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4-[4-(4-Formyl-2-methoxyphenoxy)butoxy]-3-methoxybenzaldehyde

Zhong-Yu Duan* and Wen-Jun Zhang

Hebei University of Technology, Tianjin 300130, People's Republic of China

Correspondence e-mail: duan_zhongyu@163.com

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Key indicators

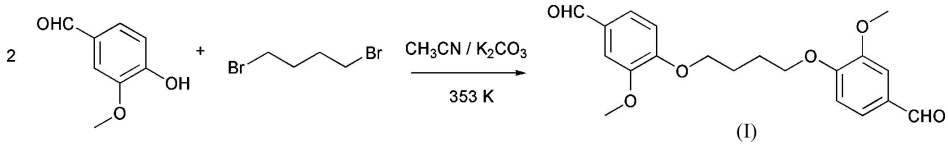
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.101
Data-to-parameter ratio = 13.7

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

The title compound, $C_{20}H_{22}O_6$, was prepared by the reaction of 4-hydroxy-3-methoxybenzaldehyde and 1,4-dibromobutane. A crystallographic center of symmetry is located at the mid-point of the central C—C bond. The four C atoms linking the two aromatic rings are coplanar and the two aromatic rings are parallel to each other.

Comment

Crystal engineering plays an important role in the preparation of crystalline solid materials, enabling their architecture and properties to be predictable (Parashar *et al.*, 1988; Tynan *et al.*, 2005). We are interested in the molecular and ionic recognition of crown ethers. As part of this study, we report the synthesis and structure of the title compound, (I), which will provide useful information on its physical and chemical properties.



(I)

A view of the molecule is shown in Fig. 1. A crystallographic center of symmetry is located at the mid-point of the C10—C10^{i} bond [symmetry code: (i) $-x$, $-y$, $2-z$]. The vanillin system (C1–C8/O1–O3) is planar, with an r.m.s. deviation for fitted atoms of 0.0289 Å. The chain of atoms C9—C10—C10^{i}—C9^{i} linking the two vanillin systems is planar and this plane makes a dihedral angle of 5.2 (2)° with the vanillin plane. The two aromatic rings in the molecule are parallel to each other. The bond lengths and angles are unexceptional.

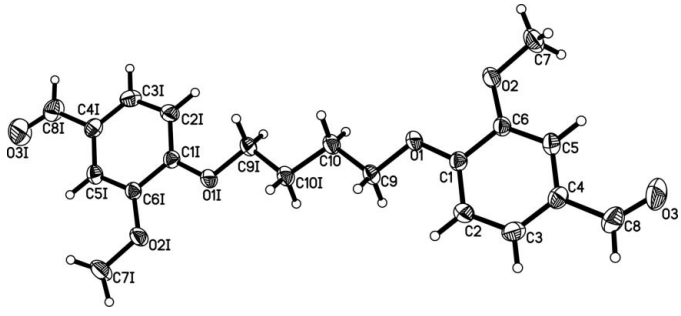


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level. [Symmetry code: (I) $-x$, $-y$, $2-z$.]

Experimental

To a solution of 4-hydroxy-3-methoxybenzaldehyde (15.2 g, 10 mmol) and potassium carbonate (13.8 g, 10 mmol) in acetonitrile (500 ml), 1,4-dibromobutane (10.8 g, 5 mmol) was added over a period of 30 min and the mixture refluxed for 24 h under nitrogen. The solvent was removed and the resultant oil poured into ice–water (500 ml). The white precipitate was then isolated and recrystallized from ethanol to give the pure compound in 63% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{20}H_{22}O_6$
M_r = 358.38
Monoclinic, $P2_1/c$
a = 7.4200 (16) Å
b = 7.6630 (16) Å
c = 16.407 (3) Å
β = 95.787 (4)°
V = 928.2 (3) Å^3
Z = 2
D_x = 1.282 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1740 reflections
θ = 2.8–26.3°
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, colorless
0.36 × 0.30 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.944, T_{max} = 0.977
4527 measured reflections
1632 independent reflections
1142 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.0°
$h = -8 \rightarrow 7$
$k = -9 \rightarrow 8$
$l = -14 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
S = 1.03
1632 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.2073P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

H atoms were included in calculated positions and refined using a riding-model approximation; C—H = 0.93 (aromatic), 0.96 (methyl) and 0.97 Å (methylene), and U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl and 1.2 for other H atoms.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); software used to prepare material for publication: *SHELXTL*.

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