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2,5-Dibenzoyl-1,4-phenylenediamine

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The title compound, $C_{20}H_{16}N_2O_2$, was synthesized from the reaction of 2,5-dibenzoylterephthalamide and sodium hypochlorite solution. The asymmetric unit contains one half-molecule, the molecule being centrosymmetric. Intra- and intermolecular N—H···O hydrogen bonds are highly effective in forming a two-dimensional layer structure.

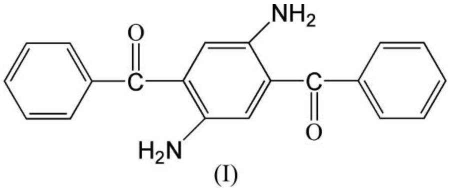
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.005 Å
R factor = 0.054
wR factor = 0.151
Data-to-parameter ratio = 12.9

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

Comment

2,5-Dibenzoyl-1,4-phenylenediamine, (I), is a significant material in the synthesis of extended lattice compounds with a centrosymmetric system. It is also an important compound in preparation of electron-transport materials (Tonzola *et al.*, 2003). The synthesis of 2,5-dibenzoyl-1,4-phenylenediamine has been reported (Imai *et al.*, 1975).



(I)

The molecular structure of (I) is shown in Fig. 1 and selected bond lengths and angles are given in Table 1. The asymmetric unit contains one half molecule, the whole molecule being centrosymmetric.

The crystal packing is stabilized by intra- and intermolecular N—H···O hydrogen bonds (Table 2), forming a two-dimensional layer structure (Fig. 2).

Experimental

Sodium hypochlorite solution (10 ml, 5.25%) was added with stirring to a mixture of 2,5-dibenzoylterephthalamide (1 g, 2.7 mmol) and potassium hydroxide solution (30 ml, 10.45%) cooled in an ice-water bath for half an hour. The mixture was stirred for an additional hour at 343–353 K and the precipitate began to separate. The resulting precipitate was filtered off, washed with hot water and dried under reduced pressure. The crude product was obtained by slow evaporation of a solution in benzene (yield: 0.6 g, 71%; m.p. 492 K).

Crystal data

$C_{20}H_{16}N_2O_2$
M_r = 316.35
Orthorhombic, *Pcab*
a = 7.4651 (15) Å
b = 13.0034 (16) Å
c = 15.9759 (18) Å
V = 1550.8 (4) Å^3
Z = 4
D_x = 1.355 Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9–12°
μ = 0.09 mm^{-1}
T = 296 (2) K
Prism, brown
0.3 × 0.3 × 0.1 mm

doi:10.1107/S1600536805019112

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (*XPREP* in *SHELXTL*; Bruker, 2000)
$T_{\min} = 0.974$, $T_{\max} = 0.991$
1519 measured reflections
1519 independent reflections
614 reflections with $I > 2\sigma(I)$
$\theta_{\max} = 26.0°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 16$
$l = 0 \rightarrow 19$
3 standard reflections every 200 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.151$
$S = 1.02$
1519 reflections
118 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.19$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0047 (19)

Table 1
Selected geometric parameters (Å, °).

O—C4	1.231 (4)	N—C1	1.393 (4)
C10—C4	1.478 (5)	C3—C4	1.491 (4)
C2—C1—N	120.1 (3)	C1$^{\rm i}$—C3—C4	120.7 (3)
C1—C2—C3	122.4 (3)	C10—C4—C3	120.9 (3)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N—H1$\cdots$O$^{\rm i}$	0.87 (4)	2.25 (4)	2.855 (5)	127 (3)
N—H1$\cdots$O$^{\rm ii}$	0.87 (4)	2.61 (4)	3.220 (5)	128 (3)

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

Atoms H1 and H3 were located in a difference synthesis and refined freely [N—H = 0.87 (4)–0.95 (5) Å]. The remaining H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(parent atom).

Data collection: *CAD-4 Software* (Enraf–Nonius,1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

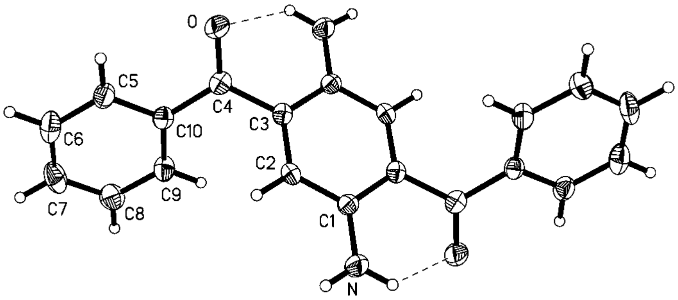


Figure 1
A drawing of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines represent hydrogen bonds. [Symmetry code for unlabelled atoms: $-x, -y, -z$.]

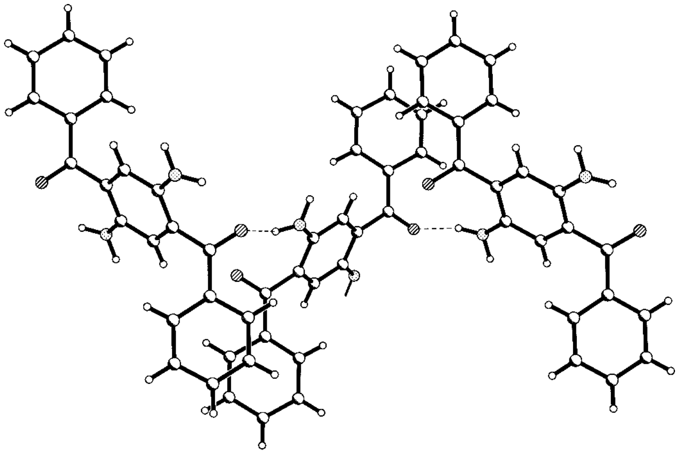


Figure 2
The two-dimensional layer structure of (I). Dashed lines indicate hydrogen bonds.

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