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2,5-Bis(2,4-diethylbenzoyl)terephthalic acid pyridine disolvate

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The asymmetric unit of the title compound, $C_{30}H_{30}O_6 \cdot 2C_5H_5N$, contains one half-molecule of 2,5-bis(2,4-diethylbenzoyl)terephthalic acid (BDTA) and one pyridine molecule; the BDTA molecule is centrosymmetric and linked to the pyridine molecule by a strong intermolecular O—H···N hydrogen bond. O—H···N and C—H···O hydrogen bonds may be effective in the stabilization of the crystal structure.

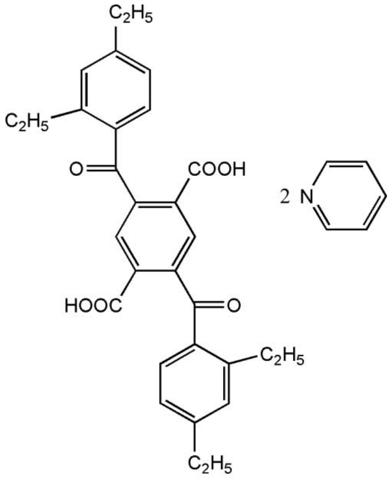
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.008 Å
R factor = 0.098
wR factor = 0.222
Data-to-parameter ratio = 16.2

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

Comment

2,5-Bis(2,4-diethylbenzoyl)terephthalic acid (BDTA) is a new compound synthesized by the literature method (Liu, Ji *et al.*, 2006). It may be viewed as a derivative of 2,5-dibenzoylterephthalic acid (DBTA), which is one of the intermediates that can be used for the syntheses of organic semiconductors and conjugated polymers (Tonzola *et al.*, 2003). We report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The asymmetric unit contains one half-molecule of BDTA and one pyridine molecule; the BDTA molecule is centrosymmetric and linked to the pyridine molecule by a strong intermolecular O—H···N hydrogen bond (Table 1).

Rings *A* (C5–C10), *B* (C12–C14/C12A–C14A) and *C* (N1/C16–C20) are, of course, planar; the dihedral angles between them are *A*/*B* = 99.9 (1)°, *B*/*C* = 125.6 (2)° and *A*/*C* = 85.3 (1)°. The O1—C11—C10—C9 [−157.9 (6)°] torsion angle is much smaller than the corresponding one [176.7 (1)°] in DBTA pyridine tetrasolvate (Liu, Heng *et al.*, 2006), probably because of the intramolecular C—H···O hydrogen bond (Table 1).

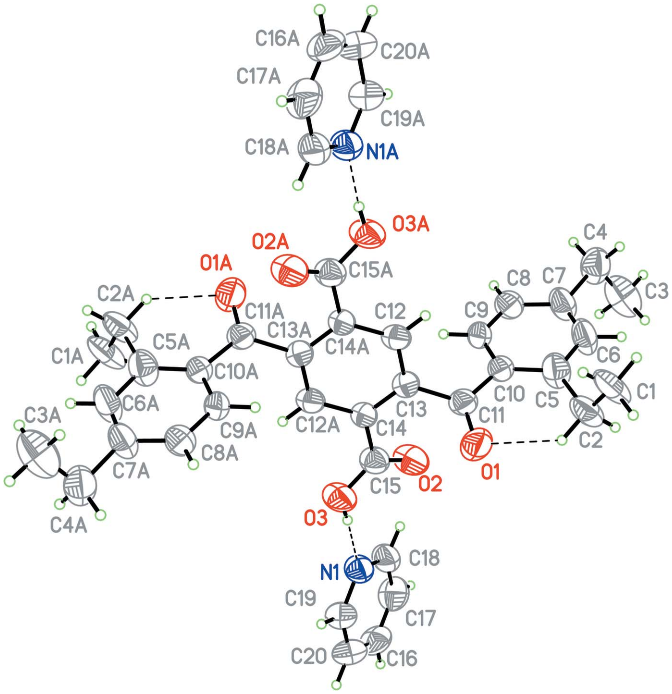


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. Hydrogen bonds are shown as dashed lines. [Symmetry code: (A) $1 - x$, $1 - y$, $-z$].

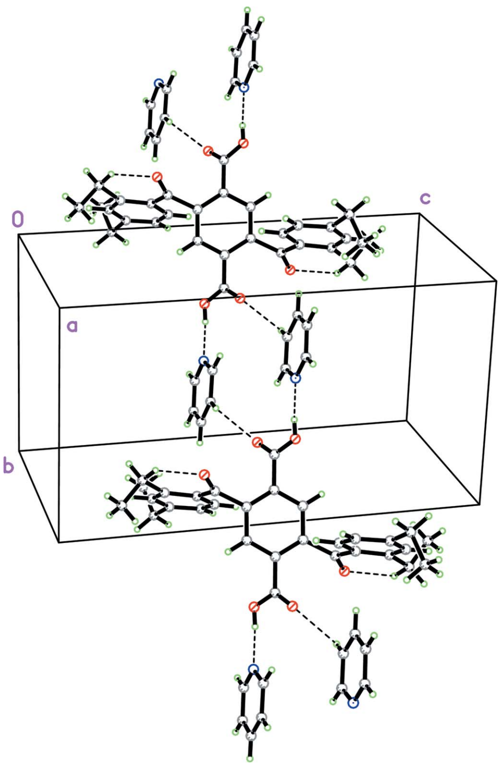


Figure 2
A partial packing diagram of (I). Hydrogen bonds are shown as dashed lines.

As can be seen from the packing diagram (Fig. 2), the pyridine molecules are also linked to BDTA by weak intermolecular C—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

BDTA was prepared by the literature method (Liu, Ji *et al.*, 2006). The crystals were obtained by dissolving BDTA (0.5 g) in pyridine (50 ml) and then allowing the solvent to evaporate slowly at room temperature for about 5 d.

Crystal data

$C_{30}H_{30}O_6 \cdot 2C_5H_5N$
$M_r = 644.74$
Monoclinic, $P2_1/n$
$a = 9.7260\ (19)$ Å
$b = 10.071\ (2)$ Å
$c = 18.285\ (4)$ Å
$\beta = 91.15\ (3)°$
$V = 1790.7\ (6)$ Å^3
$Z = 2$
$D_x = 1.196$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 294\ (2)$ K
Block, colorless
0.40 × 0.30 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.960$, $T_{max} = 0.987$
3521 measured reflections
3508 independent reflections
1619 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 26.0°$
3 standard reflections every 200 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.099$
$wR(F^2) = 0.222$
$S = 0.83$
3508 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + 9P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3D···N1^{i}	0.82	1.78	2.598 (6)	175
C2—H2B···O1	0.97	2.10	2.850 (9)	132
C17—H17A···O2^{ii}	0.93	2.51	3.271 (10)	139

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

H atoms were positioned geometrically, with O—H = 0.82 Å (for OH) and C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,O)$, where $x = 1.5$ for OH, methylene (for C2) and methyl H, and $x = 1.2$ 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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