Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,5-Dibenzoylterephthalic acid *N*,*N*-dimethylformamide disolvate

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Received 15 December 2006
Accepted 20 December 2006

The asymmetric unit of the title compound, $C_{22}H_{14}O_6\cdot 2C_3H_7NO$, contains one half-molecule of 2,5-dibenzoylterephthalic acid (DBTA) and one *N*,*N*-dimethylformamide (DMF) molecule. The DBTA molecule is centrosymmetric. The DMF molecules are linked to DBTA by strong O—H···O hydrogen bonds.

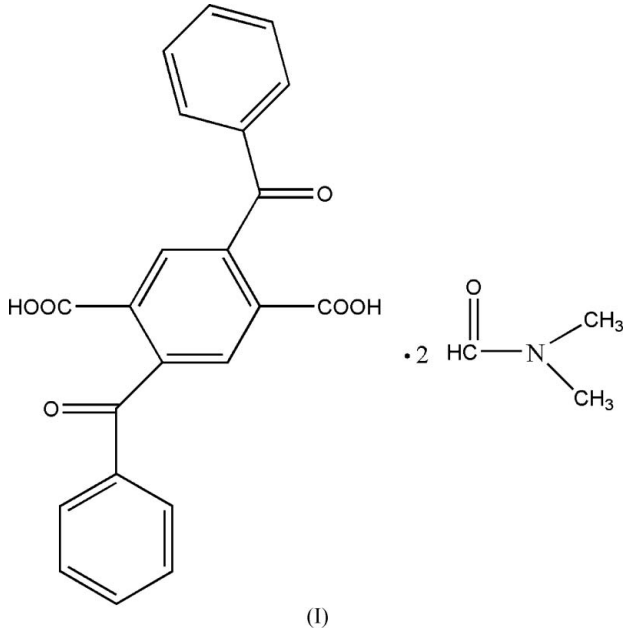
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.131
Data-to-parameter ratio = 15.0

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

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)

The asymmetric unit of (I) contains one half-molecule of DBTA with the other half generated by a centre of inversion, and one *N*,*N*-dimethylformamide (DMF) molecule (Fig. 1). The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angle between rings *A* (C1–C6) and *B* (C8–C10/C8*A*–C10*A*) [symmetry code: (*A*) 1 − *x*, 1 − *y*, 1 − *z*] is 72.30 (9)°.

The DMF molecules are linked to DBTA by strong O—H···O hydrogen bonds (Fig. 2 and Table 1), which may be effective in stabilizing the crystal structure.

Experimental

DBTA was prepared by a method we reported recently (Liu *et al.*, 2006). Single crystals were obtained by dissolving DBTA (1.0 g, 2.67 mmol) in DMF (40 ml) and then allowing the solvent to evaporate slowly at room temperature for about 15 d.

Crystal data

$C_{22}H_{14}O_6\cdot 2C_3H_7NO$
$M_r = 520.52$
Triclinic, $P\overline{1}$
$a = 6.0430\ (12)$ Å
$b = 8.5950\ (17)$ Å
$c = 13.211\ (3)$ Å
$\alpha = 95.57\ (3)^\circ$
$\beta = 101.64\ (3)^\circ$
$\gamma = 93.47\ (3)^\circ$
$V = 666.6\ (3)$ Å^3
$Z = 1$
$D_x = 1.297$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ 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)
$T_{min} = 0.963$, $T_{max} = 0.981$
2895 measured reflections
2633 independent reflections
2039 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 26.0^\circ$
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.131$
$S = 1.03$
2633 reflections
175 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.1552P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.189 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3*A*···O4	0.82	1.73	2.531 (2)	166
C13—H13*A*···O4	0.96	2.35	2.734 (3)	103

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 atoms, 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*.

The authors thank the Center for Testing and Analysis, Nanjing University, for support.

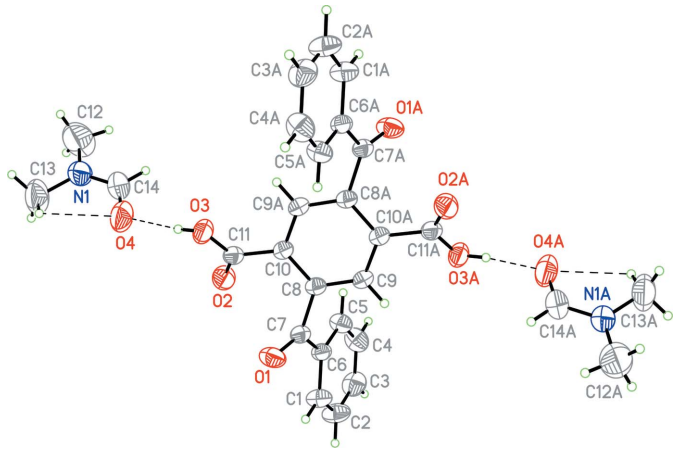


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. Atoms labelled with the suffix A are generated by the symmetry operation $(1 - x, 1 - y, 1 - z)$.

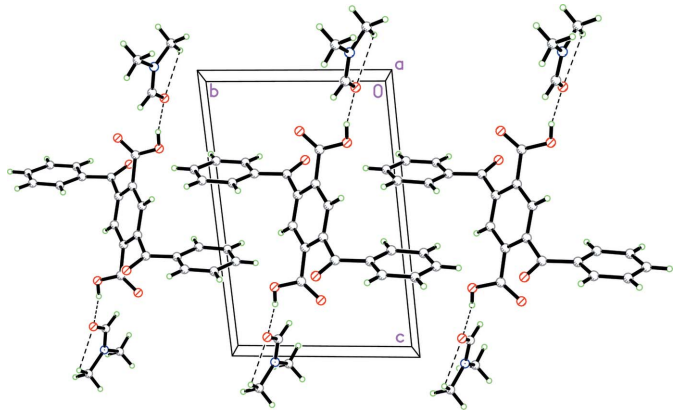


Figure 2
A packing diagram for (I). Dashed lines indicate hydrogen bonds.

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