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4-Diphenylmethoxyphthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.095
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.

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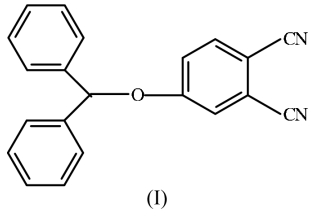
The title compound, $C_{21}H_{14}N_2O$, contains three aromatic rings. The structure is stabilized by π–π stacking interactions.

Comment

4–Diphenylmethoxyphthalonitrile, (I), is a precursor in the synthesis of 2,9,16,23-tetrahydroxyphthalocyanines (Leznoff *et al.*, 1994). For many years, phthalocyanines have attracted continued interest in various research fields, *e.g.* chemical sensors, electrochromism, batteries, applications in colours, catalysis, photodynamic therapy, semiconductive materials, liquid crystals and non-linear optics (Leznoff & Lever, 1989–1996). One of the most promising fields is the use of phthalocyanine derivatives as photosensitizers for photodynamic theraphy (PDT), an emerging new bimodal strategy for treating a large variety of diseases, such as psoriasis, cancer, dysplasia and infectious diseases, and for prevention of HIV-1 infection (Leznoff & Lever, 1989–1996; Vzorov *et al.*, 2003).



(I)

The title compound contains three aromatic rings. Rings *A* (C3–C8), *B* (C10–C15) and *C* (C16–C21) are each essentially planar. Ring *A* carries two cyano groups. Rings *B* and *C* are connected by a C atom, and the dihedral angle between them is 77.66 (7)°. All of the C≡N and C—O bond distances and angles (Table 1) are in good agreement with literature values (Atalay *et al.*, 2003). The dihedral angles between rings *A*/*B* and *A*/*C* are 8.79 (11)° and 75.90 (7)°, respectively. There are

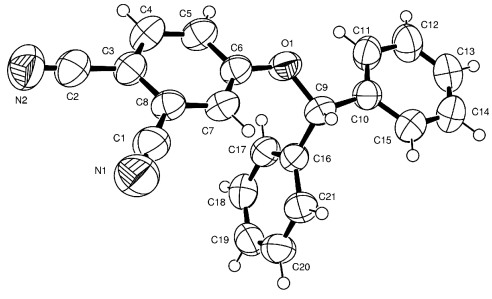


Figure 1
An *ORTEP*III (Burnett & Johnson, 1996) drawing of the molecular structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level.

π–π stacking interactions; ring *A* in the molecule at (*x*, *y*, *z*) stacks with ring *B* at $(1-x, 1-y, 1-z)$, with a distance of 3.6887 (14) Å between the ring centroids.

Experimental

4-Diphenylmethoxyphthalonitrile was synthesized according to reported procedures (Leznoff *et al.*, 1994). Single crystals were obtained from an ethanol solution by slow evaporation at room temperature.

Crystal data

$C_{21}H_{14}N_2O$
M_r = 310.34
Monoclinic, $P2_1/n$
a = 8.9005 (13) Å
b = 15.1033 (19) Å
c = 12.1253 (15) Å
β = 92.632 (11)°
V = 1628.2 (4) Å^3
Z = 4
D_x = 1.266 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6068 reflections
θ = 2.2–26.7°
μ = 0.08 mm^{-1}
T = 293 (2) K
Prism, green
0.28 × 0.21 × 0.15 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: none
15368 measured reflections
3187 independent reflections
1458 reflections with $I > 2\sigma(I)$
R_{int} = 0.084
θ_{max} = 26.0°
$h = -10 \rightarrow 10$
$k = -18 \rightarrow 18$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.095
S = 0.83
3187 reflections
218 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.0195 (18)

Table 1
Selected geometric parameters (Å, °).

O1—C6	1.368 (2)	C3—C2	1.439 (3)
O1—C9	1.447 (2)	C2—N2	1.138 (3)
C8—C1	1.440 (3)	C1—N1	1.142 (3)
C6—O1—C9	118.94 (14)	C11—C10—C9	123.08 (18)
O1—C9—C16	110.57 (15)	N2—C2—C3	178.3 (3)
O1—C9—C10	106.54 (15)	N1—C1—C8	179.1 (3)

H atoms were positioned geometrically and refined using a riding model, with an aromatic C—H distance of 0.93 Å, a C—H distance of 0.98 Å for the tertiary C atom and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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