4,5-Bis(2-*tert*-butylphenoxy)phthalonitrile

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The title compound, $C_{28}H_{28}N_2O_2$, contains three aromatic rings, which are not coplanar and which are distorted from ideal C_{2v} symmetry. The crystal structure involves four intramolecular C—H···O hydrogen bonds.

Comment

4,5-Bis(2-*tert*-butylphenoxy)phthalonitrile, (I), is a precursor in the synthesis of symmetrically and unsymmetrically substituted phthalocyanines (Leznoff & Lever, 1989–1996). Pthalocyanines possess some remarkable properties which render them important commercial commodities. The production of phthalocyanines for the use of dyes and pigments is around 80 000 tons per year (Wöhrle, 2001). In the past few years, a great deal of interest has been focused on the synthesis of phthalocyanine derivatives as a result of their application in many fields, such as chemical sensors, electrochromism, batteries, semiconductor 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 therapy (PDT), an emerging new bimodal strategy for treating a wide variety of conditions, such as psoriasis, cancer, and dysplastic and infectious diseases, and for prevention of HIV-1 infection (Leznoff & Lever, 1989–1996; Vzorov *et al.*, 2003).


(I)
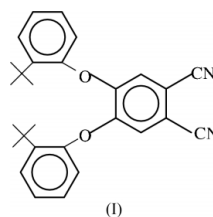
. The title compound, (I), consists of a phthalonitrile moiety carrying 2-*tert*-butylphenoxy substituents at C4 and C5 (Fig. 1). The molecular structure of (I) is shown in Fig. 1. Tables 1 and 2 list selected molecular and hydrogen-bonding geometry, respectively. The C7≡N1 and C8≡N2 bond distances are 1.139 (2) and 1.135 (2) Å, respectively, consistent with N≡C triple-bond character. They are also comparable with literature values (Öztürk *et al.*, 1999, 2000; Subbiah Pandi *et al.*, 2002; Ocak *et al.*, 2003, 2004).

The geometry of (I) is distorted from ideal C_{2v} symmetry, with a dihedral angle between rings A (C1–C6) and B (C9–C14) of 69.15 (4)°, between rings A and C (C19–C24) of 73.74 (5)°, and between rings B and C of 28.59 (6)°. While the bond lengths at oxygen are essentially equal, the C4—O1—C9—C14 and C5—O2—C19—C24 torsion angles of −125.09 (16) and 121.21 (16)°, respectively, are different. This destroys any molecular symmetry.
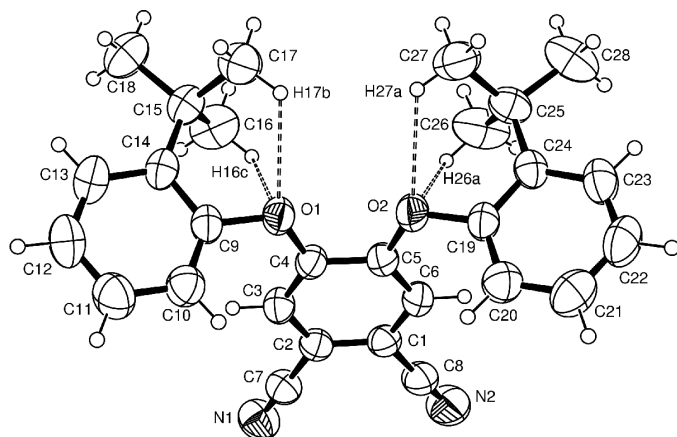
Figure 1
An *ORTEP*III drawing (Burnett & Johnson, 1996) of the title compound, showing the atomic numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 40% probability level.

There are intramolecular C—H···O interactions in the structure of (I). Firstly, atom O1 forms an intramolecular bifurcated hydrogen bond with atoms H17B and H16C. Similarly, atom O2 forms an intramolecular bifurcated hydrogen bond with atoms H27A and H26A (Fig. 1 and Table 2).

Experimental

4,5-Bis(2-*tert*-butylphenoxy)phthalonitrile was synthesized according to reported procedures with minor modifications (Matlaba & Nyokong, 2002). Single crystals were obtained by slow evaporation of an absolute ethanol solution at room temperature.

Crystal data

$C_{28}H_{28}N_2O_2$	$D_x = 1.135$ Mg m^{-3}
$M_r = 424.52$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 6510
$a = 10.8426$ (10) Å	reflections
$b = 21.704$ (2) Å	$\theta = 1.9$–$27.5°$
$c = 11.0967$ (9) Å	$\mu = 0.07$ mm^{-1}
$\beta = 107.920$ (7)°	$T = 293$ (2) K
$V = 2484.6$ (4) Å^3	Prism, green
$Z = 4$	$0.50 \times 0.35 \times 0.22$ mm

Data collection

Stoe IPDS-2 diffractometer	4880 independent reflections
ω scans	2371 reflections with $I > 2\sigma(I)$
Absorption correction: by	$R_{int} = 0.054$
integration (*X-RED*32;	$\theta_{max} = 26.0°$
Stoe & Cie, 2002)	$h = -13 \rightarrow 13$
$T_{min} = 0.971$, $T_{max} = 0.985$	$k = -26 \rightarrow 26$
17 816 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.108$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.80$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
4880 reflections	$\Delta\rho_{min} = -0.11$ e Å^{-3}
290 parameters	Extinction correction: *SHELXL*97
H-atom parameters constrained	Extinction coefficient: 0.0113 (11)

Table 1
Selected geometric parameters (Å, °).

O1—C4	1.3603 (18)	C15—C17	1.530 (3)
O1—C9	1.4031 (19)	C15—C16	1.534 (3)
O2—C5	1.3608 (18)	C15—C18	1.536 (3)
O2—C19	1.4050 (18)	C25—C28	1.532 (3)
C7—N1	1.139 (2)	C25—C26	1.533 (3)
C8—N2	1.135 (2)	C25—C27	1.536 (3)
C4—O1—C9	120.01 (12)	C14—C15—C18	112.17 (17)
C5—O2—C19	118.56 (12)	C24—C25—C28	111.67 (17)
C14—C15—C17	110.92 (15)	C24—C25—C26	109.46 (15)
C14—C15—C16	109.17 (16)	C24—C25—C27	110.17 (16)
C4—O1—C9—C14	−125.09 (16)	C5—O2—C19—C24	121.21 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17B···O1	0.96	2.35	3.004 (2)	124
C27—H27A···O2	0.96	2.36	3.022 (2)	126
C16—H16C···O1	0.96	2.43	3.063 (2)	123
C26—H26A···O2	0.96	2.39	3.054 (3)	126

The H atoms were placed geometrically and refined using a riding model, fixing the aromatic C—H distance at 0.93 Å and methyl group C—H distance at 0.96 Å. U_{iso}(H) values were calculated as $1.2U_{eq}(C_{aromatic})$ and $1.5U_{eq}(C_{methyl})$ of the parent atom.

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) and *PARST* (Nardelli, 1995).

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