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Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$

R factor = 0.041

wR factor = 0.116

Data-to-parameter ratio = 12.8

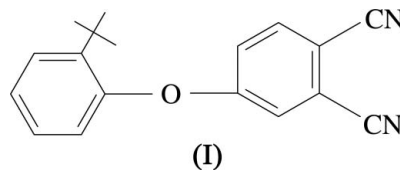
For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.4-(2-*tert*-Butylphenoxy)phthalonitrileThe molecular conformation of the title compound, $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}$, is stabilized by two intramolecular $\text{C}-\text{H}\cdots\text{O}$ interactions. The crystal packing is characterized by $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds.

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Comment

As part of an investigation of the synthesis of peripherally tetra-substituted phthalocyanines, the title compound, (I), was obtained and its structure analysed by standard analytical techniques (elemental analysis, IR). Phthalocyanine compounds have attracted attention for a long time because of their unique properties, such as semiconductivity, photoconductivity, chemical activity and the formation of liquid crystals (Leznoff & Lever, 1989–1996).

The two benzene rings of compound (I) form a dihedral angle of $78.81(1)^\circ$. The $\text{C}\equiv\text{N}$ bond lengths [$\text{N1}\equiv\text{C1} = 1.137(3) \text{ \AA}$ and $\text{N2}\equiv\text{C2} = 1.164(3) \text{ \AA}$] are close to the values reported in the literature [$1.153(4) \text{ \AA}$ in $\text{C}_6\text{H}_6\text{N}_2\text{S}$ (Çoruh *et al.*, 2003), $1.142(3) \text{ \AA}$ in $\text{C}_{15}\text{H}_{10}\text{N}_2\text{S}$ (Çoruh *et al.*, 2005) and $1.148(2) \text{ \AA}$ in $\text{C}_8\text{H}_4\text{F}_3\text{N}$ (Boitsov *et al.*, 2002)]. The $\text{N}\equiv\text{C}-\text{C}$ angles are close to linear [$\text{N1}\equiv\text{C1}-\text{C8} = 178.3(3)^\circ$ and $\text{N2}\equiv\text{C2}-\text{C3} = 179.8(3)^\circ$].The overall conformation of (I) is stabilized by two intramolecular $\text{C}-\text{H}\cdots\text{O}$ interactions (Table 2). The crystal packing is characterized by intermolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds.

Experimental

2-*tert*-Butylphenol (2.0 g, 13.33 mmol) and 4-nitrophthalonitrile (1.5 g, 8.67 mmol) were dissolved in dry dimethylformamide (40 ml). After stirring for 30 min at room temperature, dry fine-powdered potassium carbonate (2.00 g, 14.5 mmol) was added portionwise over 2 h with thorough stirring. The reaction was stirred for 24 h at room temperature and poured into ice-water (200 g). The product was filtered off and washed with NaOH solution (10% w/w) and water until the filtrate was neutral. Recrystallization from methanol gave a white product (yield 1.41 g, 59.0%). Single crystals of (I) were obtained from a solution in ethanol at room temperature *via* slow evaporation. Elemental analysis, calculated for $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}$: C 78.24, H 5.84, N 10.14%; found: C 78.20 H 5.90 N 10.10%. IR (ν_{max} , cm^{-1}): 3070–3025 (Ar–CH), 2950–2870 (CH), 2210 (CN).

Crystal data

$C_{18}H_{16}N_2O$
 $M_r = 276.33$
 Orthorhombic, $P2_12_12_1$
 $a = 10.2462$ (10) Å
 $b = 9.4543$ (12) Å
 $c = 16.1120$ (17) Å
 $V = 1560.8$ (3) Å³
 $Z = 4$
 $D_x = 1.176$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 1280 reflections
 $\theta = 2.4\text{--}29.3^\circ$
 $\mu = 0.07$ mm⁻¹
 $T = 293$ (2) K
 Tablet, colourless
 $0.50 \times 0.40 \times 0.20$ mm

Data collection

Stoe IPDS-2 diffractometer
 ω scans
 Absorption correction: none
 8384 measured reflections
 2428 independent reflections
 1280 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.065$
 $\theta_{\text{max}} = 29.3^\circ$
 $h = -13 \rightarrow 12$
 $k = -14 \rightarrow 14$
 $l = -22 \rightarrow 0$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.116$
 $S = 0.90$
 2428 reflections
 190 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.032$
 $\Delta\rho_{\text{max}} = 0.14$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

O1—C5	1.359 (3)	C2—N2	1.164 (3)
O1—C9	1.424 (3)	C1—N1	1.137 (3)
N2—C2—C3	179.8 (3)	N1—C1—C8	178.3 (3)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C16—H16B \cdots O1	0.96	2.27	3.024 (4)	135
C18—H18C \cdots O1	0.96	2.64	3.309 (4)	127
C7—H7 \cdots N1 ⁱ	0.93	2.73	3.398 (4)	129

Symmetry code: (i) $x + \frac{1}{2}, -y - \frac{1}{2}, -z + 1$.

All H atoms were located in a difference synthesis and refined as riding, with C—H = 0.93–0.96 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, or

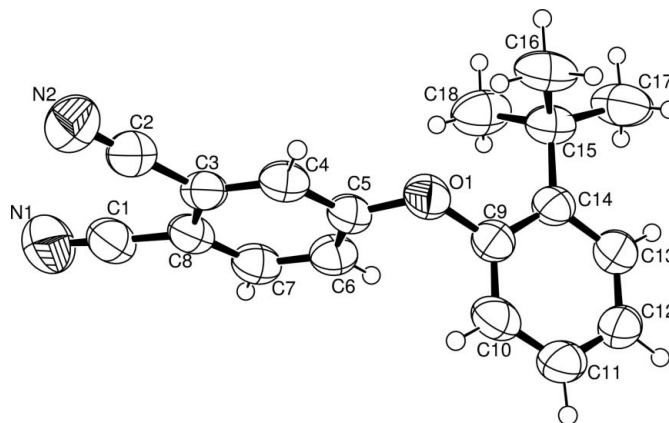


Figure 1

The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

$1.5U_{\text{eq}}(\text{C})$ for methyl H. In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

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, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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