

2,5-Dimethoxybenzene-1,4-dicarbaldehyde

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Key indicators

Single-crystal X-ray study
 $T = 122$ K
Mean $\sigma(\text{C}-\text{C}) = 0.001$ Å
 R factor = 0.046
 wR factor = 0.130
Data-to-parameter ratio = 37.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The title compound, $\text{C}_{10}\text{H}_{10}\text{O}_4$, crystallizes in the triclinic space group $P\bar{1}$ with two half-molecules in the asymmetric unit; both molecules are located on inversion centres.

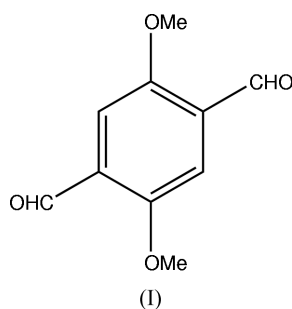
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Comment

The title compound, (I), was prepared for use as a building block in the syntheses of oligophenylenevinylenes for non-linear optical studies.



Compound (I) crystallizes in space group $P\bar{1}$, with two half-molecules in the asymmetric unit; both molecules display inversion symmetry. Equivalent bonds have essentially the same bond lengths in both molecules (Table 1) except for the terminal C—O bonds, which show differences that are slightly larger than the uncertainties. The aldehyde and methoxy groups are both coplanar with the benzene ring (Fig. 1). Phenyl–phenyl stacking along the a axis, as well as four weak C—H \cdots O hydrogen bonds (Table 2), are the most important intermolecular interactions responsible for the packing arrangement in this structure (Fig. 2).

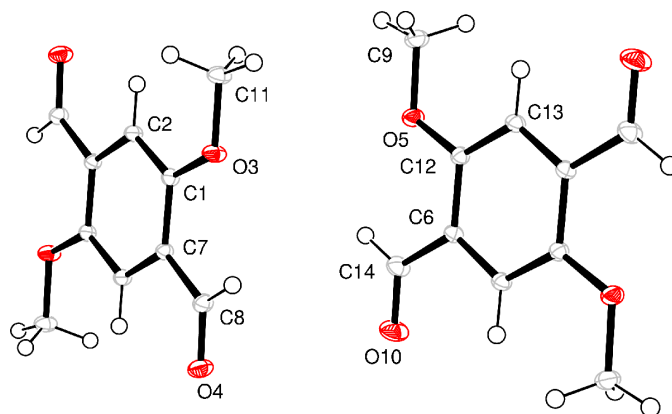


Figure 1

A view of the two independent molecules of (I). Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by $(-x, -y, -z)$ in the left molecule and $(1-x, -y, 2-z)$ in the right molecule.

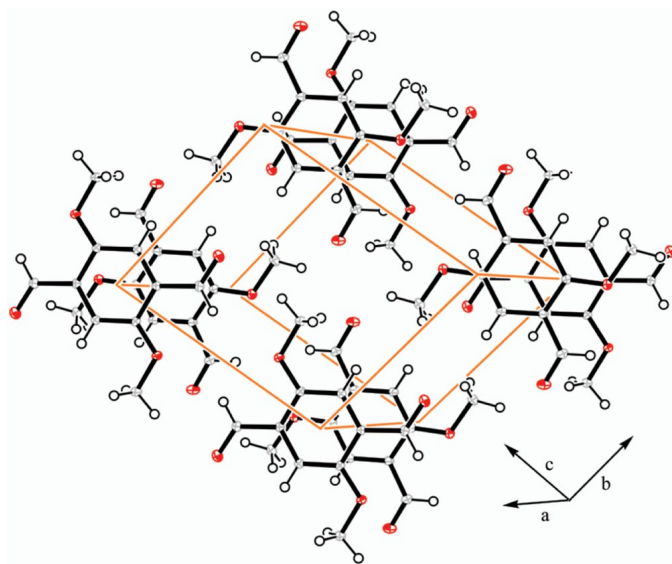


Figure 2
A view of the crystal packing in (I).

Experimental

The title compound, (I), was prepared according to the procedure given in Kuhnert *et al.* (2003). Crystals suitable for X-ray analysis were grown from a 1:5.3 *M* hydrochloric acid–THF binary mixture.

Crystal data

$C_{10}H_{10}O_4$	$Z = 2$
$M_r = 194.18$	$D_x = 1.482 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.1330 (6) \text{ \AA}$	Cell parameters from 7928 reflections
$b = 8.0050 (9) \text{ \AA}$	$\theta = 2.6\text{--}38.0^\circ$
$c = 8.4520 (11) \text{ \AA}$	$\mu = 0.12 \text{ mm}^{-1}$
$\alpha = 99.571 (9)^\circ$	$T = 122 (1) \text{ K}$
$\beta = 112.751 (6)^\circ$	Prism, yellow
$\gamma = 93.146 (8)^\circ$	$0.47 \times 0.31 \times 0.08 \text{ mm}$
$V = 435.08 (9) \text{ \AA}^3$	

Data collection

Nonius KappaCCD area-detector diffractometer	4725 independent reflections
ω and φ scans	3335 reflections with $I > 2\sigma(I)$
Absorption correction: Gaussian (Coppens, 1970)	$R_{\text{int}} = 0.045$
$T_{\text{min}} = 0.957$, $T_{\text{max}} = 0.995$	$\theta_{\text{max}} = 38.0^\circ$
20896 measured reflections	$h = -12 \rightarrow 12$
	$k = -13 \rightarrow 13$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.1289P]$
$R[F^2 > 2\sigma(F^2)] = 0.046$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.130$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.57 \text{ e \AA}^{-3}$
4725 reflections	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$
127 parameters	
H-atom parameters constrained	

Table 1
Selected bond lengths (\AA).

C1–O3	1.3611 (9)	O5–C9	1.4355 (10)
C1–C2	1.3930 (10)	C6–C13 ⁱⁱ	1.3976 (11)
C1–C7	1.4092 (10)	C6–C12	1.4094 (10)
C2–C7 ⁱ	1.3978 (10)	C6–C14	1.4796 (11)
O3–C11	1.4406 (9)	C7–C8	1.4763 (10)
O4–C8	1.2181 (10)	O10–C14	1.2136 (10)
O5–C12	1.3632 (9)	C12–C13	1.3920 (11)

Symmetry codes: (i) $-x, -y, -z$; (ii) $1-x, -y, 2-z$.

Table 2
Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C11–H11A \cdots O4 ⁱ	0.98	2.57	3.5128 (11)	162
C11–H11B \cdots O4 ⁱⁱ	0.98	2.63	3.5400 (12)	155
C9–H9A \cdots O10 ⁱⁱⁱ	0.98	2.66	3.5050 (11)	144
C9–H9B \cdots O4 ^{iv}	0.98	2.67	3.3744 (12)	129

Symmetry codes: (i) $-x, -y, 1-z$; (ii) $x, 1+y, z$; (iii) $1-x, -y, 1-z$; (iv) $1+x, 1+y, 1+z$.

H atoms were positioned geometrically ($C-H = 0.95\text{--}0.98 \text{ \AA}$) and refined as riding, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX* (Duisenberg, 1992); data reduction: *EvalCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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