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2,5-Dibenzoylterephthalic acid acetic acid disolvate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.057
wR factor = 0.169
Data-to-parameter ratio = 14.6

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

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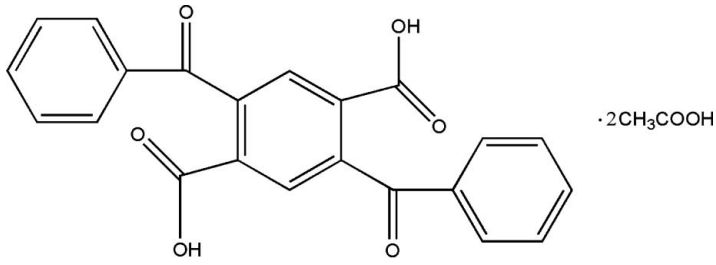
The asymmetric unit of the title compound, $C_{22}H_{14}O_6\cdot 2C_2H_4O_2$, contains one half-molecule of 2,5-dibenzoylterephthalic acid (DBTA) and one acetic acid molecule. The DBTA molecule is centrosymmetric. The acetic acid molecules are linked to DBTA by strong O—H···O hydrogen bonds, which may be effective in the stabilization of the crystal structure.

Comment

2,5-Dibenzoylterephthalic acid (DBTA), and its isomer 4,6-dibenzoylisophthalic acid (DBIA), can be utilized to synthesize organic semiconductors and conjugated polymers (Tonzola *et al.*, 2003), which are of wide current interest for applications in electronic and optoelectronic devices, including light-emitting diodes (Kolosov *et al.*, 2002), thin film transistors and photovoltaic cells (Antoniadis *et al.*, 1994). We report here the crystal structure of the title compound, (I).



(I)

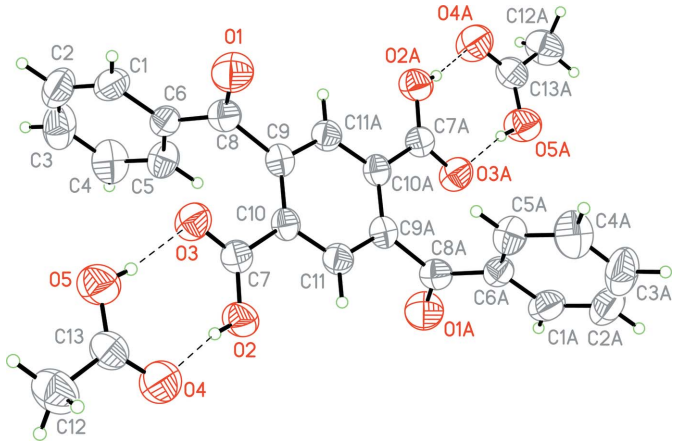


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. [Symmetry code: (A) $-x$, $1-y$, $1-z$.]

In the molecules of compound (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The asymmetric unit contains one half-molecule of DBTA and one acetic acid molecule. The DBTA molecule is centrosymmetric.

Rings *A* (C1–C6) and *B* (C9–C11/C9*A*–C11*A*) [symmetry code: (A) $-x, 1-y, 1-z$] are, of course, planar. The dihedral angle between them is 85.1 (1)°.

As can be seen from the packing diagram (Fig. 2), the acetic acid molecules are linked to DBTA by strong O—H···O hydrogen bonds (Table 1), which may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

Experimental

DBTA was prepared by the literature method of Liu *et al.* (2006). Single crystals were obtained by dissolving DBTA (1.5 g) in boiling acetic acid (100 ml) and then allowing the solvent to evaporate slowly at room temperature for about 7 d.

Crystal data

$C_{22}H_{14}O_6\cdot 2C_2H_4O_2$
M_r = 494.44
Triclinic, $P\overline{1}$
a = 5.6380 (11) Å
b = 9.889 (2) Å
c = 11.387 (2) Å
α = 79.60 (3)°
β = 78.92 (3)°
γ = 83.76 (3)°
V = 611.0 (2) Å^3
Z = 1
D_x = 1.344 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
Block, colourless
0.40 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.959, T_{max} = 0.979
2388 measured reflections
2388 independent reflections
1453 reflections with $I > 2\sigma(I)$
θ_{max} = 26.0°
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.169
S = 0.98
2388 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.09P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*B*···O4	0.82	1.82	2.633 (3)	170
O5—H5*B*···O3	0.82	1.86	2.677 (3)	171

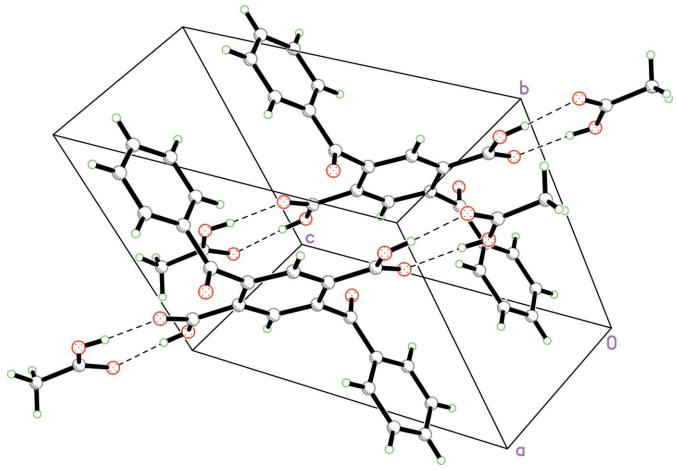


Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

H atoms were positioned geometrically, with O—H = 0.82 Å and C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and were constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,O), where x = 1.2 for aromatic H and x = 1.5 for all other H atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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