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4,4′-Oxydibenzaldehyde

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.041
wR factor = 0.074
Data-to-parameter ratio = 12.3

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

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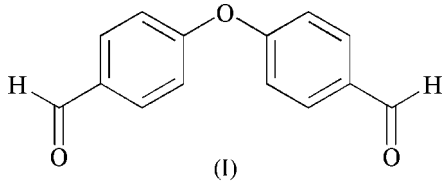
The two aromatic rings in the title compound, $C_{14}H_{10}O_3$, are approximately perpendicular to each other. One of the aldehyde groups in the title molecule is disordered over two sites with occupancies 0.80 (2) and 0.20 (2).

Comment

An X-ray single crystal structure determination of the title compound, (I), was carried out to elucidate the structure and the results are presented here. The compound was obtained as an intermediate in a synthesis.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The two aromatic rings are approximately orthogonal, forming a dihedral angle of 98.4 (2)°. The C4—C5—O2—C8 torsion angle is 177.9 (2)°, indicating that these atoms are almost coplanar. The O2—C8 bond is significantly longer than the O2—C5 bond (Table 1). The aldehyde group attached to atom C11 is disordered over two sites [occupancies 0.80 (2) and 0.20 (2)].

In the crystal structure of (I), there are no classical hydrogen bonds. The structure is stabilized by weak intermolecular C—H···O hydrogen interactions [C6—H6···O3^{i}; H6···O3^{i} = 2.45 Å, C6···O3^{i} = 3.327 (3) Å and C6—H6···O3^{i} = 158°; symmetry code: (i) −*x*, 1 − *y*, 1 − *z*].

Experimental

The title compound (I) was synthesized according to known procedures (Guilani *et al.*, 1990). Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

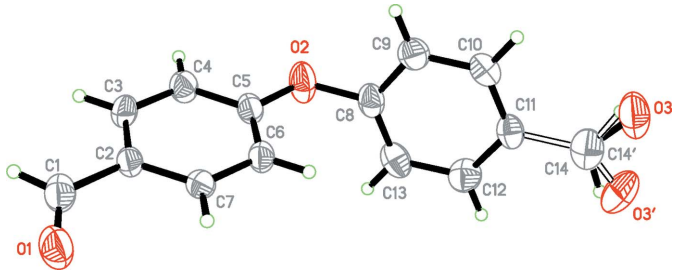


Figure 1
View of the molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. Both disorder components are shown.

Crystal data

$C_{14}H_{10}O_3$
M_r = 226.22
Monoclinic, $P2_1/n$
a = 12.662 (4) Å
b = 7.181 (2) Å
c = 12.951 (4) Å
β = 103.090 (7)°
V = 1147.0 (7) Å^3
Z = 4
D_x = 1.310 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, colourless
0.22 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.980, T_{max} = 0.991
5713 measured reflections
2020 independent reflections
1059 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.074
S = 1.14
2020 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0159P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.056 (2)

Table 1
Selected geometric parameters (Å, °).

O2—C5	1.372 (2)	O2—C8	1.400 (2)
C5—O2—C8	118.52 (15)	C9—C8—O2	118.3 (2)
O2—C5—C6	123.14 (17)		
C8—O2—C5—C4	177.9 (2)		

H atoms attached to atom C1 and to the aromatic rings were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The H atoms of the disordered aldehyde group were refined with C14—H14*A* = 0.96 Å, C14—H14*B* = 1.02 Å and U_{iso}(H) = 1.2U_{eq}(C). The aldehyde group attached to atom C11 is disordered over two sites [occupancies 0.80 (2) and 0.20 (2)].

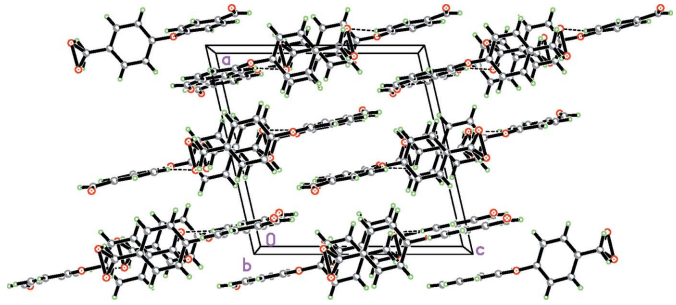


Figure 2
The packing of (I), viewed down the *b* axis, showing the intermolecular hydrogen-bonding (dashed lines).

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

References

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