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4-Nitrophenyl phenyl ether: sheets built from C—H···O and C—H···π(arene) hydrogen bonds

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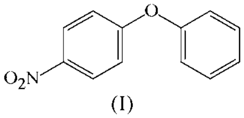
In the title compound, $C_{12}H_9NO_3$, the ether C—O—C angle is 119.65 (10)°. The molecules are linked into sheets by a combination of C—H···O and C—H···π(arene) hydrogen bonds, reinforced by an aromatic π–π stacking interaction.

Comment

We report here the molecular and supramolecular structure of the title compound, (I) (Fig. 1), a simple substituted analogue of the low-melting-point parent compound biphenyl ether, Ph_2O (m.p. *ca* 300 K), the structure of which does not appear in the Cambridge Structural Database (January 2005 release; Allen, 2002). The C—O distance to the substituted ring in (I) is significantly the shorter of the two C—O distances (Table 1), but the mean C—C distances for the two aryl rings are identical within experimental uncertainty. The C—O—C angle is strikingly larger than those typically found in water and simple ethers, which are just below the idealized tetrahedral value. The value of this angle in (I) may be compared with the corresponding C—O—C angle of 127.9 (1)° in $Ph_3C—O—CPh_3$ (Glidewell & Liles, 1978). Associated with this large angle is the concerted twist of the aryl rings away from the central C—O—C plane, as indicated by the relevant torsion angles. The dihedral angle between the ring planes is 63.2 (2)°. These geometric features are most readily ascribed to the avoidance of the mutual repulsion between the *ortho* H atoms bonded to atoms C2 and C16 (Fig. 1).



(I)

The molecules of (I) are linked into sheets by a combination of one C—H···O hydrogen bond and one C—H···π(arene) hydrogen bond, and these sheets are reinforced by an aromatic π–π stacking interaction. Aryl atom C6 in the molecule at (x, y, z) acts as hydrogen-bond donor to nitro atom O42 in the molecule at ($1 - x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$), so producing a $C(6)$ (Bernstein *et al.*, 1995) chain running parallel to the [010] direction and generated by the 2_1 screw axis along ($\frac{1}{2}$, y, $\frac{1}{4}$) (Fig. 2). A similar chain, antiparallel to the first and related to

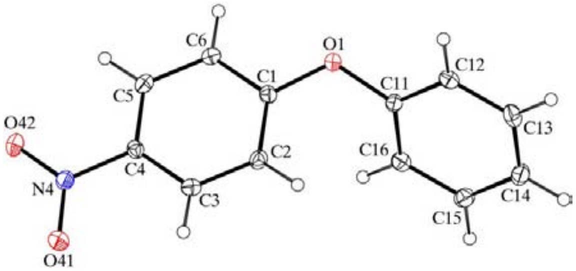


Figure 1
The molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

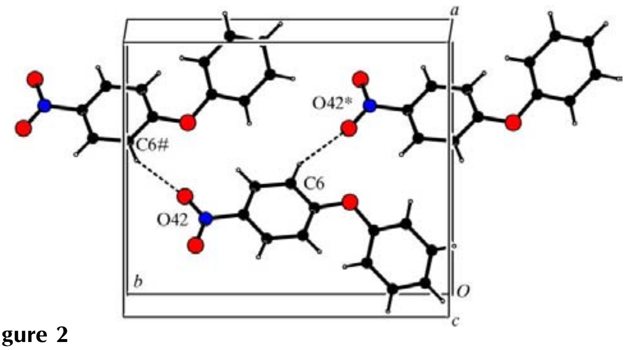


Figure 2
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded chain along [010]. Atoms marked with an asterisk (*) or hash (#) are at the symmetry positions ($1 - x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$) and ($1 - x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$), respectively.

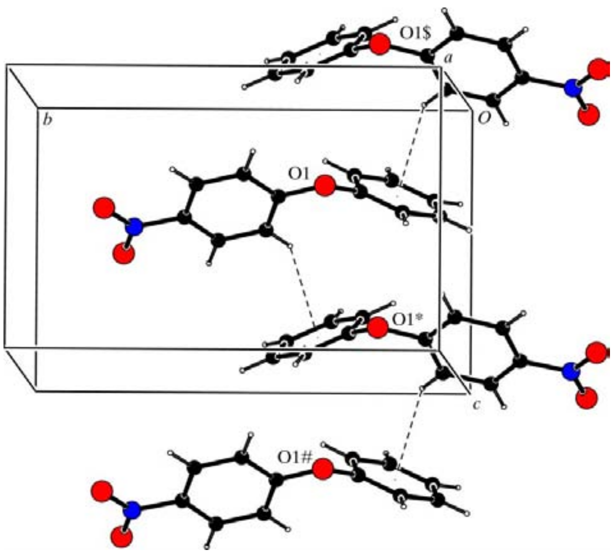


Figure 3
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded chain along [001]. Atoms marked with an asterisk (*), hash (#) or dollar sign ($) are at the symmetry positions (x, $\frac{1}{2} - y$, $\frac{1}{2} + z$), (x, y, $1 + z$) and (x, $\frac{1}{2} - y$, $z - \frac{1}{2}$), respectively.

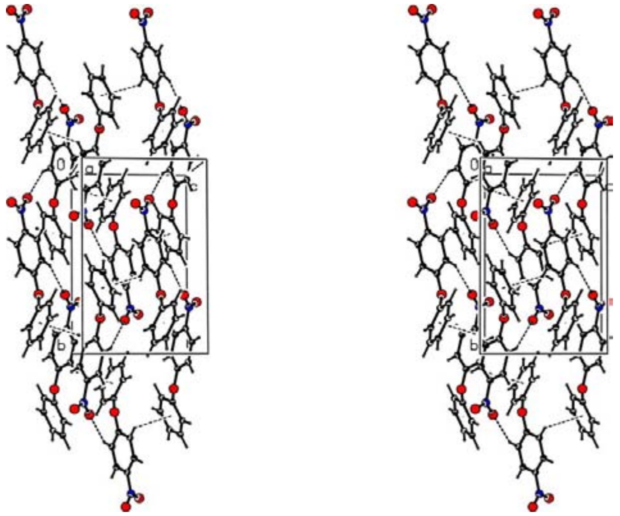


Figure 4
A stereoview of part of the crystal structure of (I), showing the formation of the (100) sheet.

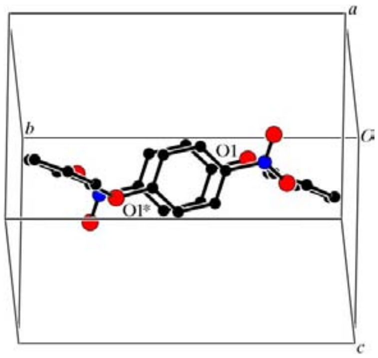


Figure 5
Part of the crystal structure of (I), showing the π–π stacking interaction. For the sake of clarity, H atoms have been omitted. The atom marked with an asterisk (*) is at the symmetry position $(1 - x, 1 - y, 1 - z)$.

it by inversion, is generated by the 2_1 screw axis along $(\frac{1}{2}, -y, \frac{3}{4})$, and these chains are linked by the C—H$\cdots\pi$(arene) hydrogen bond.

Aryl atom C2 in the molecule at (x, y, z), which forms part of the chain along $(\frac{1}{2}, y, \frac{1}{4})$, acts as hydrogen-bond donor to the unsubstituted C11–C16 ring in the molecule at $(x, \frac{1}{2} - y, \frac{1}{2} + z)$, which lies in the chain along $(\frac{1}{2}, -y, \frac{3}{4})$. In this manner, a second chain motif is produced, running parallel to the [001] direction and generated by the c-glide plane at $y = \frac{1}{4}$ (Fig. 3). The combination of the [010] and [001] chains generates a (100) chain in the form of a (4,4)-net (Batten & Robson, 1998) built from a single type of ring (Fig. 4). Just one sheet of this type passes through each unit cell.

A single aromatic π–π stacking interaction reinforces the sheet. The C1–C6 rings in the molecules at (x, y, z) and $(1 - x, 1 - y, 1 - z)$ are strictly parallel and these molecules lie in the same sheet. The interplanar spacing between these molecules is 3.296 (2) Å and the ring–centroid separation is 3.695 (2) Å, corresponding to a centroid offset of 1.670 (2) Å (Fig. 5). There are no direction-specific interactions between adjacent (100) sheets.

Experimental

A sample of the title compound was obtained from Aldrich. Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of a solution in ethanol.

Crystal data

$C_{12}H_9NO_3$
$M_r = 215.20$
Monoclinic, $P2_1/c$
$a = 10.3300\ (5)$ Å
$b = 12.2408\ (4)$ Å
$c = 7.9804\ (4)$ Å
$\beta = 96.215\ (2)^\circ$
$V = 1003.17\ (8)$ Å^3
$Z = 4$

$D_x = 1.425$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2285 reflections
$\theta = 3.1$–27.5°
$\mu = 0.10$ mm^{-1}
$T = 120\ (2)$ K
Shard, colourless
0.34 × 0.18 × 0.09 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{\min} = 0.955$, $T_{\max} = 0.991$
11 250 measured reflections

2285 independent reflections
1644 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.045$
$\theta_{\max} = 27.5^\circ$
$h = -13 \rightarrow 13$
$k = -15 \rightarrow 15$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.113$
$S = 1.04$
2285 reflections
146 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 0.0313P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.22$ e Å^{-3}
$\Delta\rho_{\min} = -0.29$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.018 (3)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.3783 (15)	O1—C11	1.3955 (15)
C1—O1—C11	119.65 (10)		
C2—C1—O1—C11	26.75 (19)	C1—O1—C11—C16	47.64 (18)

Table 2
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C11–C16 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C6—H6$\cdots$O42$^{\rm i}$	0.95	2.54	3.4033 (17)	152
C2—H2$\cdots Cg^{\rm ii}$	0.95	2.71	3.428 (2)	134

Symmetry codes: (i) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $x, \frac{1}{2} - y, z + \frac{1}{2}$.

The space group $P2_1/c$ was uniquely assigned from the systematic absences. All H atoms were located from difference maps and then treated as riding atoms, with C—H distances of 0.95 Å and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *OSCAIL for Windows* (McArdle, 2003) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); soft-

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ware used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1810). Services for accessing these data are described at the back of the journal.

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