Dimethyl 2,5-dibenzoylterephthalate

Shan Liu, Jun-Mei Tang and Hong-Jun Zhu*

Department of Applied Chemistry, College of Science, Nanjing University of Technology, Nanjing 210009, People's Republic of China

Correspondence e-mail: zhuhj@njut.edu.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.062
wR factor = 0.186
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.

The asymmetric unit of the title compound, $C_{24}H_{18}O_6$, contains one half-molecule of dimethyl 2,5-dibenzoyl-terephthalate, which is located on a centre of inversion. Intermolecular C—H···O hydrogen bonds result in the formation of a three-dimensional framework, which seems to be effective in the stabilization of the crystal structure.

Comment

Dimethyl 2,5-dibenzoylterephthalate is obtained from pseudo-2,5-dibenzoylterephthaloyl chloride, which is an intermediate used to synthesize the monomer 2,5-dibenzoyl-1,4-phenylenediamine utilized to synthesize organic semi-conductors and conjugated polymers (Tonzola *et al.*, 2003). We report here the crystal structure of the title compound, (I).

(I)
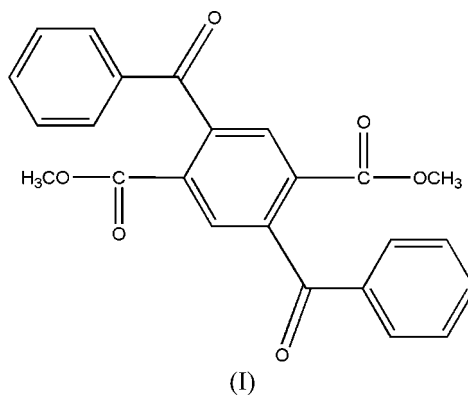
In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The asymmetric unit contains one half-molecule of dimethyl 2,5-dibenzoyl-terephthalate, which is located on a centre of inversion.

The rings *A* (C3–C5/C3*A*–C5*A*) and *B* (C7–C12) are, of course, planar and the dihedral angle between them is *A*/*B* = 79.82 (3)°.

The intermolecular C—H···O hydrogen bonds (Table 1) seem to be effective in the stabilization of the crystal structure. Hydrogen bonds play an important role in the construction of the three-dimensional framework (Fig. 2).

Experimental

Compound (I) was prepared by dissolving pseudo-2,5-dibenzoyl-terephthaloyl chloride (1.0 g, 2.4 mmol) (Liu *et al.*, 2006) in methanol (30 ml), reacting at 298 K for about 5 d. Crystals were obtained by evaporating the solvent methanol slowly at room temperature for about 20 d.

Crystal data

$C_{24}H_{18}O_6$
$M_r = 402.38$
Monoclinic, $P2_1/c$
$a = 5.391 (3)$ Å
$b = 9.192 (1)$ Å
$c = 20.656 (2)$ Å
$\beta = 93.25 (3)°$
$V = 1021.9 (6)$ Å^3

$Z = 2$
$D_x = 1.308$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 294 (2)$ K
Block, colorless
$0.40 \times 0.30 \times 0.10$ mm

Data collection

Enraf–Nonius CAD-4
  diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan
  (North et al., 1968)
  $T_{min} = 0.963$, $T_{max} = 0.991$
2218 measured reflections

1999 independent reflections
1155 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 26.0°$
3 standard reflections
  frequency: 120 min
  intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.186$
$S = 1.02$
1999 reflections
137 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.06P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Extinction correction: SHELXL97
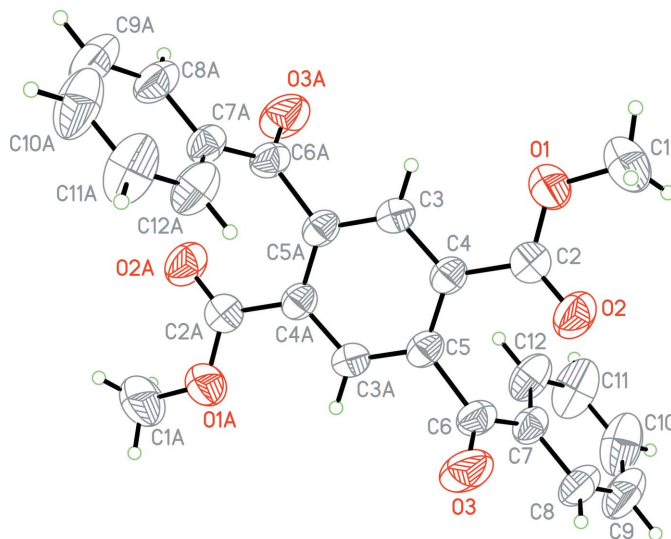Extinction coefficient: 0.048 (8)

Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (A) $2 - x$, $-y$, $-z$].
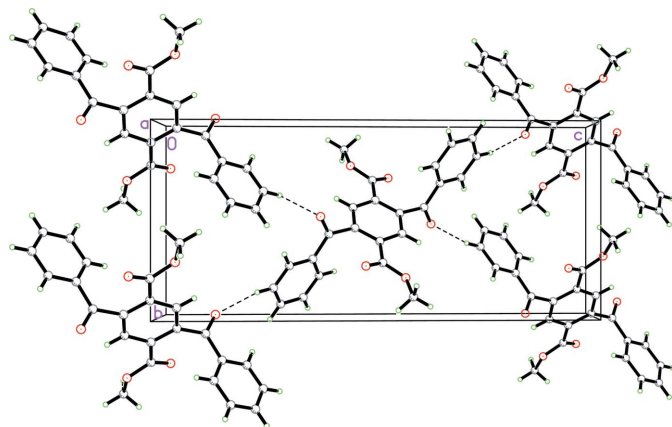

Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9A···O3^i	0.93	2.43	3.340 (5)	166

Symmetry code: (i) $-x + 1$, $y + \frac{1}{2}$, $-z + \frac{1}{2}$.

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

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.

Bruker (2000). 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.
Liu, S., Liu, J.-N., Song, G.-L., Wu, Y.-M. & Zhu, H.-J. (2006). Acta Cryst. E62, o3099–o3100.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). Acta Cryst. A24, 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.