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Methyl phenyl terephthalate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.117
Data-to-parameter ratio = 14.5

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

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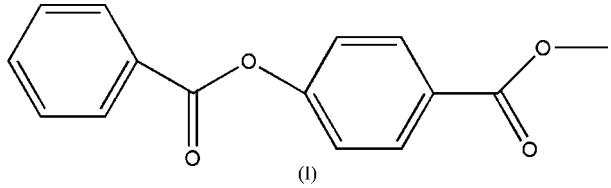
The title compound, $C_{15}H_{12}O_4$, was synthesized in an anhydrous medium. The aromatic rings make a dihedral angle of 37.43 (5)°. Weak intermolecular C—H···O hydrogen bonds involving one of the carbonyl O atoms stabilize the crystal packing.

Comment

Organic electroluminescence – the emission of light by organic molecules exposed to an electric field – has been extensively investigated in academic and industrial laboratories (Cui & Kim, 2004). The title compound, (I) (Fig. 1), prepared by our group, belongs to the family of organic electroluminescent materials. We report here its X-ray crystal structure.



(I)

The bond lengths and angles in (I) (Table 1) show normal values. The two aromatic rings make a dihedral angle of 37.43 (5)°. Weak intermolecular C—H···O hydrogen bonds (Table 2) stabilize the crystal packing (Fig. 2).

Experimental

The title compound was prepared according to a known procedure (Li *et al.*, 2000), which resulted in a colourless powder (m.p. 405–406 K). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane solution.

Crystal data

$C_{15}H_{12}O_4$
M_r = 256.25
Monoclinic, $P2_1/c$
a = 6.1654 (13) Å
b = 29.374 (6) Å
c = 7.2827 (16) Å
β = 111.188 (4)°
V = 1229.8 (5) Å^3
Z = 4
D_x = 1.384 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2124 reflections
θ = 2.8–25.8°
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, colourless
0.30 × 0.28 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.967, T_{max} = 0.980
6896 measured reflections
2526 independent reflections
1623 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 26.5°
$h = -3 \rightarrow 7$
$k = -36 \rightarrow 36$
$l = -9 \rightarrow 9$

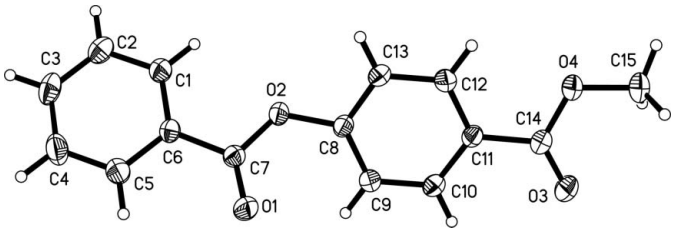


Figure 1
View of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 35% probability level.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.2662P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.043$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.117$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.19$ e Å^{-3}
2526 reflections	Extinction correction: *SHELXL97*
174 parameters	Extinction coefficient: 0.018 (2)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.194 (2)	O2—C8	1.401 (2)
O2—C7	1.352 (2)	C6—C7	1.478 (2)
C5—C6—C7	118.13 (16)	C9—C8—O2	123.42 (16)
O1—C7—C6	125.13 (16)		
C8—O2—C7—C6	177.84 (15)	C5—C6—C7—O2	174.25 (15)
C5—C6—C7—O1	−6.9 (3)	O2—C8—C9—C10	173.84 (16)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O1^{i}	0.93	2.46	3.362 (2)	164
C15—H15A···O1^{ii}	0.96	2.57	3.443 (2)	152

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

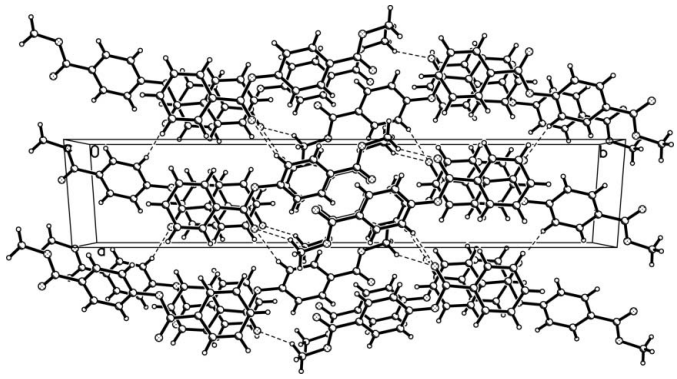


Figure 2
A packing diagram for (I). The dashed lines denote intermolecular C—H···O hydrogen bonds.

All H atoms were positioned geometrically and refined as riding (C—H = 0.93 or 0.96 Å). For CH groups, U_{iso}(H) values were set equal to $1.2U_{eq}$(C) and for the methyl groups they were set equal to $1.5U_{eq}$(C).

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: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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