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# 2,5-Dibenzoylterephthalic acid pyridine tetrasolvate

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**Key indicators**

Single-crystal X-ray study
*T* = 294 K
Mean σ(C–C) = 0.007 Å
*R* factor = 0.076
*wR* factor = 0.188
Data-to-parameter ratio = 14.7

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



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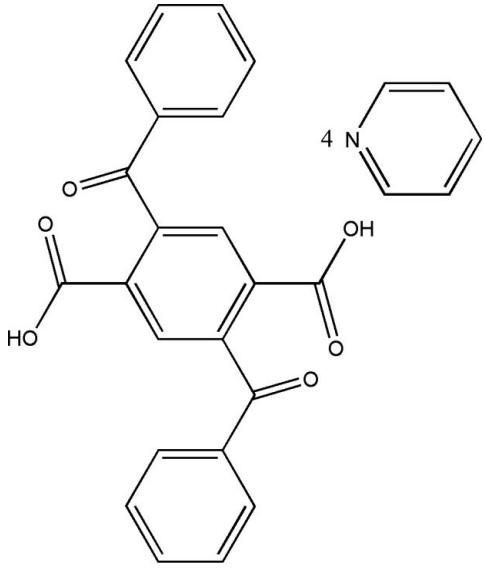
The asymmetric unit of the title compound, $C_{22}H_{14}O_6\cdot 4C_5H_5N$, contains one half-molecule of 2,5-dibenzoylterephthalic acid (DBTA) and two pyridine molecules; the DBTA molecule is centrosymmetric. The pyridine molecules are linked to DBTA by strong O—H···N and C—H···O hydrogen bonds, which 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), which is of interest to us in this field.




(I)

In the molecular structure of (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 two pyridine molecules; the DBTA molecule is centrosymmetric.

Rings *A* (C18/C19/C21/C18A/C19A/C21A), *B* (C11–C16), *C* (N1/C1–C5) and *D* (N2/C6–C10) are, of course, planar; the dihedral angles between them are *A*/*B* = 83.85 (3)° and *C*/*D* = 85.47 (4)°.

As can be seen from the packing diagram (Fig. 2), the pyridine molecules are linked to DBTA by strong O—H···N

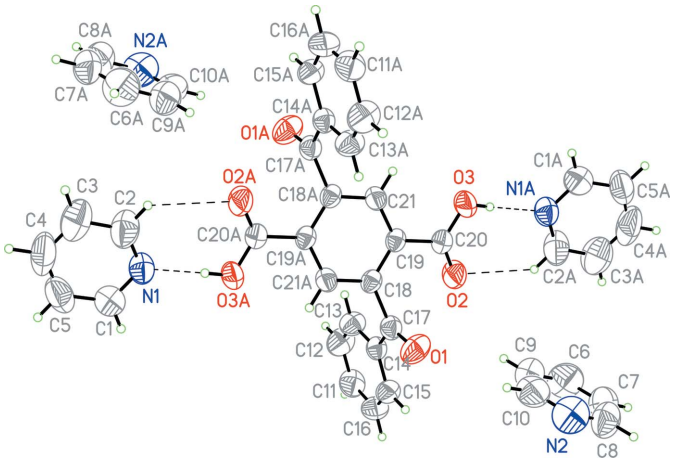



**Figure 1**
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. [Symmetry code: (A) $-x$, $1-y$, $1-z$.]

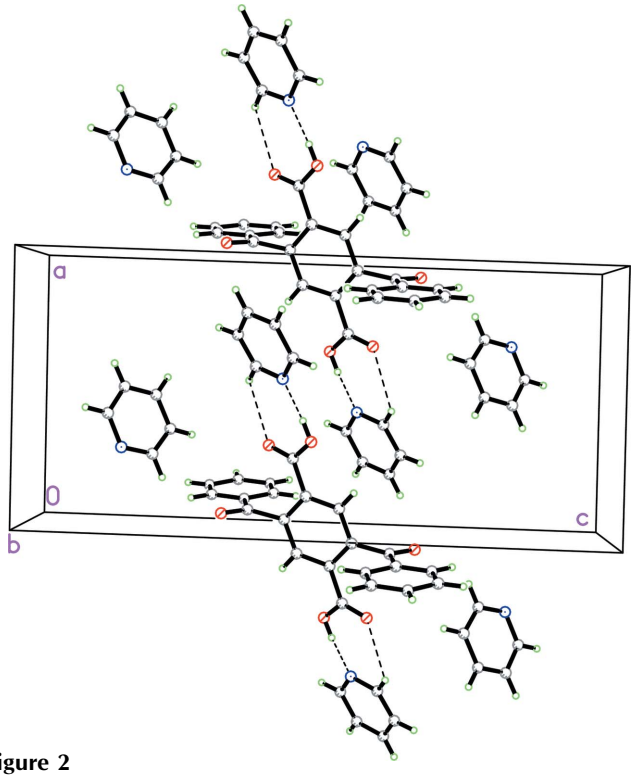



**Figure 2**
A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

and 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

DBTA was prepared by the literature method (Liu *et al.*, 2006). The crystals were obtained by dissolving DBTA (1.5 g) in pyridine (25 ml) and then allowing the solvent to evaporate slowly at room temperature for about 5 d.

*Crystal data*

$C_{22}H_{14}O_6\cdot 4C_5H_5N$
$M_r = 690.73$
Monoclinic, $P2_1/c$
$a = 9.990\ (3)$ Å
$b = 8.313\ (1)$ Å
$c = 21.437\ (2)$ Å
$\beta = 90.75\ (3)^\circ$
$V = 1780.1\ (6)$ Å$^3$
$Z = 2$
$D_x = 1.289$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm$^{-1}$
$T = 294\ (2)$ K
Block, colorless
0.30 × 0.20 × 0.20 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min} = 0.974$, $T_{max} = 0.983$
3678 measured reflections
3476 independent reflections
1385 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 26.0^\circ$
3 standard reflections
frequency: 120 min
intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.076$
$wR(F^2) = 0.188$
$S = 1.06$
3476 reflections
236 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.8P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å$^{-3}$
$\Delta\rho_{min} = -0.19$ e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.023 (2)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3$B$···N1$^{i}$ | 0.82 | 1.76 | 2.569 (5) | 168 |
| C2—H2$A$···O2$^{i}$ | 0.93 | 2.59 | 3.256 (6) | 129 |

Symmetry code: (i) $-x, -y+1, -z+1$.

H atoms were positioned geometrically, with O—H = 0.82 Å and C—H = 0.93 Å and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,O)$, where $x = 1.2$ for aromatic 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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## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–19.
Antoniadis, H., Hsieh, B. R., Abkowitz, M. A., Jenekhe, S. A. & Stolka, M. (1994). *Synth. Met.* **62**, 265–271.
Bruker (2000). *XSCANS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Enraf–Nonius (1985). *CAD-4 Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Kolosov, S., Adamovich, V., Djurovich, P., Thompson, M. E. & Adachi, C. (2002). *J. Am. Chem. Soc.* **124**, 9945–9954.

Liu, S., Ji, J.-X., Wang, D.-D. & Zhu, H.-J. (2006). *Acta Cryst.* E**62**, o1387–o1389.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tonzola, C. J., Alam, M. M., Kaminsky, W. & Jenekhe, S. A. (2003). *J. Am. Chem. Soc.* **125**, 13548–13558.