

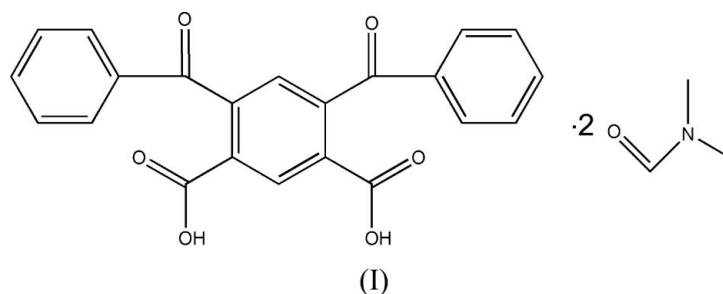
Shan Liu,^a Zhan-Mei Cao,^b
Dan-Dan Wang^a and Hong-Jun
Zhu^{a*}^aDepartment of Applied Chemistry, College of
Science, Nanjing University of Technology,
Nanjing 210009, People's Republic of China,
and ^bDepartment of Biochemistry, Yangzhou
College of Education, Yangzhou, 225002,
People's Republic of China

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

Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.079
 wR factor = 0.193
Data-to-parameter ratio = 15.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.4,6-Dibenzoylisophthalic acid *N,N*-dimethyl-
formamide disolvateIn the title compound, $\text{C}_{22}\text{H}_{14}\text{O}_6 \cdot 2\text{C}_3\text{H}_7\text{NO}$, 4,6-dibenzoyl-
isophthalic acid is linked to two *N,N*-dimethylformamide
solvent molecules *via* $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds. An intra-
molecular three-centred $\text{C}-\text{H} \cdots \text{O}$ hydrogen bond is
favoured by the *syn* conformation of both carboxyl groups.Received 17 August 2006
Accepted 26 August 2006

Comment

4,6-Dibenzoylisophthalic acid (DBIA) and its isomer 2,5-
dibenzoylterephthalic acid (DBTA) 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 opto-electronic 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).The molecular structure of (I) is shown in Fig. 1. The
dihedral angles between rings *A* (C1–C6), *B* (C17–C22) and *C*
(C9–C14) are $A/C = 112.0$ (2)°, $B/C = 74.6$ (3)° and $A/B =$
 77.0 (2)°. In the crystal structure, DBIA is linked to two *N,N*-
dimethylformamide (DMF) solvent molecules by $\text{O}-\text{H} \cdots \text{O}$
hydrogen bonds (Table 1), and the intramolecular bifurcated
 $\text{C14}-\text{H14A} \cdots \text{O2}/\text{O5}$ hydrogen bond (Fig. 1) stabilizes the
molecular conformation. DBIA molecules are also connected
to each other by $\text{C}-\text{H} \cdots \text{O}$ interactions, forming dimers
(Fig. 2).

Experimental

Compound (I) was prepared by a method we reported recently (Liu
et al., 2006). Crystals were obtained by dissolving DBIA (1.0 g,
2.67 mmol) in DMF (30 ml) and evaporating the DMF slowly at room
temperature for about 120 d.

Crystal data

$C_{22}H_{14}O_6 \cdot 2C_3H_7NO$
 $M_r = 520.52$
 Triclinic, $P\bar{1}$
 $a = 9.998(2) \text{ \AA}$
 $b = 10.940(2) \text{ \AA}$
 $c = 12.577(3) \text{ \AA}$
 $\alpha = 98.06(3)^\circ$
 $\beta = 97.67(3)^\circ$
 $\gamma = 90.72(3)^\circ$

$V = 1349.2(5) \text{ \AA}^3$
 $Z = 2$
 $D_x = 1.281 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.10 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Block, colourless
 $0.20 \times 0.20 \times 0.10 \text{ mm}$

Data collection

Nonius CAD-4 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.831$, $T_{\max} = 0.913$
 (expected range = 0.901–0.991)
 5284 measured reflections

5284 independent reflections
 2837 reflections with $I > 2\sigma(I)$
 $\theta_{\max} = 26.0^\circ$
 3 standard reflections
 every 200 reflections
 intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.079$
 $wR(F^2) = 0.193$
 $S = 0.97$
 5284 reflections
 343 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.70 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.51 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O2-H2B \cdots O8$	0.82	1.78	2.586 (5)	167
$O5-H5B \cdots O7$	0.82	1.76	2.562 (6)	167
$C11-H11A \cdots O1^i$	0.93	2.46	3.373 (5)	169
$C14-H14A \cdots O2$	0.93	2.46	2.762 (5)	99
$C14-H14A \cdots O5$	0.93	2.40	2.721 (5)	100
$C23-H23B \cdots O3^{ii}$	0.96	2.48	3.240 (8)	136
$C27-H27A \cdots O8$	0.96	2.47	2.834 (8)	102
$C27-H27B \cdots O4^{iii}$	0.96	2.57	3.358 (7)	139

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

H atoms were positioned geometrically, with $O-H = 0.82 \text{ \AA}$ and $C-H = 0.93-0.96 \text{ \AA}$, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, or $1.5U_{\text{eq}}(\text{C}, \text{O})$ for methyl and hydroxy groups. The geometric parameters of one of the DMF molecules ($C23-C25/N1/O7$) are abnormal, suggesting unresolved positional disorder.

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 Centre for Testing and Analysis, Nanjing University, for support.

References

Antoniadis, H., Hsieh, B. R., Abkowitz, M. A., Jenekhe, S. A. & Stolka, M. (1994). *Synth. Met.* **62**, 265–271.
 Bruker (2000). *XCANS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

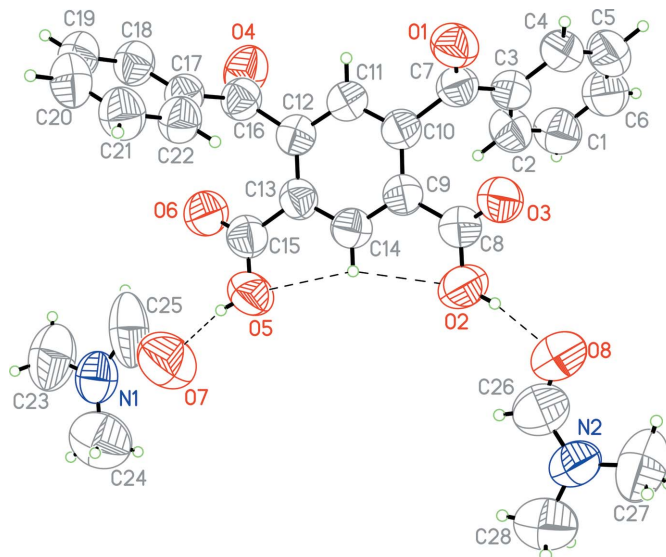


Figure 1

The asymmetric unit of (I), showing the atom-numbering scheme and displacement ellipsoids at the 50% probability level. Dashed lines indicate hydrogen bonds.

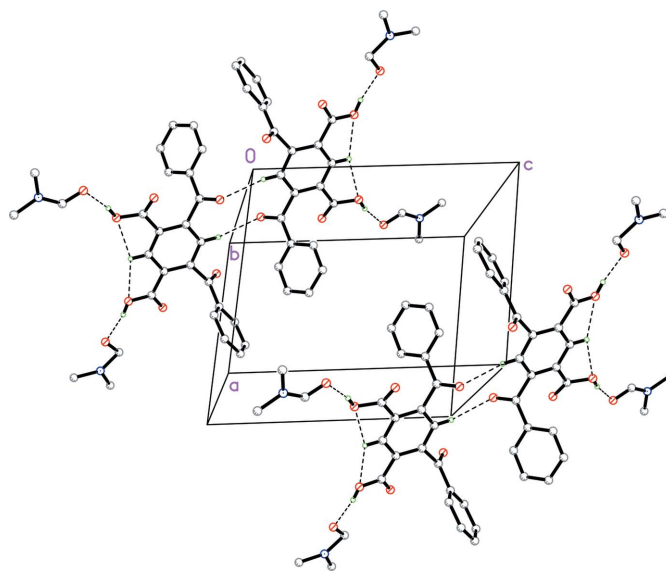


Figure 2

A partial packing diagram for (I). H atoms have been omitted unless they are involved in hydrogen bonds (dashed lines).

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., Song, G.-L., Tang, J.-M., Xu, W.-K. & Zhu, H.-J. (2006). *Acta Cryst.* **E62**, o2697–o2699.
 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.