroid = $Cg1$) and C15–C20 (centroid = $Cg2$) benzene rings with perpendicular and centroid–centroid separations of 3.640 and 3.930 (2) Å, respectively, for $Cg1\cdots Cg2^{i}$ [symmetry code: (i) $-x$, $1-y$, $2-z$], and 3.583 and 3.875 (2) Å, respectively, for $Cg1\cdots Cg2^{ii}$ [symmetry code: (ii) $1-x$, $1-y$, $2-z$]. A short intermolecular C—H···O interaction (Table 1) also occurs.

Experimental

The title compound was synthesized by the reaction of 2-benzyl-4-chlorophenol with 1-(bromomethyl)-4-nitrobenzene in the presence of sodium ethoxide (Bockmuhl & Stein, 1932). Yellow blocks of (I) (m.p. 386 K) were obtained by recrystallization from an ethyl acetate solution. Analysis calculated for $C_{20}H_{16}ClNO_3$: C 67.90, H 4.56, N 3.96%; found: C 67.87, H 4.50, N 3.93%.

Crystal data

$C_{20}H_{16}ClNO_3$
M_r = 353.79
Monoclinic, $P2_1/c$
a = 7.329 (2) Å
b = 19.023 (5) Å
c = 12.723 (3) Å
β = 101.845 (5)°
V = 1735.9 (8) Å^3
Z = 4
D_x = 1.354 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 293 (2) K
Block, yellow
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.945, T_{max} = 0.958
8820 measured reflections
3064 independent reflections
1780 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.153
S = 1.06
3064 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 0.4515P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O2^{i}	0.93	2.51	3.366 (4)	152

Symmetry code: (i) $x, y, z+1$.

All H atoms were positioned geometrically (C—H = 0.93–0.97Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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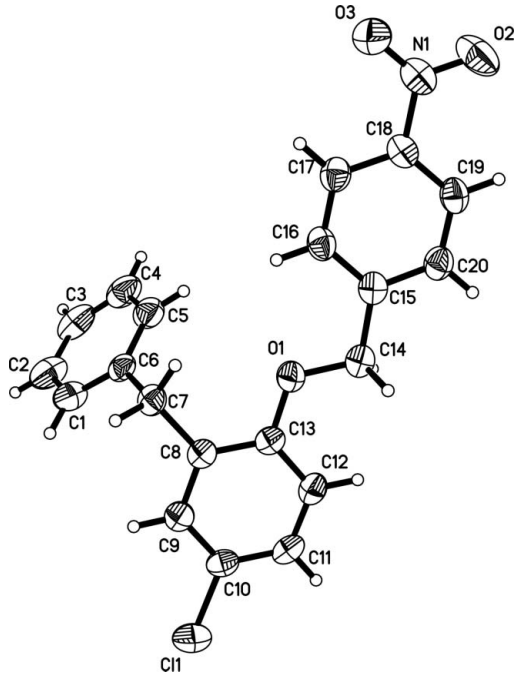

Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms).

References

Bockmuhl, M. & Stein, L. (1932). US Patent No. 1 877 756.
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