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4,4′-(Propane-1,3-diyldioxy)dibenzaldehyde

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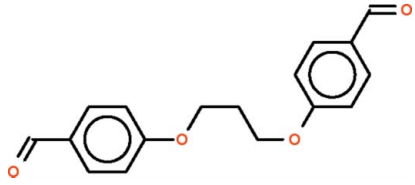
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.106; data-to-parameter ratio = 16.4.

The title compound, $C_{17}H_{16}O_4$, is a dialdehyde in which two formylphenoxy units are linked by a $-CH_2CH_2CH_2-$ chain; the molecule is V-shaped with the middle methylene C atom as the apex. The two benzene rings are aligned at 77.4 (1)°. In the crystal, molecules are linked into centrosymmetric dimers by pairs of non-classical C—H···O hydrogen bonds.

Related literature

For background to Schiff bases derived by condensing similar dialdehydes with primary amines, see: Zhang *et al.* (2008). For the crystal structure of the 2,2′-disubstituted analog, see: Hu *et al.* (2005).



Experimental

Crystal data

$C_{17}H_{16}O_4$ M_r = 284.30
Monoclinic, $P2_1/n$
a = 15.3323 (15) Å
b = 4.6173 (5) Å
c = 20.2800 (19) Å
β = 104.783 (1)°
V = 1388.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEXII diffractometer
8297 measured reflections
3113 independent reflections
2538 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.106
S = 1.03
3113 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O1^{i}	0.95	2.41	3.287 (2)	154

Symmetry code: (i) $-x+1, -y+2, -z+1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5094).

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supplementary materials

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4,4'-(Propane-1,3-diyldioxy)dibenzaldehyde

Q. Ali, M. Raza Shah and S. W. Ng

Comment

The two-arm aldehyde is intended for condensation with primary amines to form Schiff bases, which, in a subsequent step, will be reacted with *β*-cyclodextrin to furnish inclusion compounds. The idea for this theme draws on a report on such compounds of poly(Schiff bases) (Zhang *et al.*, 2008). The flexibilty of the Schiff base can be controlled by varying the position of the formyl group; the title compound has the the formyl groups in the 4,4'-positions. The crystal structure of the 2,2'-substituted compound has been reported (Hu *et al.*, 2005). The molecule of $C_{17}H_{16}O_4$ (Scheme I) is V-shaped with the middle methylene carbon as the apex (Fig. 1).

Experimental

4-Hydroxybenzaldehyde (1 g, 8.2 mmol) was dissolved in acetone (25 ml). To the solution was added potassium carbonate (2.3 g, 16.4 mmol). The mixture was heated for 1 h. 1,3-Dibromopropane (0.29 ml, 2.7 mmol) was added and the mixture heated for another hour. The mixture was set aside for 8 h. The solvent was removed and the solid material was extracted with ethyl acetate. The solvent was again removed and the product purified by column chromatography by using dichloro-methane-hexane (1:4) as mobile phase. Single crystals were obtained by recrystallization from dichloromethane.

Refinement

H atoms were placed in calculated positions [C–H = 0.95–0.99 Å] and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

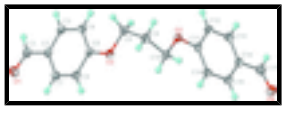


Fig. 1. Displacement ellipsoid plot (Barbour, 2001) of $C_{17}H_{16}O_4$ at the 70% probability level; H atoms are drawn as spheres of arbitrary radius.

4,4'-(Propane-1,3-diyldioxy)dibenzaldehyde

Crystal data

$C_{17}H_{16}O_4$	F(000) = 600
M_r = 284.30	D_x = 1.360 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2677 reflections
a = 15.3323 (15) Å	θ = 3.1–28.0°
b = 4.6173 (5) Å	μ = 0.10 mm^{-1}

c = 20.2800 (19) Å	T = 100 K
β = 104.783 (1)°	Plate, colourless
V = 1388.2 (2) Å^3	0.25 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART APEXII diffractometer	2538 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.027
graphite	θ_{max} = 27.5°, θ_{min} = 1.5°
ω scans	h = −19→19
8297 measured reflections	k = −5→5
3113 independent reflections	l = −19→26

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.039	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.106	H-atom parameters constrained
S = 1.02	$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 0.4617P]$ where $P = (F_o^2 + 2F_c^2)/3$
3113 reflections	$(\Delta/\sigma)_{max}$ = 0.001
190 parameters	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.33791 (6)	1.4272 (2)	0.27971 (5)	0.0247 (2)
O2	0.37445 (6)	0.5332 (2)	0.52487 (5)	0.0191 (2)
O3	0.36450 (6)	0.5695 (2)	0.70403 (5)	0.0191 (2)
O4	0.58320 (6)	1.2514 (2)	0.97043 (5)	0.0290 (3)
C1	0.28543 (9)	1.3387 (3)	0.31097 (7)	0.0193 (3)
H1	0.2260	1.4154	0.2992	0.023*
C2	0.30737 (8)	1.1217 (3)	0.36563 (7)	0.0171 (3)
C3	0.24107 (8)	1.0286 (3)	0.39613 (7)	0.0183 (3)
H3	0.1816	1.1028	0.3805	0.022*
C4	0.25983 (8)	0.8289 (3)	0.44913 (7)	0.0182 (3)
H4	0.2137	0.7657	0.4694	0.022*
C5	0.34744 (8)	0.7227 (3)	0.47213 (6)	0.0166 (3)
C6	0.41484 (8)	0.8113 (3)	0.44128 (7)	0.0188 (3)
H6	0.4742	0.7361	0.4566	0.023*
C7	0.39463 (9)	1.0082 (3)	0.38860 (7)	0.0192 (3)
H7	0.4404	1.0678	0.3676	0.023*

C8	0.30783 (8)	0.4333 (3)	0.55834 (7)	0.0182 (3)
H8A	0.2590	0.3283	0.5257	0.022*
H8B	0.2810	0.5991	0.5771	0.022*
C9	0.35588 (9)	0.2331 (3)	0.61526 (7)	0.0190 (3)
H9A	0.3901	0.0869	0.5964	0.023*
H9B	0.3103	0.1290	0.6331	0.023*
C10	0.42019 (8)	0.3892 (3)	0.67370 (7)	0.0176 (3)
H10A	0.4544	0.2486	0.7074	0.021*
H10B	0.4635	0.5084	0.6567	0.021*
C11	0.40426 (8)	0.7236 (3)	0.76107 (6)	0.0164 (3)
C12	0.34516 (8)	0.8830 (3)	0.78886 (7)	0.0189 (3)
H12	0.2821	0.8762	0.7685	0.023*
C13	0.37858 (9)	1.0507 (3)	0.84602 (7)	0.0202 (3)
H13	0.3383	1.1611	0.8647	0.024*
C14	0.47139 (8)	1.0595 (3)	0.87679 (7)	0.0187 (3)
C15	0.52930 (8)	0.8986 (3)	0.84844 (7)	0.0189 (3)
H15	0.5923	0.9038	0.8691	0.023*
C16	0.49718 (8)	0.7308 (3)	0.79069 (7)	0.0174 (3)
H16	0.5375	0.6227	0.7716	0.021*
C17	0.50495 (9)	1.2379 (3)	0.93787 (7)	0.0235 (3)
H17	0.4622	1.3516	0.9531	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0269 (5)	0.0271 (5)	0.0213 (5)	0.0011 (4)	0.0081 (4)	0.0041 (4)
O2	0.0179 (4)	0.0231 (5)	0.0158 (5)	0.0023 (4)	0.0036 (4)	0.0036 (4)
O3	0.0165 (4)	0.0234 (5)	0.0163 (5)	0.0004 (4)	0.0020 (3)	−0.0030 (4)
O4	0.0248 (5)	0.0375 (6)	0.0228 (6)	−0.0053 (4)	0.0027 (4)	−0.0083 (5)
C1	0.0220 (6)	0.0177 (6)	0.0168 (7)	0.0004 (5)	0.0027 (5)	−0.0033 (5)
C2	0.0200 (6)	0.0162 (6)	0.0139 (6)	−0.0002 (5)	0.0020 (5)	−0.0036 (5)
C3	0.0168 (6)	0.0190 (6)	0.0169 (7)	0.0015 (5)	0.0006 (5)	−0.0027 (5)
C4	0.0171 (6)	0.0207 (6)	0.0165 (7)	−0.0013 (5)	0.0039 (5)	−0.0019 (5)
C5	0.0197 (6)	0.0166 (6)	0.0118 (6)	0.0005 (5)	0.0010 (5)	−0.0027 (5)
C6	0.0166 (6)	0.0212 (7)	0.0177 (7)	0.0022 (5)	0.0026 (5)	−0.0018 (5)
C7	0.0189 (6)	0.0211 (7)	0.0180 (7)	−0.0012 (5)	0.0055 (5)	−0.0017 (5)
C8	0.0187 (6)	0.0199 (7)	0.0158 (7)	−0.0021 (5)	0.0039 (5)	−0.0018 (5)
C9	0.0208 (6)	0.0174 (6)	0.0181 (7)	−0.0019 (5)	0.0035 (5)	−0.0009 (5)
C10	0.0184 (6)	0.0182 (6)	0.0160 (7)	0.0010 (5)	0.0038 (5)	−0.0005 (5)
C11	0.0191 (6)	0.0155 (6)	0.0135 (6)	−0.0013 (5)	0.0022 (5)	0.0025 (5)
C12	0.0154 (6)	0.0218 (7)	0.0192 (7)	−0.0006 (5)	0.0037 (5)	0.0012 (5)
C13	0.0194 (6)	0.0205 (7)	0.0221 (7)	0.0011 (5)	0.0077 (5)	−0.0014 (6)
C14	0.0205 (6)	0.0190 (6)	0.0163 (7)	−0.0018 (5)	0.0037 (5)	0.0006 (5)
C15	0.0160 (6)	0.0204 (7)	0.0186 (7)	−0.0006 (5)	0.0015 (5)	0.0027 (5)
C16	0.0165 (6)	0.0190 (6)	0.0173 (7)	0.0016 (5)	0.0053 (5)	0.0009 (5)
C17	0.0242 (7)	0.0258 (7)	0.0214 (7)	−0.0022 (6)	0.0073 (5)	−0.0026 (6)

Geometric parameters (Å, °)

O1—C1	1.2152 (16)	C8—H8A	0.99
O2—C5	1.3620 (15)	C8—H8B	0.99
O2—C8	1.4389 (15)	C9—C10	1.5167 (17)
O3—C11	1.3623 (15)	C9—H9A	0.99
O3—C10	1.4382 (15)	C9—H9B	0.99
O4—C17	1.2145 (17)	C10—H10A	0.99
C1—C2	1.4682 (19)	C10—H10B	0.99
C1—H1	0.95	C11—C12	1.3931 (18)
C2—C3	1.3863 (18)	C11—C16	1.3981 (17)
C2—C7	1.4014 (18)	C12—C13	1.3796 (19)
C3—C4	1.3894 (19)	C12—H12	0.95
C3—H3	0.95	C13—C14	1.4009 (17)
C4—C5	1.3938 (18)	C13—H13	0.95
C4—H4	0.95	C14—C15	1.3895 (19)
C5—C6	1.3989 (18)	C14—C17	1.4674 (19)
C6—C7	1.3765 (19)	C15—C16	1.3859 (18)
C6—H6	0.95	C15—H15	0.95
C7—H7	0.95	C16—H16	0.95
C8—C9	1.5153 (18)	C17—H17	0.95
C5—O2—C8	117.78 (10)	C10—C9—H9A	108.9
C11—O3—C10	118.66 (9)	C8—C9—H9B	108.9
O1—C1—C2	124.65 (12)	C10—C9—H9B	108.9
O1—C1—H1	117.7	H9A—C9—H9B	107.7
C2—C1—H1	117.7	O3—C10—C9	105.71 (10)
C3—C2—C7	118.83 (12)	O3—C10—H10A	110.6
C3—C2—C1	119.72 (11)	C9—C10—H10A	110.6
C7—C2—C1	121.44 (12)	O3—C10—H10B	110.6
C2—C3—C4	121.36 (12)	C9—C10—H10B	110.6
C2—C3—H3	119.3	H10A—C10—H10B	108.7
C4—C3—H3	119.3	O3—C11—C12	115.02 (11)
C3—C4—C5	118.95 (12)	O3—C11—C16	124.28 (11)
C3—C4—H4	120.5	C12—C11—C16	120.69 (12)
C5—C4—H4	120.5	C13—C12—C11	119.74 (11)
O2—C5—C4	124.25 (12)	C13—C12—H12	120.1
O2—C5—C6	115.34 (11)	C11—C12—H12	120.1
C4—C5—C6	120.40 (12)	C12—C13—C14	120.51 (12)
C7—C6—C5	119.66 (12)	C12—C13—H13	119.7
C7—C6—H6	120.2	C14—C13—H13	119.7
C5—C6—H6	120.2	C15—C14—C13	118.95 (12)
C6—C7—C2	120.77 (12)	C15—C14—C17	121.73 (12)
C6—C7—H7	119.6	C13—C14—C17	119.32 (12)
C2—C7—H7	119.6	C16—C15—C14	121.44 (12)
O2—C8—C9	106.81 (10)	C16—C15—H15	119.3
O2—C8—H8A	110.4	C14—C15—H15	119.3
C9—C8—H8A	110.4	C15—C16—C11	118.67 (12)
O2—C8—H8B	110.4	C15—C16—H16	120.7

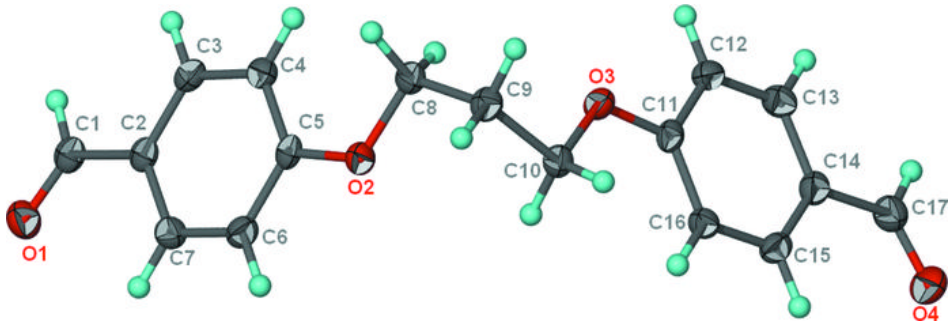
C9—C8—H8B	110.4	C11—C16—H16	120.7
H8A—C8—H8B	108.6	O4—C17—C14	124.94 (13)
C8—C9—C10	113.45 (11)	O4—C17—H17	117.5
C8—C9—H9A	108.9	C14—C17—H17	117.5
O1—C1—C2—C3	−177.57 (13)	C11—O3—C10—C9	176.03 (10)
O1—C1—C2—C7	3.3 (2)	C8—C9—C10—O3	65.84 (13)
C7—C2—C3—C4	0.75 (19)	C10—O3—C11—C12	−177.41 (11)
C1—C2—C3—C4	−178.41 (12)	C10—O3—C11—C16	3.47 (18)
C2—C3—C4—C5	0.48 (19)	O3—C11—C12—C13	−178.89 (12)
C8—O2—C5—C4	0.89 (18)	C16—C11—C12—C13	0.26 (19)
C8—O2—C5—C6	−179.69 (11)	C11—C12—C13—C14	−0.7 (2)
C3—C4—C5—O2	178.02 (12)	C12—C13—C14—C15	0.6 (2)
C3—C4—C5—C6	−1.37 (19)	C12—C13—C14—C17	−179.52 (13)
O2—C5—C6—C7	−178.41 (11)	C13—C14—C15—C16	0.0 (2)
C4—C5—C6—C7	1.0 (2)	C17—C14—C15—C16	−179.92 (12)
C5—C6—C7—C2	0.2 (2)	C14—C15—C16—C11	−0.42 (19)
C3—C2—C7—C6	−1.1 (2)	O3—C11—C16—C15	179.37 (12)
C1—C2—C7—C6	178.04 (12)	C12—C11—C16—C15	0.29 (19)
C5—O2—C8—C9	−178.76 (10)	C15—C14—C17—O4	−3.7 (2)
O2—C8—C9—C10	70.22 (13)	C13—C14—C17—O4	176.44 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O2^{i}	0.95	2.57	3.508 (2)	168
C16—H16···O1^{ii}	0.95	2.41	3.287 (2)	154

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+2, −*z*+1.

Fig. 1


C3
C4
C1
C2
C5
C8
C9
O3
C12
C13
C11
C14
C10
O2
C16
C17
C6
C7
C15
O1
O4