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4-(2,3,5-Trimethylphenoxy)phthalonitrile

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Wae) = 0.000 Å
R factor = 0.036
wR factor = 0.100
Data-to-parameter ratio = 13.9

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

The crystal structure of the title compound, $C_{17}H_{14}N_2O$, is stabilized by weak van der Waals interactions.

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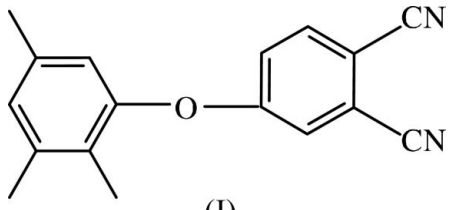
Comment

Substituted phthalonitriles are generally used for preparing symmetrically and unsymmetrically peripherally substituted phthalocyanine complexes and subphthalocyanines (McKeown, 1998; Leznoff & Lever, 1989–1996). Phthalocyanines, whose production for the use of dyes and pigments is around 80 000 tons per year (Worhle, 2001), are excellent pigments with good thermal and chemical stabilities. 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 large variety of illnesses, such as psoriasis, cancer, dysplastic, infectious diseases and prevention of HIV-1 infection (Leznoff & Lever, 1989–1996; Vzorov *et al.*, 2003).



(I)

The triple-bond lengths are in agreement with reported values (Petek *et al.*, 2004; Büyükgüngör *et al.*, 2005). The dihedral angle between the C2–C7 and C9–C14 rings is 85.12 (5)°.

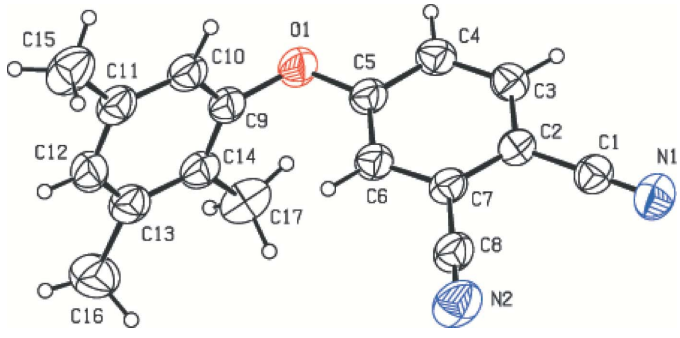


Figure 1
The structure of the title compound, (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

2,3,5-Trimethylphenol (1.17 g, 8.59 mmol) and 4-nitrophthalonitrile (1.0 g, 5.78 mmol) were dissolved in dry dimethylformamide (50 ml). After stirring for 1 h at room temperature, dry fine-powdered potassium carbonate (1.40 g, 10.0 mmol) was added portionwise over a period of 2 h with stirring. 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 (I) (yield 1.11 g, 73.51%). Single crystals were obtained from absolute ethanol at room temperature by slow evaporation (m.p. 373 K); elemental analysis calculated for $C_{17}H_{14}N_2O$: C 77.84, H 5.38, N 10.68%; found: C 75.70 H 5.46 N 10.60%.

Crystal data

$C_{17}H_{14}N_2O$
$M_r = 262.30$
Orthorhombic, *Pbca*
$a = 7.8929$ (8) Å
$b = 29.415$ (4) Å
$c = 12.4679$ (14) Å
$V = 2894.7$ (6) Å^3
$Z = 8$
$D_x = 1.204$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10756 reflections
$\theta = 1.4$–$26.0°$
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.38 × 0.20 × 0.20 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.926$, $T_{max} = 0.970$
15698 measured reflections
2841 independent reflections
1343 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 26.0°$
$h = -9 \rightarrow 9$
$k = -36 \rightarrow 36$
$l = -15 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.100$
$S = 0.80$
2841 reflections
205 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.09$ e Å^{-3}
$\Delta\rho_{min} = -0.10$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0030 (6)

Table 1
Selected geometric parameters (Å, °).

O1—C5	1.3621 (19)	C1—N1	1.142 (2)
O1—C9	1.4097 (19)	C8—N2	1.134 (2)
C6—C5	1.388 (2)		
N1—C1—C2	179.3 (2)	N2—C8—C7	179.1 (2)

The aromatic H atoms were found in a difference Fourier map and were refined isotropically [C—H = 0.877 (19)–0.991 (19) Å]. The methyl H atoms were placed in geometrically idealized positions (C—H = 0.96 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(methyl 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).

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