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4,5-Bis(5-isopropyl-2-methylphenoxy)-phthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.052
wR factor = 0.167
Data-to-parameter ratio = 15.2

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

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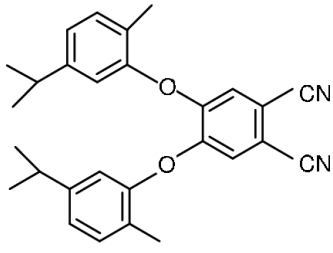
The phthalonitrile derivative, $C_{28}H_{26}N_2O_2$, contains three aromatic rings, which are mutually almost orthogonal. The structure is stabilized by π–π stacking interactions.

Comment

Phthalonitriles such as the title compound 4,5-bis(5-isopropyl-2-methylphenoxy)phthalonitrile, (I), are generally used for the synthesis of symmetrically and unsymmetrically substituted phthalocyanines and subphthalocyanines (Leznoff & Lever, 1989–1996). Phthalocyanines have been the subject of research due to their wide applications, such as in organic pigments, chemical sensors, electrochromic display devices, photovoltaic cells, xerography, optical disks, catalysis, and nonlinear optics (McKeown, 1998). The title compound, (I), consists of a phthalonitrile moiety carrying two 4-isopropyl-2-methylphenoxy groups at positions 4 and 5 (Fig. 1). The lengths of the two C≡N triple bonds [C8—N2 = 1.138 (3) Å and C7—N1 = 1.140 (3) Å] are consistent with those found in similar compounds (Ocak *et al.*, 2003, 2004; Atalay *et al.*, 2003; Erdem *et al.*, 2004). The angles subtended at the O atoms of the 5-isopropy-2-methylphenoxy substituents are equivalent [C4—O1—C15 = 117.38 (14)° and C3—O2—C9 = 117.84 (14)°], but the ring C15—C20 is approximately perpendicular to the other aromatic rings, with a dihedral angle of 87.41 (8)° with respect to ring C1–C6 and 87.02 (9)° with respect to C9–C14. Although there are no hydrogen bonds in the structure, there is evidence for π–π stacking interactions between the C1–C6 rings; the perpendicular interplanar distance is 3.7676 (11) Å (Fig. 2).



(I)

Experimental

5-Isopropyl-2-methylphenol (1.54 g, 10.26 mmol) and 4,5-dichloro-1,2-dicyanobenzene (1.00 g, 5.08 mmol) were heated at 333 K in dry dimethyl sulfoxide (50 ml) with stirring under N_2. Dry fine-powdered potassium carbonate (1.70 g, 12.32 mmol) was added in portions (12 × 1 mmol) every 10 min. The mixture was heated for a further 48 h. After cooling, the mixture was 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 the final product (yield 1.19 g, 55.35%). Single crystals were obtained from absolute ethanol at room temperature *via* slow evaporation (m.p. 366 K); elemental analysis calculated for $C_{28}H_{26}N_2O_2$: C 79.22, H 6.65, N 6.60%; found: C 79.10 H 6.50 N 6.70%. IR (ν_{max}, cm^{-1}): 3110–3035 (Ar-CH), 2958–2870 (CH), 2229 (CN), 1599, 1568, 1494, 1459, 1414, 1390, 1319, 1292, 1265, 1234, 1196, 1176, 1111, 1068, 997, 939, 885, 869, 816, 767, 732, 710.

Crystal data

$C_{28}H_{26}N_2O_2$	D_x = 1.134 Mg m^{-3}
M_r = 424.52	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 13663 reflections
a = 15.5339 (13) Å	θ = 1.4–26.4°
b = 11.1141 (7) Å	μ = 0.07 mm^{-1}
c = 15.7665 (15) Å	T = 293 (2) K
β = 114.061 (7)°	Prism, colourless
V = 2485.5 (4) Å^3	0.72 × 0.45 × 0.24 mm
Z = 4	

Data collection

Stoe IPDS-2 diffractometer	4891 independent reflections
ω scans	2849 reflections with $I > 2\sigma(I)$
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)	R_{int} = 0.052
	θ_{max} = 26.0°
	$h = -19 \rightarrow 19$
T_{min} = 0.957, T_{max} = 0.984	$k = -13 \rightarrow 13$
34735 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1056P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.053	$(\Delta/\sigma)_{max}$ = 0.026
$wR(F^2)$ = 0.167	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
S = 0.94	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
4891 reflections	Extinction correction: *SHELXL*97
321 parameters	Extinction coefficient: 0.021 (2)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C4	1.376 (2)	O2—C9	1.411 (2)
O1—C15	1.397 (2)	N2—C8	1.138 (3)
O2—C3	1.362 (2)	N1—C7	1.140 (3)
C4—O1—C15	117.38 (14)	C3—O2—C9	117.84 (14)

H atoms were positioned geometrically and refined using a riding model, fixing the aromatic C—H distances at 0.93 Å and the methyl-group C—H distances at 0.96 Å. U_{iso}(H) values were calculated as 1.5U_{eq}(methyl group) or 1.5U_{eq}(C). Large displacement parameters for the methyl C atoms of both isopropyl groups in the molecule were indicative of positional disorder. This was partially resolved by refining two unique positions for atoms C23, C25, C26 and C27 with occupancy factors of 0.668:0.332 (17). Even with this disorder model, the displacement parameters remain very high and details of the geometry in these portions of the molecule remain somewhat unreliable.

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).

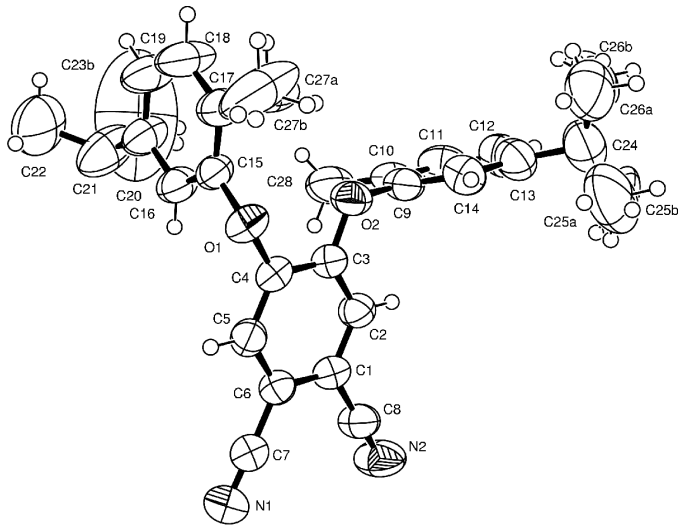


Figure 1
An *ORTEP*III drawing (Burnett & Johnson, 1996) of (I), showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level. Both disorder components are shown.

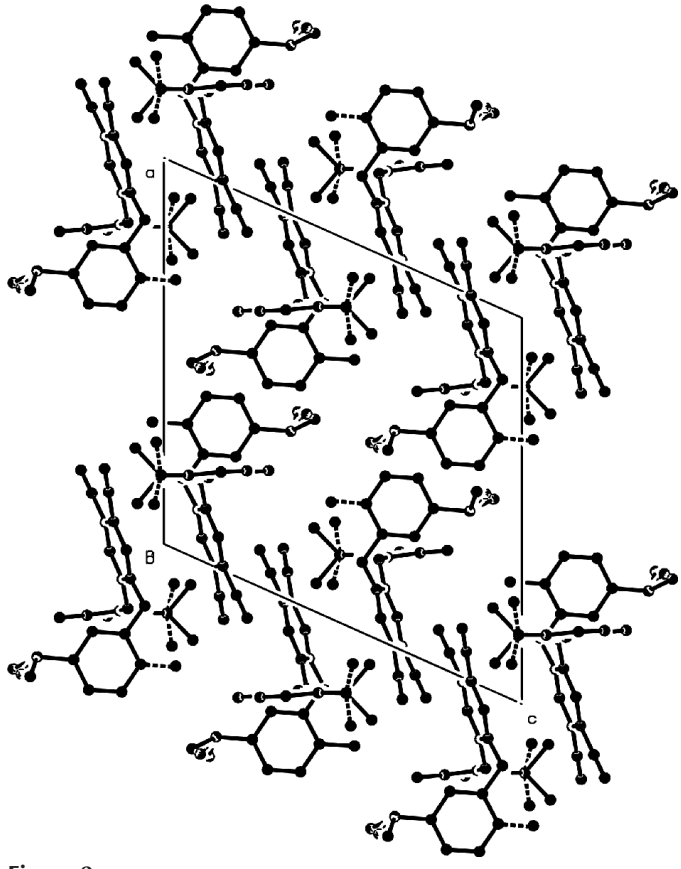


Figure 2
The unit-cell contents of (I), viewed down the *b* axis

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