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(*E*)-4,4′-(But-2-ene-1,4-diyldioxy)bis(3-methoxybenzaldehyde)

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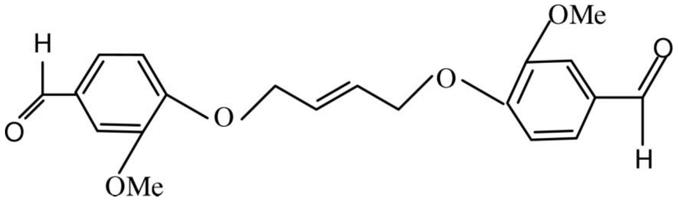
Key indicators: single-crystal X-ray study; *T* = 294 K; mean σ(C–C) = 0.004 Å; *R* factor = 0.054; *wR* factor = 0.139; data-to-parameter ratio = 11.2.

The molecule of the title compound, $C_{20}H_{20}O_6$, has a centre of symmetry located at the mid-point of the C=C double bond. The aldehyde C, oxy O, methoxy O and aldehyde O atoms lie in the benzene ring plane.

Related literature

For general backgroud, see: Allen *et al.* (1987); Du *et al.* (2002); Dugas & Penney, 1981; Easmon *et al.* (2001); Finch *et al.* (1999); Greenbaum *et al.* (2004); Jones *et al.* (1979); Sancak *et al.* (2007); Sengottuvelan *et al.* (2002); Vigato & Tamburini (2004); Wilson *et al.* (1974). For a related structure see: Ustabaş *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{20}O_6$
M_r = 356.36
Monoclinic, $P2_1/n$
a = 4.0639 (9) Å
b = 15.617 (3) Å
c = 13.735 (3) Å
β = 92.212 (4)°
V = 871.0 (3) Å^3
Z = 2
Mo *K*α radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
0.42 × 0.19 × 0.16 mm

Data collection

Bruker CCD area-detector diffractometer
Absorption correction: none
3568 measured reflections
1368 independent reflections
836 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.139
S = 1.04
1368 reflections
122 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max}$ = 0.16 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.359 (3)	O2—C8	1.408 (3)
O1—C9	1.438 (3)	O3—C7	1.210 (4)
O2—C2	1.366 (3)		
C3—C2—O2	124.9 (2)	O2—C2—C1	115.3 (2)
C3—C2—C1	119.8 (3)		

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2231).

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supplementary materials

Acta Cryst. (2007). E**63**, o2452 [**doi:10.1107/S1600536807018181**]

(*E*)-4,4'-(But-2-ene-1,4-diyldioxy)bis(3-methoxybenzaldehyde)

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Comment

Benzaldehyde and its derivatives are the major important compounds to obtain biologically active compounds. The aldehyde (thio)semicarbazones are a class of small molecules that have been evaluated over the last 50 years as antiviral, anticancer (Finch *et al.*, 1999) and antiparasitical (Greenbaum *et al.*, 2004; Wilson *et al.*, 1974; Du *et al.*, 2002; Easmon *et al.*, 2001). Benzaldehyde derivatives are important starting materials for obtaining Schiff bases and oxime-type ligands and their transition metal complexes (Vigato & Tamburini, 2004; Sancak *et al.*, 2007). These types of ligands display a wide variety of structures with different flexibility and electronic nature and the presence of additional donor atoms besides imino nitrogen. Further finetuning of their coordination characteristics can be achieved by varying the nature and positions of the substituents. Some Schiff bases and their complexes have been studied because of catalytic activities in hydrogenation of olefins (Jones *et al.*, 1979) and photochromic properties (Dugas & Pennev, 1981). Many reports have demonstrated the potential of Schiff base or oxime complexes in the construction of polynuclear aromatic compounds (Sengottuvelan *et al.*, 2002).

In the molecule of (I), (Fig. 1), the bond lengths and angles (Table 1) are generally within normal ranges (Allen *et al.*, 1987). It has a centre of symmetry located at the mid-point of the C═C double bond. The atoms C7, O1, O2 and O3 lie in the benzene ring plane, while atoms C8, C9 and C10 are 0.134 (3), 0.089 (2) and 0.142 (3) Å away, respectively. The O3═C7 bond [1.210 (4) Å] agrees with the corresponding value [1.200 (3) Å] in 2,2'-[2,3-bis(1-formyl-2-naphthyloxymethyl)-but-2-ene-1,4-diyldioxy]bis- (naphthalene-1-carbaldehyde) (Ustabaş *et al.*, 2006).

Experimental

For the preparation of the title compound, the corresponding 4-hydroxy-3-methoxy benzaldehyde (3.04 g, 10 mmol) was refluxed with potassium hydroxide (1.121 g, 10 mmol) in absolute ethanol (100 ml) for 1 h. Then, trans 1,4-dichloro2-butene (2.138 g, 40 mmol) was added and refluxed for an additional 26 h. The precipitate was filtered off, washed with water and recrystallized from chloroform/acetone (1:1) (yield; 2.145 g, 60%, m.p. 444-445 K).

Refinement

H10 was located in difference syntheses and refined isotropically [C—H = 0.90 (3) Å and U_{iso}(H) = 0.056 (9) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

Figures

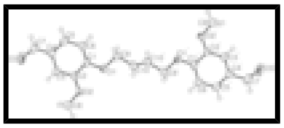


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Primed atoms are related to the unprimed atoms by the symmetry operator: 2 - x, 2 - y, 2 - z.

(*E*)-4,4'-(But-2-ene-1,4-diyldioxy)bis(3-methoxybenzaldehyde)

Crystal data

$C_{20}H_{20}O_6$

$M_r = 356.36$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 4.0639$ (9) Å

$b = 15.617$ (3) Å

$c = 13.735$ (3) Å

$\beta = 92.212$ (4)°

$V = 871.0$ (3) Å^3

$Z = 2$

$F_{000} = 376$

$D_x = 1.359$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 836 reflections

$\theta = 2.0$–25.0°

$\mu = 0.10$ mm^{-1}

$T = 294$ (2) K

Prism, colorless

0.42 × 0.19 × 0.16 mm

Data collection

Bruker CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 294(2)$ K

φ and ω scans

Absorption correction: none

3568 measured reflections

1368 independent reflections

836 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\text{max}} = 25.0$°

$\theta_{\text{min}} = 2.0$°

$h = -4\to4$

$k = -18\to13$

$l = -16\to13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.054$

$wR(F^2) = 0.139$

$S = 1.04$

1368 reflections

122 parameters

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0692P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.16$ e Å^{-3}

$\Delta\rho_{\text{min}} = -0.18$ e Å^{-3}

Extinction correction: none

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.2583 (5)	0.83308 (11)	0.95737 (14)	0.0456 (6)
O2	1.4321 (5)	0.69144 (11)	1.03941 (14)	0.0528 (6)
O3	1.9445 (7)	0.51354 (15)	0.76387 (18)	0.0788 (9)
C1	1.3981 (7)	0.77503 (15)	0.8979 (2)	0.0368 (7)
C2	1.4979 (7)	0.69800 (15)	0.9429 (2)	0.0382 (7)
C3	1.6459 (7)	0.63623 (16)	0.8898 (2)	0.0432 (8)
H3	1.7129	0.5853	0.9197	0.052*
C4	1.6976 (7)	0.64900 (16)	0.7908 (2)	0.0418 (8)
C5	1.6001 (8)	0.72447 (18)	0.7472 (2)	0.0490 (8)
H5	1.6336	0.7330	0.6813	0.059*
C6	1.4525 (7)	0.78787 (17)	0.8007 (2)	0.0447 (8)
H6	1.3901	0.8392	0.7710	0.054*
C7	1.8599 (8)	0.5833 (2)	0.7339 (3)	0.0585 (10)
H7	1.9016	0.5963	0.6695	0.070*
C8	1.5004 (10)	0.61245 (19)	1.0854 (3)	0.0714 (12)
H8A	1.4426	0.6156	1.1524	0.107*
H8B	1.7309	0.5998	1.0819	0.107*
H8C	1.3743	0.5681	1.0531	0.107*
C9	1.1295 (8)	0.91024 (15)	0.9134 (2)	0.0440 (8)
H9A	0.9700	0.8965	0.8614	0.053*
H9B	1.3059	0.9434	0.8862	0.053*
C10	0.9710 (7)	0.95961 (17)	0.9906 (2)	0.0401 (8)
H10	0.830 (7)	0.9284 (18)	1.025 (2)	0.056 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0663 (15)	0.0312 (11)	0.0405 (14)	0.0094 (9)	0.0170 (10)	0.0012 (9)

O2	0.0896 (16)	0.0399 (11)	0.0303 (13)	0.0138 (11)	0.0198 (11)	0.0025 (9)
O3	0.102 (2)	0.0513 (15)	0.085 (2)	0.0161 (14)	0.0317 (17)	−0.0153 (13)
C1	0.0444 (18)	0.0317 (15)	0.0352 (19)	−0.0031 (12)	0.0125 (14)	−0.0046 (12)
C2	0.0543 (19)	0.0326 (15)	0.0283 (18)	0.0017 (13)	0.0102 (14)	−0.0015 (12)
C3	0.059 (2)	0.0293 (15)	0.042 (2)	−0.0005 (13)	0.0147 (15)	−0.0020 (13)
C4	0.051 (2)	0.0380 (17)	0.0371 (19)	−0.0078 (13)	0.0144 (15)	−0.0104 (13)
C5	0.065 (2)	0.0490 (19)	0.0344 (19)	−0.0097 (15)	0.0164 (16)	−0.0047 (14)
C6	0.061 (2)	0.0362 (16)	0.0373 (19)	0.0002 (14)	0.0138 (15)	0.0028 (13)
C7	0.074 (2)	0.052 (2)	0.051 (2)	−0.0059 (18)	0.0274 (19)	−0.0176 (16)
C8	0.120 (3)	0.055 (2)	0.041 (2)	0.023 (2)	0.016 (2)	0.0109 (17)
C9	0.0533 (19)	0.0331 (15)	0.046 (2)	0.0032 (13)	0.0079 (15)	0.0017 (13)
C10	0.0435 (19)	0.0335 (14)	0.044 (2)	−0.0011 (14)	0.0118 (15)	0.0035 (14)

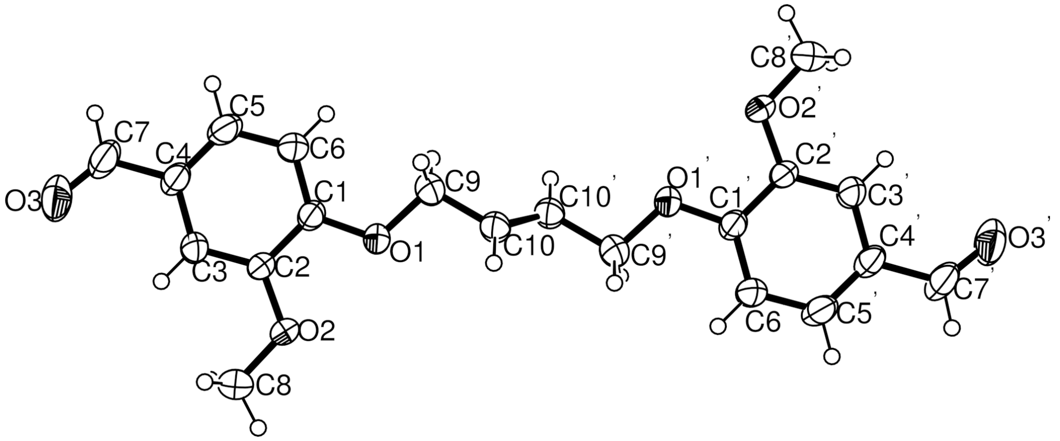
Geometric parameters (Å, °)

O1—C1	1.359 (3)	C5—H5	0.9300
O1—C9	1.438 (3)	C6—C5	1.383 (4)
O2—C2	1.366 (3)	C6—H6	0.9300
O2—C8	1.408 (3)	C7—H7	0.9300
O3—C7	1.210 (4)	C8—H8A	0.9600
C1—C6	1.376 (4)	C8—H8B	0.9600
C1—C2	1.405 (3)	C8—H8C	0.9600
C2—C3	1.363 (4)	C9—H9A	0.9700
C3—C4	1.398 (4)	C9—H9B	0.9700
C3—H3	0.9300	C10—C10^{i}	1.307 (5)
C4—C7	1.462 (4)	C10—C9	1.479 (4)
C5—C4	1.373 (4)	C10—H10	0.90 (3)
C1—O1—C9	117.4 (2)	C5—C6—H6	120.0
C2—O2—C8	117.3 (2)	O3—C7—C4	125.3 (3)
O1—C1—C6	124.9 (2)	O3—C7—H7	117.3
O1—C1—C2	115.3 (2)	C4—C7—H7	117.3
C6—C1—C2	119.8 (2)	O2—C8—H8A	109.5
C3—C2—O2	124.9 (2)	O2—C8—H8B	109.5
C3—C2—C1	119.8 (3)	H8A—C8—H8B	109.5
O2—C2—C1	115.3 (2)	O2—C8—H8C	109.5
C2—C3—C4	120.3 (3)	H8A—C8—H8C	109.5
C2—C3—H3	119.8	H8B—C8—H8C	109.5
C4—C3—H3	119.8	O1—C9—C10	107.3 (2)
C5—C4—C3	119.7 (3)	O1—C9—H9A	110.3
C5—C4—C7	119.8 (3)	C10—C9—H9A	110.3
C3—C4—C7	120.5 (3)	O1—C9—H9B	110.3
C4—C5—C6	120.4 (3)	C10—C9—H9B	110.3
C4—C5—H5	119.8	H9A—C9—H9B	108.5
C6—C5—H5	119.8	C10^{i}—C10—C9	124.4 (4)
C1—C6—C5	120.0 (3)	C10^{i}—C10—H10	122 (2)
C1—C6—H6	120.0	C9—C10—H10	113.5 (19)
C9—O1—C1—C6	6.3 (4)	O2—C2—C3—C4	179.1 (3)
C9—O1—C1—C2	−175.4 (2)	C1—C2—C3—C4	−0.3 (5)

C1—O1—C9—C10	176.0 (2)	C2—C3—C4—C5	0.4 (5)
C8—O2—C2—C3	−5.0 (4)	C2—C3—C4—C7	179.2 (3)
C8—O2—C2—C1	174.4 (3)	C5—C4—C7—O3	−177.1 (3)
O1—C1—C2—C3	−178.9 (3)	C3—C4—C7—O3	4.1 (5)
C6—C1—C2—C3	−0.5 (4)	C6—C5—C4—C3	0.2 (5)
O1—C1—C2—O2	1.7 (4)	C6—C5—C4—C7	−178.6 (3)
C6—C1—C2—O2	−179.9 (3)	C1—C6—C5—C4	−1.0 (5)
O1—C1—C6—C5	179.3 (3)	C10^{i}—C10—C9—O1	129.2 (4)
C2—C1—C6—C5	1.1 (4)		

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+2.

Fig. 1


C8'
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C6
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O2
C8