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# 3-Benzoyl-1,2-diphenyl-1*H*-benz[*f*]indole-4,9-dione

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.005 Å
*R* factor = 0.050
*wR* factor = 0.151
Data-to-parameter ratio = 12.6

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



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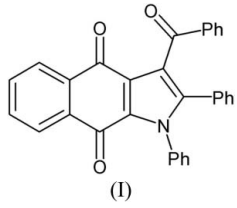
In the title compound, $C_{31}H_{19}NO_3$, the benz[*f*]indole-4,9-dione unit is essentially planar. The crystal structure exhibits intermolecular C—H···O contacts.

## Comment

Naturally occurring quinones constitute an important class of natural products that have a wide range of biological activities (Bolton *et al.*, 2000). A basic structural unit in these quinone natural products is the indolequinone group. The synthesis of benzannulated indolequinones, benz[*f*]indole-4,9-diones, attracts much current attention (Hu *et al.*, 2006). In our ongoing research work on the direct one-pot syntheses of benz[*f*]indole-4,9-diones, we have prepared the title compound, (I), by a *C*,*N*-dialkylation reaction between 2,3-dichloro-1,4-naphthoquinone and 1,3-diphenyl-3-(phenylamino)-2-propen-1-one.




(I)

In the molecule of (I) (Fig. 1), the benz[*f*]indole-4,9-dione unit is essentially planar, with the benzene (C1–C6) and pyrrole rings forming dihedral angles of 4.2 (3) and 2.7 (3)°, respectively, with the mean plane through the benzoquinone unit.

The crystal structure of (I) exhibits intermolecular C—H···O contacts (Table 1).

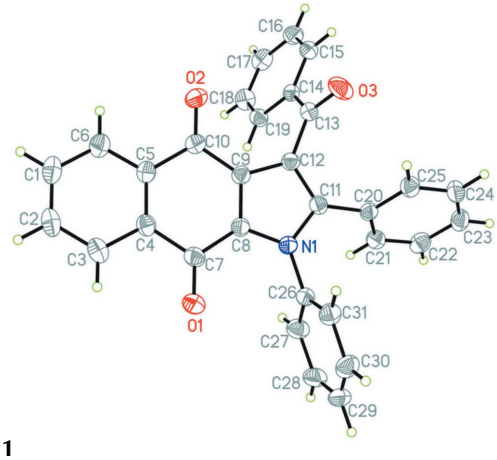



**Figure 1**
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level.

## Experimental

A mixture of 2,3-dichloro-1,4-naphthoquinone (0.250 g, 1.1 mmol), 1,3-diphenyl-3-(phenylamino)-2-propen-1-one (0.299 g, 1 mmol) and $Na_2CO_3$ (0.345 g, 2.5 mmol) in dimethylformamide (15 ml) was stirred at 353 K for 6 h. After evaporation of the solvent, compound (I) was isolated using silica-gel column chromatography with petroleum ether–ethyl acetate (4:1) as eluents (yield 40%). Single crystals of (I) were obtained by slow evaporation of a petroleum ether–ethyl acetate (3:1 *v*/*v*) solution of (I).

*Crystal data*

$C_{31}H_{19}NO_3$
$M_r$ = 453.47
Triclinic, $P\overline{1}$
$a$ = 10.481 (2) Å
$b$ = 10.916 (2) Å
$c$ = 11.948 (3) Å
$\alpha$ = 63.29 (2)°
$\beta$ = 68.99 (3)°
$\gamma$ = 73.49 (3)°
$V$ = 1127.5 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 293 (2) K
0.40 × 0.31 × 0.22 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (*XCAD4*; Harms & Wocadlo, 1995)
$T_{min}$ = 0.966, $T_{max}$ = 0.973
4212 measured reflections
3969 independent reflections
2890 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.014
3 standard reflections
every 200 reflections
intensity decay: none

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.151
$S$ = 1.00
3969 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C17—H17···O1$^{i}$ | 0.93 | 2.57 | 3.340 (4) | 140 |
| C31—H31···O2$^{ii}$ | 0.93 | 2.57 | 3.475 (4) | 166 |

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

H atoms were placed in calculated positions and allowed to ride during refinement, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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