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1,3-Bis(3,5-dimethylphenoxy)propane

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.050
wR factor = 0.135
Data-to-parameter ratio = 19.0

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

The molecular structure of the title compound, $C_{19}H_{24}O_2$, exhibits great similarity to that of the previously published non-derivatized molecule, the greatest difference being seen in the central torsion angles and ring orientations. The structure additionally features a π–π stacking interaction and a weak C—H$\cdots\pi$ interaction.

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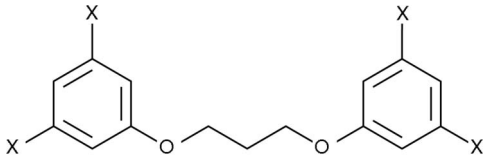
Comment

The title compound, (I), was characterized as a precursor for oxidation to isophthalaldehyde donor ligands, as part of an ongoing series of investigations (Zondervan *et al.*, 1997).



(I) X = CH_3 (II) X = H

The aliphatic linker between the aromatic rings is not in a fully stretched conformation, but has adopted an (*anti*, −*gauche*,−*gauche*,*anti*) conformation. This is directly comparable to the published (Sasanuma *et al.*, 2004) non-derivatized ligand, *viz*. 1,3-diphenoxypropane, (II), which adopts a nearly identical conformation (Fig. 2).

The main difference between the two molecules is in the torsion angles around the bonds which share the central atom of the propane linker. In (I), these are −73.50 (15) and −72.70 (16)°, whereas in (II) they are both −57.1 (2)° by symmetry. This difference in torsion angle results in a significant change in the pitch of the two sets of benzene rings. This ring orientation should not be attributed to the torsion angles

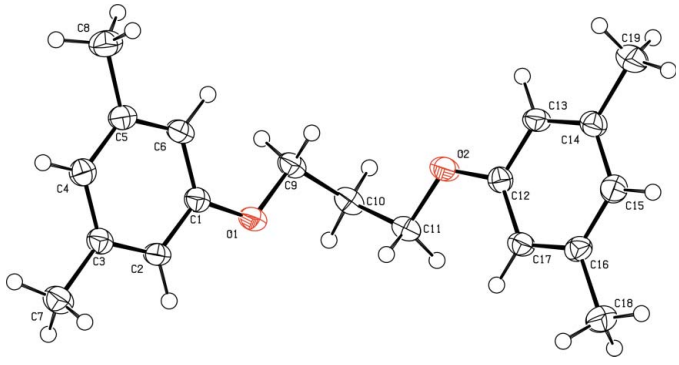


Figure 1
View of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

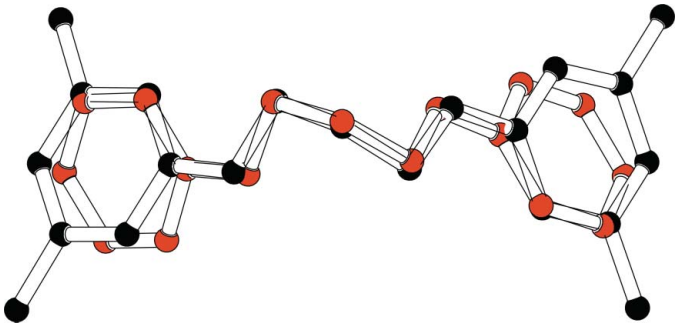


Figure 2
Quaternion fit based on the five linking O and C atoms of the title compound (black) with the previously published non-derivatized molecule (red).

around the ring C—O bonds, which are actually quite comparable; 173.70 (13) and 177.51 (13)° in (I), and 177.2 (2)° for both rings in (II).

Although there are a number of rings in the structure of (I), there is only one instance of π–π stacking, between the C1–C6 ring and its symmetry equivalent at $(1-x, -y, 2-z)$. The two rings are parallel by symmetry with a perpendicular separation of 3.411 (1) Å and a horizontal slippage of 1.16 Å (Fig. 3).

There is, additionally, a weak C—H$\cdots\pi$ interaction between H11*B* and the C12–C17 ring system, with a hydrogen to ring centroid (*Cg*) distance of 2.88 Å and a C—H$\cdots$*Cg* angle of 157° (Fig. 4).

Experimental

Single crystals, with a melting point of 308 K, were obtained by recrystallization from acetone.

Crystal data

$C_{19}H_{24}O_2$
M_r = 284.38
Triclinic, $P\overline{1}$
a = 8.7906 (12) Å
b = 9.6774 (11) Å
c = 10.7788 (12) Å
α = 82.410 (9)°
β = 78.47 (1)°
γ = 63.796 (9)°
V = 805.11 (17) Å^3
Z = 2
D_x = 1.173 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10.0–15.2°
μ = 0.07 mm^{-1}
T = 150 (2) K
Block, colourless
0.5 × 0.5 × 0.4 mm

Data collection

Nonius CAD-4-Turbo diffractometer
ω scans
Absorption correction: none
4628 measured reflections
3689 independent reflections
2710 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.5°
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 9$
3 standard reflections
frequency: 60 min
intensity decay: 0.8%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.135
S = 1.03
3689 reflections
194 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.2118P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

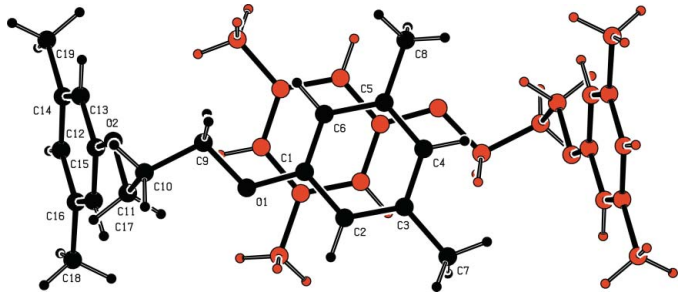


Figure 3
π–π stacking of the C1–C6 ring. The view is perpendicular to the ring mean plane.

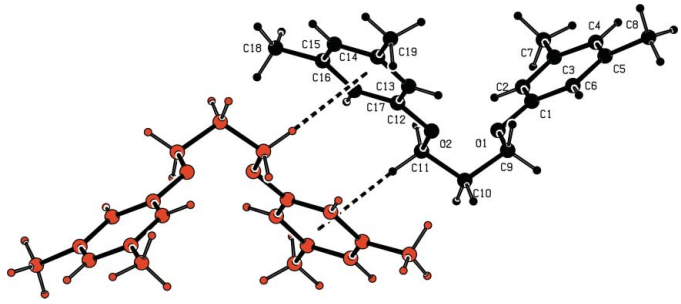


Figure 4
Weak C—H$\cdots\pi$ interaction (dashed lines) between H11*B* and the C12–C17 ring.

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.3673 (18)	O2—C11	1.4397 (18)
O1—C9	1.4351 (18)	C9—C10	1.508 (2)
O2—C12	1.3647 (18)	C10—C11	1.509 (2)
C9—O1—C1—C2	173.70 (13)	C12—O2—C11—C10	−179.40 (13)
C1—O1—C9—C10	179.91 (12)	C9—C10—C11—O2	−72.70 (16)
O1—C9—C10—C11	−73.50 (15)	C11—O2—C12—C13	177.51 (13)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and U_{iso}(H) = 1.2U_{eq}(C) for all other H atoms.

Data collection: locally modified *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *SET4* (de Boer & Duisenberg, 1984); data reduction: *HELENA* (Spek, 1997); program(s) used to solve structure: *SHELXS96* (Sheldrick, 1996); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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