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Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(C-C)$ = 0.005 Å

R factor = 0.039

wR factor = 0.113

Data-to-parameter ratio = 7.7

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

4-(2,6-Dimethylphenoxy)phthalonitrile

In the title compound, $C_{16}H_{12}N_2O$, two benzene rings are linked by an O atom. One of the benzene rings carries two cyano groups. The compound crystallizes with two independent molecules in the asymmetric unit. The crystal structure is stabilized by weak van der Waals interactions.

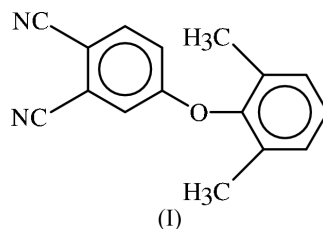
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Comment

Monosubstituted phthalonitriles, such as the title compound, 4-(2,6-dimethylphenoxy)phthalonitrile, (I), are generally used for the synthesis of symmetrically and unsymmetrically substituted phthalocyanines and subphthalocyanines (Leznoff & Lever, 1996). Phthalocyanines have been the subject of constant research as a result of their widespread applicability, such as in organic pigments, chemical sensors, electrochromic display devices, photovoltaic cells, xerography, optical disks, catalysis and non-linear optics (McKeown, 1998). We present here the structure of (I).



An *ORTEP-3* view (Farrugia, 1997) of (I) and a packing diagram are shown in Figs. 1 and 2, respectively. Selected bond lengths and angles are given in Table 1. The triple-bond lengths are in agreement with reported values (Ocak *et al.*, 2004; Atalay *et al.*, 2003; Çoruh *et al.*, 2002; Petek *et al.*, 2004). The bond lengths and angles of the two molecules in the asymmetric unit are very similar.

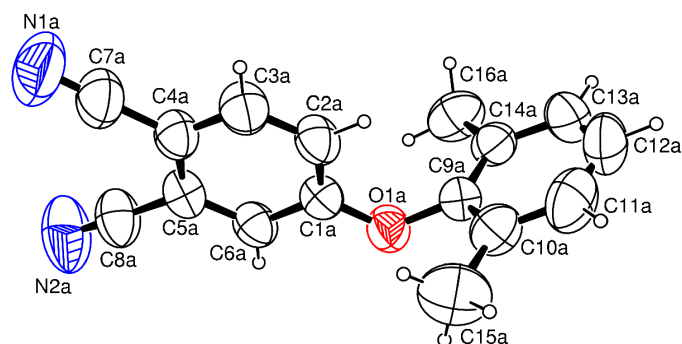


Figure 1

A view of one molecule of the asymmetric unit of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.

Experimental

4-(2,6-Dimethylphenoxy)phthalonitrile was synthesized according to a reported procedure (Sakaguchi *et al.*, 1999). Single crystals were obtained from methanol at room temperature *via* slow evaporation.

Crystal data

$C_{16}H_{12}N_2O$	$Z = 2$
$M_r = 248.28$	$D_x = 1.204 \text{ Mg m}^{-3}$
Triclinic, $P1$	Mo $K\alpha$ radiation
$a = 8.160 (5) \text{ \AA}$	Cell parameters from 10 590 reflections
$b = 8.451 (5) \text{ \AA}$	$\theta = 1.9\text{--}29.3^\circ$
$c = 11.629 (5) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$\alpha = 97.921 (5)^\circ$	$T = 293 (2) \text{ K}$
$\beta = 108.234 (5)^\circ$	Prism, colourless
$\gamma = 110.548 (5)^\circ$	$0.50 \times 0.40 \times 0.25 \text{ mm}$
$V = 685.0 (7) \text{ \AA}^3$	

Data collection

Stoe IPDS-2 diffractometer	2681 independent reflections
ω scans	2415 reflections with $I > 2\sigma(I)$
Absorption correction: by integration (<i>X-RED32</i> ;	$R_{\text{int}} = 0.075$
Stoe & Cie, 2002)	$\theta_{\text{max}} = 26.0^\circ$
$T_{\text{min}} = 0.964$, $T_{\text{max}} = 0.981$	$h = -10 \rightarrow 10$
13 674 measured reflections	$k = -10 \rightarrow 9$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0767P)^2 + 0.0109P]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.113$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
2681 reflections	$\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$
348 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

C1b—O1b	1.367 (3)	C8b—N2b	1.136 (3)
C1a—O1a	1.360 (3)	C8a—N2a	1.140 (4)
C1a—C6a	1.382 (3)	C9b—O1b	1.392 (3)
C7b—N1b	1.134 (4)	C9a—O1a	1.404 (3)
C7a—N1a	1.134 (5)		
N1b—C7b—C3b	179.1 (3)	N2b—C8b—C4b	178.2 (3)
N1a—C7a—C4a	178.8 (4)	N2a—C8a—C5a	177.0 (4)

All H atoms were refined using a riding model, with $C_{\text{sp}^2}\text{—H} = 0.93 \text{ \AA}$, methyl $C\text{—H} = 0.96 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2$ or 1.5 times $U_{\text{eq}}(\text{C})$. In addition, the methyl groups were allowed to rotate but not to tip. The Friedel opposites were merged in the absence of significant anomalous scattering effects.

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

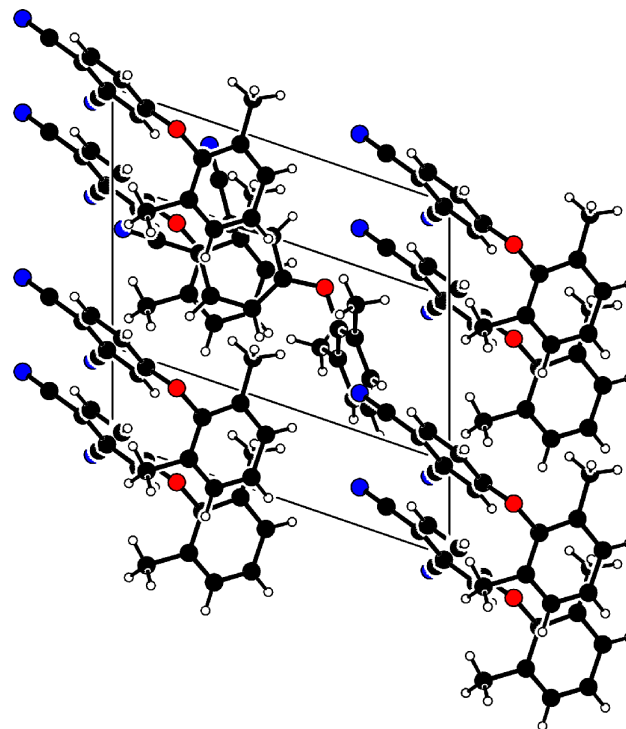


Figure 2

A packing diagram of (I), viewed approximately along the b axis.

graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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