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4-[6-(4-Formyl-2-methoxyphenoxy)hexyloxy]-3-methoxybenzaldehyde

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.178
Data-to-parameter ratio = 16.4

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

The title compound, $C_{22}H_{26}O_6$, was prepared by the reaction of 4-hydroxy-3-methoxybenzaldehyde and 1,6-dibromohexane, displays molecular symmetry C_i, and has a crystallographic centre of inversion located at the mid-point of the C—C bond of the aliphatic chain. The zigzag aliphatic chain is coplanar with the aromatic rings of the vanillin groups.

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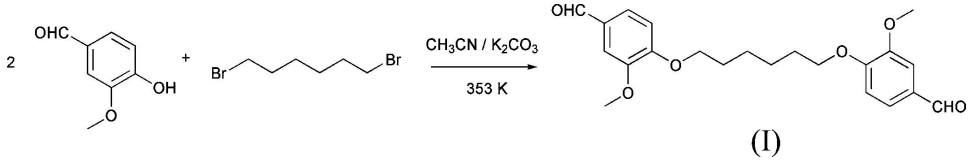
Comment

Since the first syntheses of macrocyclic crown ethers that are capable of forming stable and selective complexes with alkali and alkaline earth metal ions were performed by Pedersen (1967), a number of studies have been made to understand the factors that control the thermodynamic and kinetic stability and selectivity of the resulting complexes (Kim *et al.*, 1999). 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). A view of the molecule is shown in Fig. 1. A crystallographic centre of symmetry is located at the mid-point of the C11—C11^{i} bond [symmetry code: (i) $-x, -y, -z$]. Each vanillin group (C1–C8/O1/O2) is planar, with an r.m.s. deviation for fitted atoms of 0.028 Å. The chain of atoms C9–C11/C11^{i}–C9^{i} linking the two vanillin systems is planar, with an r.m.s. deviation for fitted atoms of 0.003 Å. The C6—C1—O1—C9 torsion angle is 177.3 (2)°, confirming the coplanarity of the aliphatic and aromatic groups. The geometry is similar to that in 4-[4-(4-formyl-2-methoxyphenoxy)butoxy]-3-methoxybenzaldehyde (Duan *et al.*, 2005). However, the dihedral angle between the plane (C9–C11/C11^{i}–C9^{i}) and the vanillin plane is 3.0 (3)°, in contrast to the value of 5.2 (2)° in 4-[4-(4-formyl-2-methoxyphenoxy)butoxy]-3-methoxybenzaldehyde.



(I)

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), 1,6-dibromohexane (12.2 g, 5 mmol) was added over a period of 30 min, and the mixture was refluxed for 24 h under nitrogen. The solvent was removed and the resulting oil was poured into ice–water (500 ml). The white precipitate was isolated and recrystallized from ethanol to give a pure compound in 54% yield.

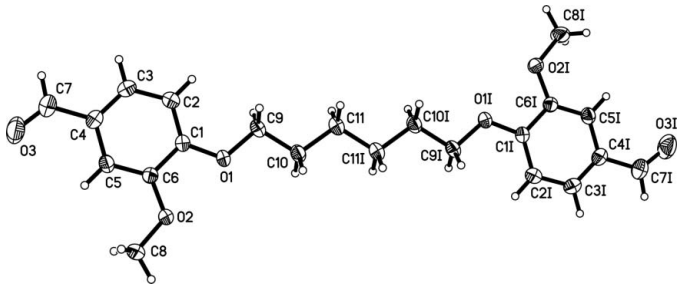


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level. [Symmetry code: (I) $-x, -y, -z$.]

Colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{22}H_{26}O_6$	D_x = 1.246 Mg m^{-3}
M_r = 386.43	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1658 reflections
a = 9.588 (2) Å	θ = 3.0–26.1°
b = 7.8313 (17) Å	μ = 0.09 mm^{-1}
c = 13.721 (3) Å	T = 294 (2) K
β = 91.311 (4)°	Prism, colourless
V = 1030.0 (4) Å^3	0.40 × 0.36 × 0.20 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	2103 independent reflections
φ and ω scans	1248 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.035
T_{min} = 0.962, T_{max} = 0.982	θ_{max} = 26.4°
5586 measured reflections	$h = -11 \rightarrow 11$
	$k = -8 \rightarrow 9$
	$l = -15 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0979P)^2 + 0.1851P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.050	
$wR(F^2)$ = 0.178	
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
2103 reflections	$\Delta\rho_{max}$ = 0.51 e Å^{-3}
128 parameters	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
H-atom parameters constrained	

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

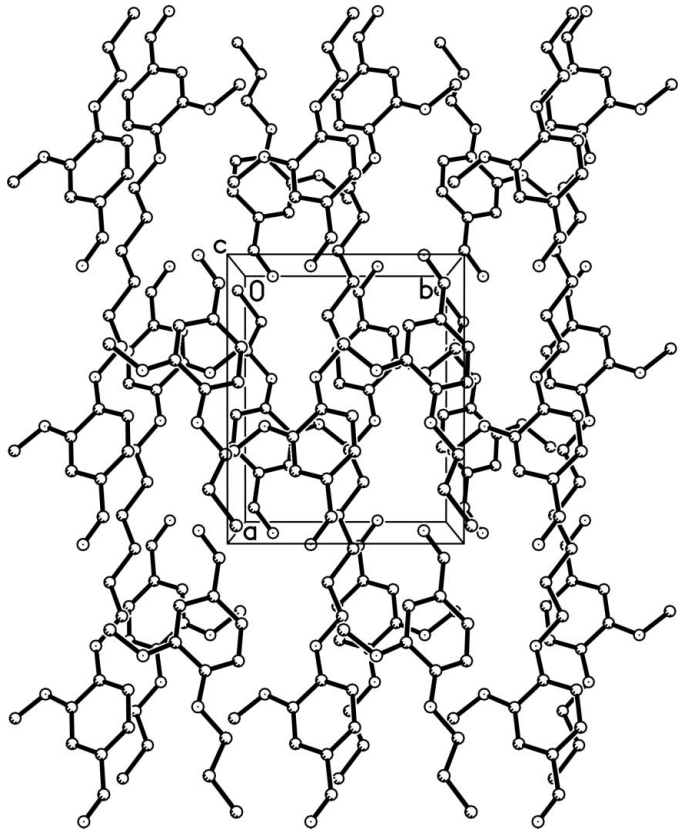


Figure 2
A view, down the c axis, of the packing arrangement in the crystal structure of (I). H atoms have been omitted.

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