electronic reprint

Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368
Editors: **W. Clegg and D. G. Watson**

2,5-Dimethoxybenzene-1,4-dicarbaldehyde

Christian B. Nielsen, Michael Pittelkow and Henning Osholm Sørensen

Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,5-Dimethoxybenzene-1,4-dicarbaldehyde

Christian B. Nielsen,[a]* Michael Pittelkow[b] and Henning Osholm Sørensen[c]

[a]The Danish Polymer Center, Risø National Laboratory, PO Box 49, DK-4000 Roskilde, Denmark, [b]University of Copenhagen, Department of Chemistry, Universitetsparken 5, 2100 Copenhagen, Denmark, and [c]Center for Fundamental Research: Metal Structures in Four Dimensions, Risø National Laboratory, PO Box 49, DK-4000 Roskilde, Denmark

Correspondence e-mail: christian.nielsen@risoe.dk

Key indicators

Single-crystal X-ray study
T = 122 K
Mean σ(C–C) = 0.001 Å
R factor = 0.046
wR factor = 0.130
Data-to-parameter ratio = 37.2

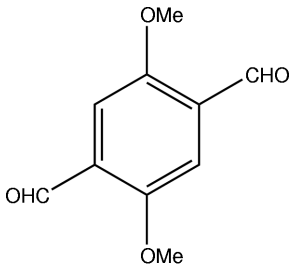
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 January 2005
Accepted 20 January 2005
Online 29 January 2005

The title compound, $C_{10}H_{10}O_4$, crystallizes in the triclinic space group $P\overline{1}$ with two half-molecules in the asymmetri unit; both molecules are located on inversion centres.

Comment

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



(I)

Compound (I) crystallizes in space group $P\overline{1}$, 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···O hydrogen bonds (Table 2), are the most important intermolecular interactions responsible for the packing arrangement in this structure (Fig. 2).

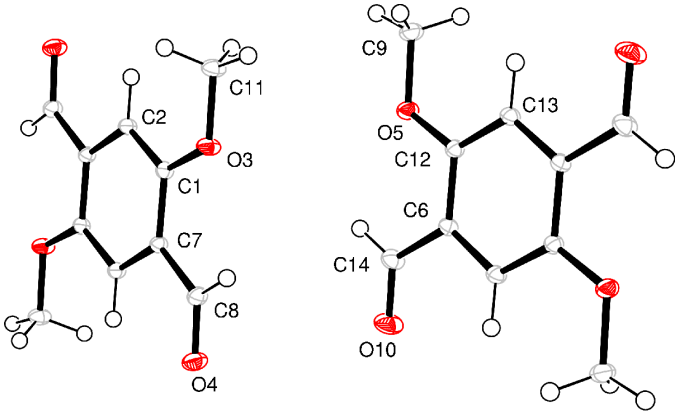


Figure 1
A view of the two independent molecules of (I). Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by $(-x, -y, -z)$ in the left molecule and $(1-x, -y, 2-z)$ in the right molecule.

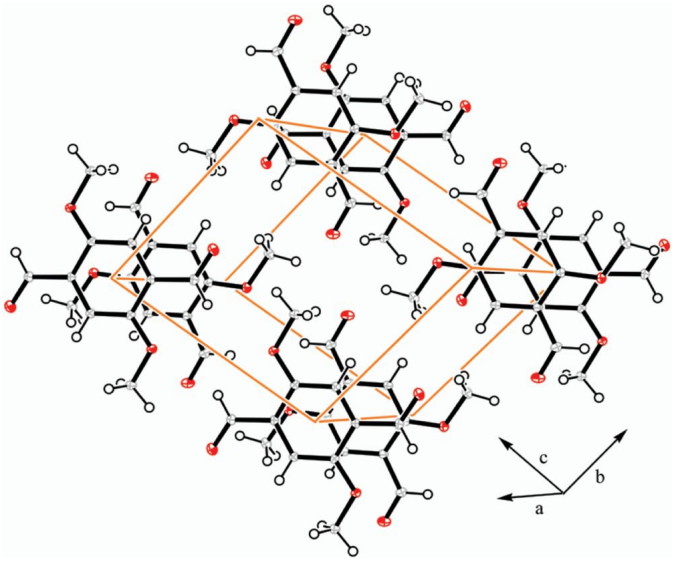


Figure 2
A view of the crystal packing in (I).

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

$C_{10}H_{10}O_4$
M_r = 194.18
Triclinic, $P\overline{1}$
a = 7.1330 (6) Å
b = 8.0050 (9) Å
c = 8.4520 (11) Å
α = 99.571 (9)°
β = 112.751 (6)°
γ = 93.146 (8)°
V = 435.08 (9) Å^3
Z = 2
D_x = 1.482 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7928 reflections
θ = 2.6–38.0°
μ = 0.12 mm^{-1}
T = 122 (1) K
Prism, yellow
0.47 × 0.31 × 0.08 mm

Data collection

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

Refinement

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

Table 1
Selected bond lengths (Å).

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 (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11A···O4^{i}	0.98	2.57	3.5128 (11)	162
C11—H11B···O4^{ii}	0.98	2.63	3.5400 (12)	155
C9—H9A···O10^{iii}	0.98	2.66	3.5050 (11)	144
C9—H9B···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 = 0.95–0.98 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq(C)}$.

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*.

The authors thank Flemming Hansen for collecting the diffraction data and the Centre for Crystallographic Studies for the use of their equipment.

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Coppens, P. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall and C. P. Huber, pp. 255–270. Copenhagen: Munksgaard.
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
Kuhnert, N., Rossignolo, G. M. & Lopez-Periago, A. (2003). *Org. Biomol. Chem.* **7**, 1157–1170.
Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.