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4-(2-Benzoylphenoxy)phthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.033
wR factor = 0.085
Data-to-parameter ratio = 13.2

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

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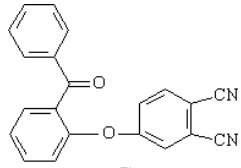
The title compound, $C_{21}H_{12}N_2O_2$, contains three aromatic rings, which are not coplanar. The benzene ring and phthalonitrile group are connected by a bridging O atom, and the dihedral angle between them is 71.26 (4)°.

Comment

4-(2-Benzoylphenoxy)phthalonitrile, (I), is a starting material in the synthesis of symmetrically and unsymmetrically tetra-substituted phthalocyanines (McKeown, 1998). Phthalocyanines have, for many years, been the subject of research due to their wide range of application fields, such as organic pigments, chemical sensors, electrochromic display devices, photovoltaic cells, xerography, optical disks, catalysis, and non-linear optics (Leznoff & Lever, 1989–1996).



(I)

The three aromatic rings in (I) are not coplanar. The bond distances and angles are normal and the average C—N bond distance of 1.445 (2) Å is short enough to indicate their triple-bond character and is consistent with a similar bond length in 4,4′-(*N*-phenyl-2,2′-iminodiethoxy)diphthalonitrile (Ocak *et al.*, 2003). The C—O bond distances are comparable to those in Işık *et al.* (2003). The dihedral angle between rings C9–C14 and C3–C8 is 71.26 (4)°, that between rings C16–C21 and C3–C8 is 47.22 (1)°, and that between rings C9–C14 and C16–C21 is 68.91 (4)°.

Experimental

2-Benzoylphenol (1.71 g, 8.63 mmol) and 4-nitrophthalonitrile (1.00 g, 5.78 mmol) were dissolved in dry dimethylformamide (40 ml) with stirring under N_2. Dry fine-powdered sodium carbonate (1.5 g, 10.87 mmol) was added in portions (10 × 1 mmol) every 10 min. The reaction mixture was stirred for 48 h at room temperature and poured into ice–water (200 g). The product was filtered off and washed with (10% *w*/*w*) NaOH solution and water until the filtrate was neutral. Recrystallization from ethanol gave a white product (yield 1.60 g, 85.56%). Single crystals of (I) were obtained from absolute ethanol at room temperature by slow evaporation (m.p. 386 K). Elemental analysis calculated for $C_{21}H_{12}N_2O_2$: C 77.77, H 3.73, N 8.64%; found: C 77.56 H 3.80 N 8.56%. ^{1}H NMR ($CDCl_3$): δ 7.03–7.75 (*m*, 12H, Ar). ^{13}C NMR ($CDCl_3$): 108.87, 114.78 (CN), 115.25 (CN), 117.31, 121.01, 121.33, 122.03, 126.33, 128.46, 129.74, 131.00, 132.16, 132.94, 133.66, 135.15, 136.63, 151.11, 161.50, 193.96 (C═O).

Crystal data

$C_{21}H_{12}N_2O_2$
M_r = 324.33
Monoclinic, $P2_1/c$
a = 8.6894 (7) Å
b = 24.3903 (15) Å
c = 7.8153 (6) Å
β = 100.460 (6)°
V = 1628.8 (2) Å^3
Z = 4
D_x = 1.323 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12 373 reflections
θ = 1.7–25.6°
μ = 0.09 mm^{-1}
T = 293 (2) K
Prism, colourless
0.3 × 0.2 × 0.1 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: by integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.926, T_{max} = 0.970
10 996 measured reflections
2995 independent reflections
2427 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 25.5°
$h = -10 \rightarrow 10$
$k = -29 \rightarrow 29$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.085
S = 1.04
2995 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 0.2033P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0138 (17)

Table 1
Selected geometric parameters (Å, °).

O1—C5	1.3719 (14)	N2—C2	1.1455 (17)
O1—C9	1.3972 (15)	C1—N1	1.1440 (17)
O2—C15	1.2193 (15)		
C5—O1—C9	119.73 (10)	C11—C12—C13	119.94 (13)
C16—C15—C10	118.72 (10)		

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

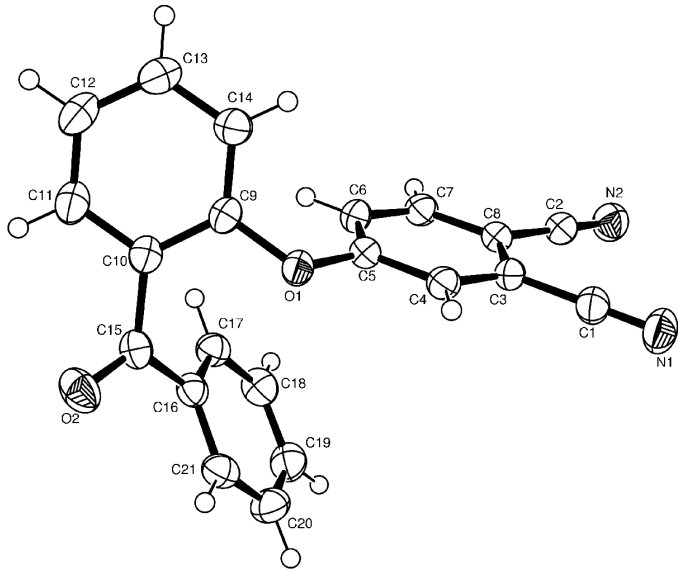


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

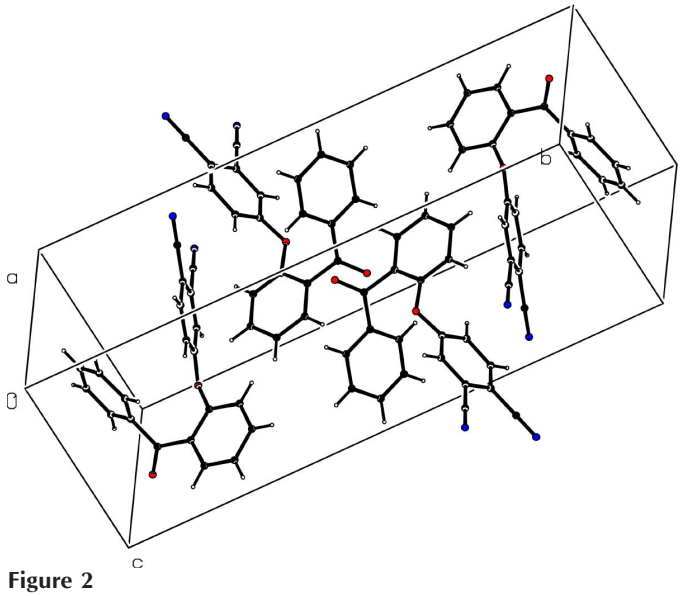


Figure 2
The crystal packing of (I).

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