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

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Key indicators

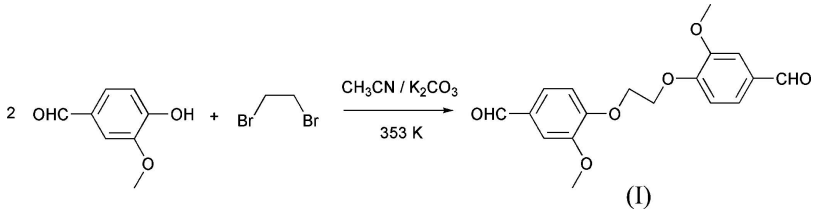
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.062
wR factor = 0.191
Data-to-parameter ratio = 12.7

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

The title compound, $C_{18}H_{18}O_6$, was prepared by the reaction of 4-hydroxy-3-methoxybenzaldehyde and 1,2-dibromoethane. There are one and a half molecules in the asymmetric unit; one has C_1 molecular symmetry and the other C_i, with the centre of inversion at the mid-point of the aliphatic C—C bond. The ethylenedioxy groups are coplanar with the aromatic systems of the vanillin groups.

Comment

Attention has been paid to the syntheses and crystal structures of compounds of the same type as the title compound, (I), owing to their role in crystal engineering (Parashar *et al.*, 1988; Tynan *et al.*, 2005). In the present study, we report the synthesis and structure of (I) (Fig. 1).



(I)

In molecule 1, each vanillin group is planar, with r.m.s. deviations for the fitted atoms of 0.0139 Å (C1–C7/O1/O3) and 0.0175 Å (C11–C16/C18/O2/O5). The dihedral angle between the two vanillin planes is 3.89 (10)°. In molecule 2, each vanillin group is planar with the r.m.s. deviation for the fitted atoms of 0.0105 Å and the two vanillin groups are exactly parallel by symmetry.

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), 1,2-dibromoethane (9.4 g, 5 mmol) was added over a period of 30 minutes and the mixture was refluxed for 24 h under nitrogen. The solvent was removed and the resultant oil was poured into ice–water (500 ml). A white precipitate was isolated and recrystallized from ethanol to give a pure compound in 65% yield. Colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{18}H_{18}O_6$
M_r = 330.32
Monoclinic, $P2_1/n$
a = 14.692 (4) Å
b = 7.805 (2) Å
c = 22.048 (6) Å
β = 108.551 (4)°
V = 2396.8 (11) Å^3
Z = 6
D_x = 1.373 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4375 reflections
θ = 2.8–26.3°
μ = 0.10 mm^{-1}
T = 294 (2) K
Prism, colourless
0.30 × 0.24 × 0.22 mm

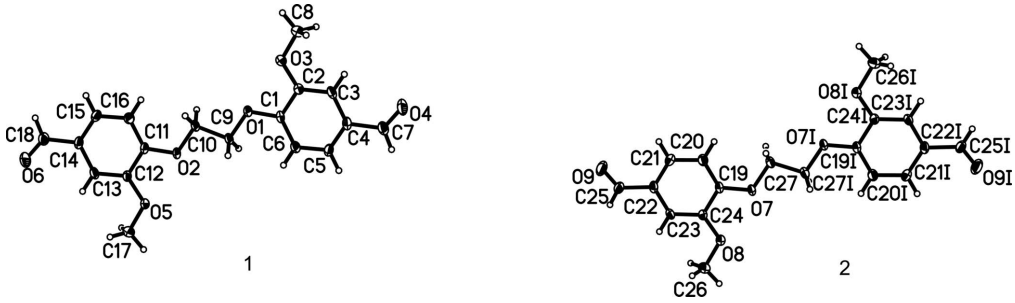


Figure 1
The structure of the two independent molecules of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level [symmetry code: (I) $2-x, -y, -z$.].

Data collection

Bruker SMART CCD area-detector diffractometer	4170 independent reflections
φ and ω scans	2809 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)	$R_{int} = 0.038$
$T_{min} = 0.960$, $T_{max} = 0.978$	$\theta_{max} = 25.0^\circ$
11241 measured reflections	$h = -17 \rightarrow 10$
	$k = -9 \rightarrow 8$
	$l = -23 \rightarrow 26$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0898P)^2 + 1.1951P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.062$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.191$	$\Delta\rho_{max} = 0.44$ e Å^{-3}
$S = 1.08$	$\Delta\rho_{min} = -0.33$ e Å^{-3}
4170 reflections	
328 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.364 (3)	O5—C17	1.425 (3)
O1—C9	1.428 (3)	O6—C18	1.190 (3)
O2—C11	1.358 (3)	O7—C19	1.360 (3)
O2—C10	1.433 (3)	O7—C27	1.430 (3)
O3—C2	1.352 (3)	O8—C24	1.355 (3)
O3—C8	1.433 (3)	O8—C26	1.426 (3)
O4—C7	1.185 (3)	O9—C25	1.185 (3)
O5—C12	1.360 (3)		
C1—O1—C9	116.68 (18)	C12—O5—C17	117.21 (19)
C11—O2—C10	116.97 (18)	C19—O7—C27	117.84 (18)
C2—O3—C8	117.3 (2)	C24—O8—C26	117.09 (19)

H atoms were included in calculated positions and refined using a riding-model approximation. The constrained C—H bond lengths and U_{iso}(H) parameters were 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C) for aromatic H atoms, and 0.96 Å and U_{iso}(H) = $1.5U_{eq}$(C) for methyl 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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